



XV RUSSIAN CONFERENCE
(with international participation)
ON THERMOPHYSICAL PROPERTIES OF
SUBSTANCES
(RCTP-15)
October 15–17, 2018

BOOK OF ABSTRACTS

Moscow, 2018

CONTENTS

1. PLENARY REPORTS

A-514. <i>Iosilevskiy I.L.</i> Entropic phase transitions and accompanying anomalous thermodynamics regions in nonideal plasmas	15
A-716. <i>Stankus S.V., Abdullaev R.N., Agazhanov A.Sh., Kozlovskii Yu.M., Savchenko I.V., Samoshkin D.A., Khairulin R.A., Yatsuk O.S.</i> Experimental study of thermophysical properties and phase transitions of metals and alloys in solid and liquid states	16
A-707. <i>Petrov V.A.</i> Spectral and temperature dependence of absorption coefficient of molten aluminum oxide	16
A-704. <i>Belonoshko A. B.</i> State of iron in the earth core: paradigm change	17
A-697. <i>Grigoriev B.A., Gerasimov A.A., Alexandrov I.S.</i> Prediction of thermodynamic properties and phase equilibria of oil hydrocarbons and petroleum products based on the multiparameter fundamental equations of state	18
A-628. <i>Baidakov V.G., Kaverin A.M., Andbaeva V.N., Khotienkova M.N.</i> Surface tension of solutions of liquefied gases: experiment, theory, and simulation	18
A-619. <i>Sheindlin M.A.</i> Recent advances in investigation of thermophysical properties of ultra high temperature ceramics (uhtcs) with the aid of laser heating	19
A-611. <i>Belov G.V., Dyachkov S.A., Levashov P.R., Mezinov N.S., Minakov D.V., Morozov I.V., Smirnov V.N.</i> Thermodynamic database for pure substances IVTANTHERMO-Online	20
A-566. <i>Levashov P.R., Minakov D.V.</i> Estimation of critical parameters of refractory metals based upon first-principle simulation	20
A-537. <i>Dmitriev A.S.</i> Thermophysical properties of thermal interface nanomaterials for thermal stabilization of energy and electronic devices	21

2. EQUATIONS OF STATE, PHASE TRANSITIONS AND CRITICAL PHENOMENA

I-646. <i>Khomkin A.L., Shumikhin A.S.</i> Equation of state and metallization in metal vapors and inert gases	22
I-782. <i>Norman G.E., Saitov I.M.</i> Plasma phase transition in hydrogen at high pressures.	22
I-649. <i>Bezverkhii P. P., Martynets V. G., Kaplun A. B., Meshalkin A. B.</i> Extended description thermal properties of carbon dioxide using equation of state with a small number of parameters	23
I-713. <i>Maevskii K.K.</i> Numerical modeling of thermodynamic parameters for mixtures with a small parametric equation of state of their components	24
I-594. <i>Magomedov R.A., Akhmedov E.N., Meilanov R.R., Beybalaev V.D., Aliverdiev A.A.</i> Calculation of thermophysical properties of krypton and xenon based on fractal equation of state	24
O-654. <i>Kuznetsov K.I., Sukhikh A.A., Granchenko P.P., Skorodumov S.V.</i> Calculation of thermodynamic functions based on the joint thermal and acoustic measurements	25
O-669. <i>Bilalov T.R., Gumerov F.M.</i> Determination of saturated vapor pressure of aromatic hydrocarbons on experimental data of their solubility in supercritical carbon dioxide	26
O-673. <i>Rykov V.A., Rykov S.V., Sverdlov A.V.</i> The fundamental equation of state for R1234yf	26

O-693.	<i>Petrik G.G.</i> About round dates, acute questions and solving problems of low-parametric equations of state by logical abduction	27
O-699.	<i>Kulikov V.D., Belyakov M. Yu.</i> Isoplene equations of a binary mixture in the vicinity of vapor-liquid critical point in the framework of scaling theory	28
O-702.	<i>Rykov V.A., Kudryavtseva I.V., Rykov S.V.</i> The fundamental equation of state for argon satisfying the scale hypothesis for the region of high temperatures and pressures	28
O-719.	<i>Martynova I.A., Iosilevskiy I.L.</i> Effect of non-linear screening on complex plasma thermodynamic stability regions	29
O-741.	<i>Fleita D.Iu., Norman G.E., Pisarev V.V.</i> The singularity of the two-particle correlator in the vicinity of the phase transition point of the pure metal melt	30
O-515.	<i>Emelyanov A.N.</i> Estimation of critical point parameters of tungsten and copper from experiments on isentropic expansion of shock-compressed porous metals	30
O-815.	<i>Ochkov V.F., Ustyuzhanin E.E., Znamensky B.E., Rykov S.V., Rykov V.A.</i> Investigation of the liquid density, the gas density and the pressure: some modern models and numerical data on the saturation line of H ₂ O	31
O-519.	<i>Kaptilnyi A.G., Kondratyev A.M., Pletnev A.E., Rakhel A.D.</i> The sound velocity measurements for fluid iron in the vicinity of the metal-nonmetal transition	31
O-547.	<i>Ternovoi V.Ya., Nikolaev D.N., Ostriuk A.V.</i> Determination of the critical point parameters of liquid-gas transition for boron.	32
O-555.	<i>Milyutin V.A.</i> Experimental study of the density of the gas system helium-nitrogen-neon at low temperatures.	32
O-565.	<i>Osmanova B.K., Bazaev E.A., Bazaev A.R.</i> Calculation of thermodynamic properties of water+aliphatic alcohol system using experimental values of	33
O-571.	<i>Chigvintsev A.Yu., Iosilevskiy I.L., Noginova L.Yu.</i> Anomalies of spatial ions distribution in trap in local equation of state approximation	33
O-617.	<i>Abdulagatov I.M., Bazaev A.R., Bazaev E.A., Osmanova B.K.</i> Phase transitions and bulk properties of the ternary system water-1-propanol-n-hexane near the critical point	34
P-691.	<i>Yarullin L.Y., Zaripov Z.I., Gumerov F.M.</i> Thermal effects during processing of the main components of natural biosystems in the environment of supercritical carbon dioxide	35
P-805.	<i>Voronov V.P., Podnek V.P.</i> Adiabatic calorimetry investigation of supercooled state of liquid water	35
P-803.	<i>Davydov A.G., Tkachev N.K.</i> Analysis of dimerization equilibrium deviations from ideality in mixtures with interaction in the form of the square well	36
P-624.	<i>Ismagambetova T.N., Gabdullin M.T., Ramazanov T.S.</i> Equation of state of dense non-isothermal plasma	37
P-526.	<i>Ahmetzyanov T.R., Khayrutdinov V.F., Gabitov F.R., Gumerov F.M.</i> Investigation of phase equilibrium of binary system “naphthalene-SCF-solvent”	37
P-736.	<i>Hazipov M.R., Galimova A.T., Gatin R.S., Sagdeev A.A.</i> The solubility of anthracene in supercritical carbon dioxide	38
P-732.	<i>Kudryavtseva I.V., Rykov S.V., Rykov V.A.</i> Analysis of methods for constructing a phase equilibrium line for different models of mean diameter	38
P-731.	<i>Peshkina K.G., Tkachev N.K.</i> Statistical thermodynamic analysis of complex formation in salt melts	39
P-576.	<i>Molodets A.M.</i> Thermophysical properties of the boron carbide melt at the megabar shock pressures	40
P-561.	<i>Rykov S.V., Kudryavtseva I.V., Rykov V.A.</i> Method of construction of the fundamental equation of state for SF ₆	40

P-573. <i>Vasserman A.A., Halkin V.N.</i> Equations for calculations liquid-vapor equilibrium in binary mixtures containing methane	41
P-690. <i>Bezgomonova E.I., Saidov S.M.</i> Isochoric heat capacity and phase equilibrium lines in the binary system n-hexane + water in the concentration range 0-0.2566 m.f. H ₂ O	42
P-633. <i>Davydov A.G., Tkachev N.K.</i> Thermodynamic characteristics of molten salts considering polarization effects	42
 3. TRANSPORT, OPTICAL AND RADIATION PROPERTIES OF SUBSTANCES	
O-539. <i>Olyanina N.V., Belyukov A.L., Ladyanov V.I.</i> Viscosity of liquid alloys of cobalt with silicon and boron	44
O-676. <i>Kondratyuk N.D., Pisarev V.V.</i> Shear viscosity calculation for liquid hydrocarbons using molecular dynamics methods	44
O-644. <i>Gabitov I.R., Zaripov Z.I.</i> Viscosities of acetic acid, butyric acid and their aqueous solutions	45
O-679. <i>Borshev N.O., Antonov V.A., Beliauskii A.E.</i> The solution of the inverse coefficient problem for the search for reflective-radiative characteristics by tikhonov's regularization method	46
O-610. <i>Povolotskiy I.I., Volosnikov D.V., Skripov P.V.</i> Thermal resistance of superheated aqueous solutions	46
O-608. <i>Senchenko V.N., Belikov R.S.</i> Investigation of the spectra of highly oriented pyrolytic graphite	47
O-685. <i>Murlieva Zh.Kh., Palchayev D.K., Iskhakov M.E., Rabadanov M.Kh.</i> Correlation of electrical resistance and thermal expansion of intermetallide ti₃al	47
O-593. <i>Nikolaev D.N., Ternovoi V.Ya., Shutov A.V., Ostriuk A.V.</i> Specific electrical conductivity of sapphire at shock compression up to 750 gpa	48
O-592. <i>Palchayev D.K.</i> The nature of the formation of the temperature dependence of the resistivity in conductors	49
O-695. <i>Bogatyrev A.F., Kucherenko M.A., Makeenkova O.A.</i> Transport properties of dilute gases and gas mixtures. diffusion	49
O-572. <i>Galkin D.A., Povolotskiy I.I., Skripov P.V.</i> Investigation of thermal conductivity of oils	50
O-540. <i>Skripov P.V.</i> Heat conduction of solutions: superheated and unstable states	51
O-666. <i>Prima A.I., Ding L., Zhang Q., Zhang Z.C.</i> Influence of fast radiation processes on cooling of a metal target after irradiation by a powerful ion beam	51
P-795. <i>Lepeshkin A.R.</i> Method for investigation of thermal conductivity of metal materials at action of ultrasonic oscillations	52
P-804. <i>Borshchev N.O., Antonov V.A., Belyavsky E.A.</i> The solution of the inverse coefficient problem for the search for the heat conductivity tensor by the gradient method of conjugate directions	52
P-668. <i>Laptev Yu.A., Tsvetkov O.B., Pyatakov G.L., Zainullina E.R.</i> Thermal conductivity for the co ₂ +r1234yf and co ₂ +r1234ze(z) binary gaseous mixtures at low pressure	53
P-647. <i>Molodets A.M., Savinykh A.S., Golyshev A.A.</i> Mechanical properties of glassy carbon under shock wave loading in the area of its abnormal compressibility.	53
P-639. <i>Kochurov D.S., Eletskiy I.A., Kotova E.S.</i> Calculation of transport properties of helium based gas mixtures in application to experimental determination of the temperature recovery factor	54

P-599.	<i>Raschektaeva E.P., Stankus S.V., Verba O.I.</i> Thermal conductivity investigation of R-125/R-134a (39/61) mixture in the vapor phase	55
P-580.	<i>Mitropov V.V., Tsvetkov O.B., Laptev Yu.A., Babich A.Yu</i> Thermodynamic assessment of low global warming potential refrigerant alternatives	55
P-575.	<i>Beltyukov A.L., Menshikova S.G., Lad'yanov V.I., Korepanov A.Yu.</i> The influence of small additions of ni, co, fe on the viscosity of liquid aluminum	56
P-543.	<i>Tsvetkov O.B., Laptev Yu.A., Prostorova F.O., Vinzarevich A.V.</i> Maxwell factor for gaseous 2.3.3.3-tetrafluoropropene and zis-1.3.3.3-tetrafluoropropene at zero density	57
P-847.	<i>Shapiyeva A.Ye., Kunakov S.K., Son E.Ye.</i> Fission fragments and energy spectra of primary electrons in a fissioning plasma	57

4. THERMODYNAMIC PROPERTIES OF SUBSTANCES IN THE CONDENSED STATE

I-727.	<i>Guluzade A., Safarov J., Hassel E., Abdulagatov I.</i> Thermophysical properties of 1-butyl-3-methylimidazolium trifluoromethanesulfonate	59
O-672.	<i>Vervevko V.N., Vervevko M.V.</i> Structural features of aromatic hydrocarbons clusters in a wide range of state parameters	59
O-703.	<i>Borisenko D.I., Kuznecov K.I., Sukhikh A.A., Shish A.I.</i> Experimental study of the thermal expansion coefficient of heat-conducting gaskets	60
O-710.	<i>Faizullin M.Z., Vinogradov A.V., Tomin A.S., Koverda V.P.</i> Hot crystallization centers in gas-saturated layers of amorphous ice	61
O-720.	<i>Egorov G.I., Makarov D.M.</i> Thermodynamic properties of aqueous solutions of urea and its alkyl derivatives in a wide range of the parameters of state	61
O-621.	<i>Radchenko A.K., Shakhov A.V., Neruchev Y.A.</i> Clusters in the "simple" and "normal" fluids	62
O-794.	<i>Sobol O.V.</i> Thermodynamic properties of aqueous solutions of sodium thiosulfatum	63
O-597.	<i>Kulyamina E. Yu., Zitserman V.Yu., Fokin L.R.</i> Melting curve of titanium. thermodynamic data consistency assessment	63
O-595.	<i>Lesev V.N., Alchagirov B.B., Dadashev R.Kh., Kyasova O.Kh., Uzdenova A.N.</i> On the possibility of the existence of a double maximum on the adsorption isotherm of binary metallic systems	64
O-586.	<i>Pakhomov E.P.</i> Defective structure of crystalline lattice of zirconium carbide	65
O-527.	<i>Neruchev Yu.A., Korotkovskii V.I., Ryschkova O.S.</i> The energy of intermolecular forces in liquid haloalkanes and their binary mixtures	65
O-548.	<i>Gribchenkova N.A., Smirnov A.S., Alikhanyan A.S.</i> Enthalpies of formation of mixed oxides in ZnO-based transparent conductive oxide systems by knudsen effusion mass spectrometry	66
O-564.	<i>Taova T.M., Khokonov Kh.B., Shebzukhova I.G., Alchagirov B.B.</i> Methods and devices for measuring surface energy and surface tension of metals and alloys	66
O-581.	<i>Pashchenko L.L., Miroshnichenko E.A.</i> Thermodynamic study of some azidonitrocompounds. energies of reorganization of radicals	67
O-584.	<i>Sineva M.A., Aristova N.M., Belov G.V., Morozov I.V.</i> A new code for joint approximation of enthalpy increments and heat capacity data	68
P-774.	<i>Safarov M.M., Sobirov J.F.</i> Behavior and thermodynamic characteristics of a gete semiconductor in a ferrous and paraphase condition sobirov j.f., safarov m.m.	68
P-838.	<i>Syzdykova A.B., Belov M.P., Abrikosov I.A.</i> Thermodynamic properties of the gray and white tin	69
P-839.	<i>Sidnov K., Vorotilo S.</i> Ab-initio modeling and experimental investigation of the properties of ultra-high temperature solid solutions $Ta_xZr_{1-x}C$	69

P-706.	<i>Kostanovskiy A.V., Kostanovskaya M.E.</i> Experimental dependence of the density of local entropy rate of production of change of the temperature in time	70
P-694.	<i>Kalazhokov Z.K., Kalazhokov K.K., Sherieva E.K.</i> Analytical description of experimental isotherms for surface tension of binary metal systems which form stable chemical compounds	71
P-522.	<i>Kalazhokov Z.K., Dzugurova L.K., Zhanimova D.A., Karamurзов B.S., Kalazhokov K.K.</i> The study of binary alloy systems Sn-Pb and In-Pb by xps . .	71
P-661.	<i>Rusanov B.A., Sidorov V.E., Moroz A.I., Svec P., Janickovic D.</i> Glass-forming ability and crystallization behavior of Al-Ni-Co-Nd (Sm) amorphous alloys . . .	72
P-530.	<i>Tatarinov A.S., Kobelev M.A., Stepanov V.P.</i> Molecular dynamics study of isothermal compressibility of binary molten potassium halides	73
P-553.	<i>Melent'ev V.V.</i> Experimental study of the elastic properties of 1-chloro-substituted n-alkanes and the possibility of their prediction	73
P-598.	<i>Sulimov A.V., Kosova D.A., Druzhinina A.I., Tiflova L.A.</i> Thermodynamic properties of sodium and potassium methanesulfonates	74
P-620.	<i>Rakhmanova P.A., Vasilyov V.A., Solovyov S.N., Novikov A.N., Doronin Ya.I., Skorba V.R.</i> Heat capacity of ions cadmium and barium in dimethylsulfoxide at 298,15 k	74
P-622.	<i>Actov A. U., Zaripov Z. I., Usmanov R. A., Nakipov R. R.</i> Thermodynamic characteristics of an aqueous oleic acid emulsion	75
P-631.	<i>Andrusova N.N., Zhavoronok E.S., Legon'kova O.A., Kedik S.A.</i> Modified compositions for endoprostheses	76
P-843.	<i>Mukhamedov B.O., Saenko I.S., Fabrichnaya O.B, Abrikosov I.A.</i> Theoretical and experimental study on thermodynamic properties intermetallic compounds in the Zr-Fe binary system	76
P-642.	<i>Matskevich N.I., Wolf T.A., Samoshkin D.A., Stankus S.V., Vyazovkin I.V.</i> Heat capacity of (er, in)-doped barium cerate in the temperature range of 200-700 k .	77
P-657.	<i>Kosova D.A., Sulimov A. V., Tiflova L.A., Monaenkova A.S.</i> Thermodynamic properties of copper and zinc methanesulfonates	77
P-660.	<i>Zakiryanov D.O., Kobelev M.A., Tkachev N.K.</i> Melting characteristics of sodium halides: a molecular dynamics simulation	78
Q-636.	<i>Ovchinnikov V.V., Kulakov A.A., Maltseva S.A.</i> Analysis of thermochemical data of fatty organic acids	79

5. THERMOPHYSICAL PROPERTIES OF SUBSTANCES AT HIGH TEMPERATURES

I-705.	<i>Dunaev A.M., Motalov V.B., Kudin L.S.</i> Comprehensive study of evaporation of BMImBF ₄ ionic liquid	80
I-722.	<i>Brykin M. V.</i> Calculation of the temperature in 3d carbon-carbon composite material.	80
I-711.	<i>Vervikishko P.S., Sheindlin M.A.</i> Recent advances in laser-pulse melting of graphite at pressure up to 6 kbar	81
I-578.	<i>Falyakhov T.M., Brykin M.V., Petukhov S.V., Sheindlin M.A.</i> Zirconium carbide phase diagram. experimental research and mathematical modeling.	82
I-677.	<i>Savvatimskiy A.I., Onufriev S.V.</i> Physical properties of the most refractory substances (graphite and carbides) in the temperature range 2000-7000 k	82
O-627.	<i>Chernoskutov M. Yu., Ivliyev A. D., Meshkov V. V.</i> High-temperature thermophysical properties of solid solutions of the Y-Ho system	83
O-674.	<i>Maltsev M.A., Morozov I.V., Osina E.L.</i> Thermodynamic properties of diatomic argon compounds	84

O-781.	<i>Minakov D.V., Levashov P.R.</i> Heat of fusion of refractory hcp metals from first-principle simulations and trouton's rule	84
O-723.	<i>Bgasheva T.V., Vervikishko P.S., Sheindlin M.A., Valiano G.E.</i> Investigations of liquid carbon at pressures above 200 bar	85
O-726.	<i>Frolov A.M., Sheindlin M.A.</i> Mass-spectrometric analysis of laser-induced evaporation of pyrographite up to 4400 k	85
O-618.	<i>Kondratyev A.M., Rakhel A.D.</i> A technique for determining the active component of the voltage drop across a sample in pulsed joule heating experiments	86
O-560.	<i>Petukhov S.V., Frolov A.M., Sheindlin M.A., Falyakhov T.M.</i> High-temperature (up to 4000 k) investigation of vapor composition of nonstoichiometric zrc_x and tac_x in the vicinity of the homogeneity domain	87
O-521.	<i>Kudin L.S., Motalov V.B., Dunaev A.M.</i> Thermodynamics of the sublimation of lanthanoid triiodides	87
O-528.	<i>Nagmutdinova A.I., Zaycev N.G., Mazilin I.V.</i> Influence of the rare earth metals on the thermophysical properties of the thermobarrier coatings	88
O-529.	<i>Vasin A.A., Frolov A.M., Sheindlin M.A.</i> Observation of graphite melting during laser heating in vacuum	89
O-583.	<i>Konyukhov S.A., Onufriev S.V., Savvatimskiy A.I.</i> Melting of anisotropic graphite with volume limitation	89
O-536.	<i>Seredkin N.N., Onufriev S.V., Savvatimskiy A.I., Muboyadzhyan S.A., Evdokimov S.A.</i> Properties of carbides in solid and liquid condition (2000 to 6000 k)	90
P-775.	<i>Rabadanova A.E., Gadzhimagomedov S.Kh., Palchaeu D.K., Ragimkhanov G.B., Isakaev E.Kh., Gadzhiev M.Kh., Demirov N.A.</i> Structure and properties of ybco before and after short-term exposure to the plasma flow	90
P-614.	<i>Roshchupkin V.V., Lyakhovitskii M.M., Pokrasin M.A., Minina N.A., Kudryavtsev E.M.</i> Influence of quenching on ultrasound speed in steels	91
P-568.	<i>Popov D.A., Lebedev A.V., Ryazantseva A.A., Malkin A.I.</i> The effect of the mechanical activation on thermophysical properties of powdered metals	91
P-655.	<i>Abdulagatova Z.Z., Abdulagatov I.M., Kallaev S.N., Omarov Z.M., Bakmaev A.G.</i> Effect of temperature on the thermal diffusivity and heat capacity of sandstone .	92
P-645.	<i>Dzhapparov T.A-G., Bazaev A.R.</i> Experimental determination of destruction of thermally unstable substances	92
P-638.	<i>Kachalov V.V.</i> Density and surface tension of alloy uranium–chromium in liquid phase	93
P-613.	<i>Rusanov B.A., Sidorov V.E., Mikhailov V.A., Popel P.S.</i> Density and magnetic susceptibility of CoFeSiBNb alloy	94
P-520.	<i>Akhtyamov E.R., Polev V.F., Korshunov I.G., Kurichenko A.A., Gorbatov V.I.</i> Thermal diffusivity of the ni-v system with vanadium content up to 22 at.% at high temperatures	95

6. EXTREME STATES OF MATTER

I-730.	<i>Rososhok A., Efimov S., Tewari S., Yanuka D., Krasik Ya.E.</i> On phase transitions in different metals	96
O-640.	<i>Struleva E.V., Komarov P.S.</i> Ablation of titanium by femtosecond laser pulses .	96
O-616.	<i>Bogdanov E.N., Zhernokletov M.V., Kozlov G.A., Medvedev A.B., Rodionov A.V.</i> Microwave doppler diagnostics of shock-compressed argon plasma	97
O-563.	<i>Apfelbaum E.M.</i> Thermophysical properties of the low-temperature plasma of metals	97
O-550.	<i>Korobenko V.N., Rakhel A.D.</i> Thermophysical properties of dense lead plasma .	98

O-535.	<i>Gryaznov V.K., Iosilevskiy I.L.</i> Thermophysical properties of dense molecular gases in quasichemical representation	98
O-532.	<i>Golyshev A.A., Sobolev D.V., Molodets A.M.</i> Electrical conductivity of polytetrafluoroethylene in the megabar range of quasi-isentropic compression . .	99
P-643.	<i>Shalenov E.O., Dzhumagulova K.N., Ramazanov T.S., Röpke G., Reinholz H.</i> Dynamical conductivity of the nonideal plasma on the basis of the effective potential	100
P-689.	<i>Kavyrshin D.I., Kutuzov D.S., Chinnov V.F.</i> Experimental observation of decrease in probability of atomic highly excited state realization in helium arc plasma at atmospheric pressure	100
P-518.	<i>Kodanova S.K, Ramazanov T.S., Issanova M.K.</i> Transport properties of hot dense plasma	101

7. DATABASES ON THERMOPHYSICAL PROPERTIES OF SUBSTANCES

O-634.	<i>Ochkov V.F., Ustyuzhanin E.E., Znamensky B.E., Rykov S.V., Rykov V.A.</i> Development of online resources to assess the effectiveness of some gas turbine plants	102
O-648.	<i>Dudarev V.A., Kiselyova N.N.</i> On importance of the multi-level chemical objects description in ontologies for information systems integration in inorganic materials science	102
O-651.	<i>Kosinov A.V., Erkimbaev A.O., Zitserman V.Yu., Kobzev G.A.</i> Ontology-based methods of thermophysical data integration	103
O-700.	<i>Kiselyova N.N., Dudarev V.A., Stolyarenko A.V.</i> Information systems for inorganic materials science	104
P-551.	<i>Gorokhov L.N., Osina E.L., Kovtun D.M.</i> Evaporation thermodynamics of yttrium trifluoride in the form of molecules YF_3 and Y_2F_6	105
P-737.	<i>Gorokhov L.N., Osina E.L., Osin S.B.</i> Thermodynamic functions and energy stability of yttrium trichloride and its dimer	105

8. NANOMATERIALS, NANOFLUIDS, INTERPHASE PHENOMENA

I-681.	<i>Rudyak V.Ya.</i> Thermophysical properties of nanofluids. expectations and reality .	106
I-579.	<i>Fokin L.R., Alchagirov B.B., Kokov Z.A., Korotkov P.K., Elimkhanov D.Z.</i> Surface tension of liquid mercury in vacuum, in the medium of oxygen. experiment . . .	106
I-696.	<i>Abdulagatov I.M., Polikhronidi N.G., Batyrova R.G.</i> Effect of instability on the critical behavior of heat capacity for ethanol + diamond nanofluid	107
I-630.	<i>Alchagirov B.B., Kyasova O.Kh., Uzdenova A.N.</i> Surface tension of lithium alloys: state of research (review)	108
O-729.	<i>Magomedov M. N.</i> Change in the phase diagram of a simple matter with a decrease in the size of the nanosystem	108
O-688.	<i>Kalazhokov K.K., Kalazhokov Z.K., Kalazhokov Z.K.</i> Equation of isotherm of surface tension of binary metal systems	109
O-849.	<i>Zakatilova E.I., Efremov V.P.</i> Nanodiamon dgraphitization at heating and irradiation	110
O-678.	<i>Akhmedov E.N.</i> Size dependence of molybdenum melting and crystallization temperatures	110
O-675.	<i>Khvesyuk V.I.</i> A generalized model of the kapitza resistance	111
P-837.	<i>Shulyatev D.A., Ponomareva A.V., Mukhamedov B., Abrikosov I.A., Bozhko S.I., Ionov A.M., Mazilkin A.A., Smirnova I.A., Walls B., Shvets I.V.</i> Nano-scale inhomogeneity in NiO	112

P-582.	<i>Prokofjev S.I.</i> Empirical estimations of surface tension of grain boundaries in pure substances	112
P-596.	<i>Barinov A.A., Liu B.</i> Heat capacity and thermal conductivity of semiconductor nanofilms and nanowires	113
P-652.	<i>Skryabin A.S., Vesnin V.R., Tsygankov P.A., Chirkov A.Yu.</i> Study of the absorbing spectra of nanostructured materials based on thin films of metal oxides in the middle ir range	113
P-687.	<i>Khasanova R.R., Zhavoronok E.S., Shabatin A.V., Senchikhin I.N.</i> Study of novel epoxy compositions with silver nanoparticles by differential scanning calorimetry and refractometry ¹	114
P-684.	<i>Pryazhnikov M.I., Minakov A.V., Rudyak V.Ya.</i> Experimental investigation of viscosity coefficient of nanofluids	115
P-683.	<i>Vervikishko D.E., Kochanova S.A., Dolzhenko A.V., Shkolnikov E.I.</i> Nanoporous carbon materials for supercapacitors	115
P-662.	<i>Kosakovich E.O., Zhavoronok E.S., Safonov A.V., Senchikhin I.N.</i> Biocidal activity of hydrophobicated oligohexamethylenuganidines in epoxy systems . . .	116
P-554.	<i>Orazbayev S.A., Zhumadylov R.E., Zhunisbekov A.T., Ramazanov T.S., Gabdullin M.T., Dosbolayev M.K., Batryshev D.G.</i> Influence of gas temperature on nucleation and growth of dust nanoparticles in high-frequency plasma	117

9. THERMOPHYSICAL MEASUREMENT TECHNIQUES

O-525.	<i>Osadchii S.M., Potapov B.G., Sokolov N.A.</i> Measuring of heat flux in the range from 5 up to 2500 kilowatt per meter squared	118
O-714.	<i>Chernoskutov M.Yu., Ivliev A.D., Meshkov V.V.</i> Signal processing algorithms for measuring thermophysical properties using temperature waves method	118
O-712.	<i>Ermishkin V.A., Minina N.A., Kudryavtsev E.M., Pokrasin M.A.</i> Definition of the temperature conductivity of a carbon film based on the data of photometric analysis of the spectra of brightness of the reflection from its surface.	119
O-692.	<i>Kurichenko A. A., Gorbatov V. I., Ivliyev A. D.</i> Digital system for the collection and processing of information and management of the thermophysical high temperature installation	120
O-667.	<i>Senchenko V.N., Konovalov P.A., Ilichev M.V., Kapustin D.I.</i> Infrared system for thermal resistance measurement of microobjects	120
O-801.	<i>Kuryakov V.N., Ivanova D.D.</i> Investigation of phase transitions of n-alkanes nanoemulsions by means of dynamic and static light scattering	121
O-615.	<i>Sukhikh A.A., Kuznetsov K.I., Skorodumov S.V.</i> Experimental study of thermal conductivity of thermally conductive strips for electronic equipment	121
O-600.	<i>Divin A.G., Ponomarev S.V., Lyubimova D.A.</i> Methods and means of thermophysical characteristics measurement for vegetables and fruits tissues . . .	122
O-588.	<i>Ermishkin V.A., Mikhaylov D.L., Minina N.A., Belousov O.K., Palyi N.A.</i> Investigation of the diffusion of alloying elements in multi component alloys of the cr-ni system using the photometric analysis of the radiation brightness spectra	123
O-559.	<i>Artamonov A.V., Mazilin I.V., Zaitsev N.G.</i> High-temperature test bench for thermal shock resistance control ceramic coatings	123
P-607.	<i>Kostanovskiy A.V., Pronkin A.A., Zeodinov M.G., Kostanovskaya M.E.</i> Features of ohmic heating of the siliconized silicon carbide at measurement of thermal properties in the field of high temperatures	124
P-791.	<i>Prorokova M.V., Bukhmirov V.V., Gaskov A.K., Suleymanov M.G.</i> Thermophysical properties of thin film coatings based on the hollow microspheres	124

P-718.	<i>Grigorenko A.V., Belyaev G.E., Vlaskin M.S., Lipatova I.A., Zhuk A.Z.</i> Increasing chemical purity fused by high temperature annealing in vacuum	125
P-562.	<i>Mendeleyev V.Ya., Kachalov V.V.</i> Influence of the background radiance on the measured total direct power of pt-10%rh alloy specimen	125
P-567.	<i>Blagonravov L.A., Modenov A.A.</i> Precision measurements of thermodynamic parameters of low-boiling metallic liquids	126
P-585.	<i>Rusin S.P.</i> On the determination of the true temperature of refractory metals by radiation in the "gray" approximation	127
P-658.	<i>Komarov P.S., Struleva E.V.</i> Interference diagnostics the dynamics of the target surface movement during ablation using a frequency-modulated laser pulse	127
P-650.	<i>Sviridenko V. I.</i> Investigation of thermal properties of the plexiglass on the apparatus tau-5	128

10. COMPUTER SIMULATIONS IN THERMOPHYSICS

I-777.	<i>Kalinichev A.G.</i> New opportunities in the application of the ClayFF force field for atomistic computer modeling of natural and synthetic nanoporous materials and their hydrated interfaces	129
I-728.	<i>Pisarev V.V.</i> Viscosity of liquid hydrocarbon mixtures: molecular dynamics simulations and mixing rules	129
I-591.	<i>Khvesyuk V.I., Barinov A.A., Qiao W.</i> The influence of interactions between phonons on heat transfer	130
I-603.	<i>Apfelbaum M.S., Gadzhiev M.Kh., Doludenko A.N.</i> Numerical and experimental investigation of formation of weakly conductive liquid dielectric flows caused by a high nonuniform electrical field	131
O-721.	<i>Shults O.V.</i> Compound thermodynamic properties evaluation model	131
O-810.	<i>Meshkov E.A., Novoselov I.I., Yanilkin A.V.</i> On-lattice models to study evolution of HEA at atomic scale	132
O-682.	<i>Zakharov S.A., Pisarev V.V., Chudanov V.V.</i> Continual fluid filtration model . .	132
O-664.	<i>Skurikhin A.V., Kostanovsky A.V.</i> Numerical estimation of thermal conductivity of exfoliated vermiculite	133
O-659.	<i>Nedyalkov Yu.V., Postnikov E.B.</i> Computational approaches to determining isothermal compressibility and fluctuation parameter of liquids	133
O-841.	<i>Fortova S.V.</i> Kolmogorov flow and its numerical simulation in a flat channel . . .	134
O-557.	<i>Ivanov P.P., Vlaskin M.S., Zhuk A.Z.</i> Modeling of the alumina cleaning by means of high temperature evaporation into vacuum	134
O-842.	<i>Shepelev V.V., Fortova S.V., Inogamov N.A.</i> Application of Turbulence Problem Solver (TPS) software complex for for the numerical simulation of the effects of femtosecond lasers on metallic substrates.	135
P-523.	<i>Belov G.V., Aristova N.M.</i> On the development of thermodynamic modeling tools for complex high-temperature systems	136
P-734.	<i>Barbin N.M., Sidash I.A., Terentev D.I., Alekseev S.G.</i> Computer simulation of the thermophysical properties of the radioactive graphite-co ₂ system	136
P-715.	<i>Paukova A.E., Shults O.V., Peshkichev I.V., Pugachev V.Yu.</i> Thermodynamic modelling in computing back-end material balance	137
P-626.	<i>Rozhdestvensky A.V.</i> Development of the database of thermodynamic functions of air in a wide range of temperatures and pressures for software packages of hypersonic flow simulation	138
P-546.	<i>Kuanishev V.T., Sachkov I.N., Sorogin I.G., Sorogina T.I.</i> Synergetic mechanism of thermal destruction of two-phase contact materials	138

P-844. <i>Fortova S.V., Utkin P.S.</i> Three-dimensional numerical modeling of development of the instability of the contact surface of colliding metallic plates in gas dynamics approach	139
--	-----

11. THERMOPHYSICAL PROPERTIES OF MATERIALS FOR NUCLEAR POWER ENGINEERING

I-604. <i>Rutin S.B., Skripov P.V.</i> Heat transfer in supercritical water	140
O-819. <i>Likhanskii V.V.</i> Models describing evolution in UO ₂ fuel properties under irradiation	140
O-840. <i>Chusov I.A., Didenko V.I., Obysov N.A., Novikov G.E., Pronyaev V.G.</i> Processing of heterogeneous data of experiments and construction of recommended relations	141

12. THERMOPHYSICAL PROPERTIES OF MATERIALS FOR AVIATION, ROCKET AND SPACE TECHNOLOGIES

O-738. <i>Khromov M.A., Chinnov V.F., Sargsyan M.A., Kavirshin D.I., Scherbakov V.M., Efimov A.V.</i> Analysis of the nitrogen plasma jet destructive effect on the heat-resistant materials	142
O-827. <i>Kashapov N.F., Kashapov R.N., Kashapov L.N.</i> Thermophysical and physicomechanical properties of products obtained by selective laser melting . . .	143

13. THERMOPHYSICAL PROPERTIES OF OILS, GAS CONDENSATES, GAS HYDRATES AND NATURAL GAS

I-790. <i>Buleiko V.M., Grigoriev B.A.</i> Calorimetric investigation of phase behavior of hydrocarbon mixtures with low content of high molecular components (C ₄ +) . .	144
I-549. <i>Bazaev A.R., Bazaev E.A.</i> Phase transitions and critical properties of 1-propanol — n-hexane system	145
O-511. <i>Lukyanov K.V., Kotov A.N., Starostin A.A., Skripov P.V.</i> Effect of moisture on heat transfer in liquid hydrocarbons under impulse heating of a wire	146
O-698. <i>Zhukov S.A., Yanovskiy L.S., Molokanov A.A., Il'ina M.A.</i> Investigation of heat flux in hydrocarbon fuels at the film and bubble boiling	146
O-708. <i>Director L.B., Sinelshchikov V.A.</i> Thermophysical properties of volatile products of biomass low temperature pyrolysis	147
O-709. <i>Yanovsky L.S., Varlamova N.I., Kazakov A.I., Molokanov A.A., Plishkin N.A., Popov I.M., Il'ina1 M.A., Ezhov V.M.</i> Manometrical investigation of the saturated vapor pressure and critical temperatures of hydrocarbon compounds .	147
O-735. <i>Subbotin D.I., Popov V.E., Safronov A.A., Popov S.D., Surov A.V., Kuchina J.A., Obraztsov N.B., Serba E.O., Nakonechny Gh.V., Spodobin V.A.</i> Interaction of methane with thermal carbon dioxide plasma obtained in the ac plasma torch . .	148
O-739. <i>Nikitin E.D., Bogatishcheva N.S., Popov A.P., Faizullin M.Z.</i> Thermophysical properties of components of biodiesel fuel and raw materials for its production .	149
O-792. <i>Bogdanov A.V., Grigoriev E.B., Sokotushenko V.N.</i> Determining the speed of multicomponent hydrocarbon mixture phase transitions in the free volume Al ₂ O ₃ & MgO	149
O-605. <i>Igolnikov A.A., Skripov P.V.</i> Study of superheat and critical parameters of diesel fuel with adding castor oil	150
O-589. <i>Zaripov Z. I., Usmanov R. A., Gumerov F. M.</i> Properties of thermodynamic systems participating in the process of obtaining biodiesel fuel in sub- and supercritical fluid conditions	151

O-533.	<i>Khairutdinov V.F., Gumerov F.M., Farakhov M.I.</i> Thermodynamic bases of the process of extraction of hydrocarbons from oil sludge using scf propane-butane mixture	151
O-806.	<i>Kiyachenko Yu.F., Deshabo V.A., Kosov V.I., Yudin D.I., Yudin I.K., Podnek V.E.</i> Dew-bubble curve determination of near-critical hydrocarbon mixtures using light-scattering method	152
O-556.	<i>Faizullin M.Z., Vinogradov A.V., Tomin A.S., Koverda V.P.</i> Hydrate formation in supersonic jets of vapor and gas	153
P-570.	<i>Nakipov R.R., Zaripov Z.I.</i> Thermophysical properties of system high-molecular organic connection (rock-oil) - water-scf solvent	153
P-587.	<i>Anishchanka Yu.V., Loktionov E.Yu.</i> Exhaust composition at laser ignition of combustible gas mixtures under controlled conditions	154
P-544.	<i>Mirskaya V.A., Nazarevich D.A., Ibayov N.V.</i> Experimental investigation of the pressure of the system of n-heptan-water (99:1)	155
P-625.	<i>Mazanov S.V., Zaripov Z.I., Gumerov F.M.</i> The experimental investigation of the isobaric heat capacity of the reaction mixture "ethanol / rapeseed oil" in the presence of a heterogeneous catalyst	155
P-517.	<i>Sagdeev D.I., Gabitov I.R., Fomina M.G., Alyaev V.A., Minkin V.S., Abdulagatov I.M.</i> Viscosity and density of vacuum working fluids for diffusion pumps	156
P-552.	<i>Ibayov N.V., Mirskaya V.A., Nazarevich D.A.</i> Isochoric heat capacity and pvt properties of binary azeotropic system n-heptane-water	156

**14. DATA DRIVEN APPROACHES IN MATERIALS DESIGN:
THEORY MEETS EXPERIMENT (MISIS)**

I-776.	<i>Colinet C., Tedenac J.P.</i> Enthalpies of formation of transition metal and rare-earth borides. a first principles study.	158
I-740.	<i>Richter K.W.</i> Modelling of phases with general nias-type structure: what can we learn from powder xrd?	158
I-612.	<i>Kim G., Gu Q., Jia H., Meschel S., Chen W., Nash P.</i> Experimental database development for data-driven materials design	159
I-680.	<i>Chen Q., Wu K., Jeppsson J., Engstrom A.</i> Precipitation simulation enabled by thermodynamic and kinetic databases	159
O-809.	<i>Ilatovskaia M., Fabrichnaya O.</i> Thermodynamic assessment of the Al ₂ O ₃ -MgO-TiO ₂ system	160
O-808.	<i>Saenko I., Ilatovskaia M., Fabrichnaya O.</i> Experimental investigation and thermodynamic modeling of the ZrO ₂ -TiO ₂ -MgO system	161
I-516.	<i>Eriksson O.</i> Data-mining approaches to find new functional materials	162
O-541.	<i>Gordeev I.S.</i> Study of the phase diagram of zirconium by molecular dynamics method	162
O-641.	<i>Smirnova D.E., Starikov S.V., Gordeev I.S.</i> Development of atomistic model for prediction of properties of binary zr-nb system	163
O-590.	<i>Gornostyrev Yu.N., Korzhvyi P., Gorbatov O.I., Katsnelson M.I.</i> Metastable embedded nanoparticles in metallic alloys. general concepts and atomistic modeling.	163
O-606.	<i>Todorova M., Yoo S., Neugebauer J.</i> Electrochemical surface phase diagrams: solvation effects and selectivity	164
O-601.	<i>Vekilova O.Yu., Eriksson O., Herper H.C.</i> Theoretical study of magnetic properties of the 1:12 alloys	164
O-524.	<i>Simak S.I.</i> Diffusion in ionic conductors from ab initio molecular dynamics	165

O-663.	<i>Ehteshami H., Smirnova E.A., Sun W., Korzhavyi P.A.</i> Atomic diffusion mechanisms in titanium carbide	166
I-717.	<i>Pisch A.</i> Development of new materials using an integrated approach of dft calculations, calphad modeling and key experiments	166
I-807.	<i>Gavrichev K.S., Guskov V.N., Nikiforova G.E.</i> Thermodynamic properties of re-containing tbc materials	167
O-742.	<i>Bajenova I.A., Kondratiev A.V., Khvan A.V., Dinsdale A.T.</i> Third-generation thermodynamic description of SiO ₂	168
O-538.	<i>Kolotova L.N., Starikov S.V.</i> Atomistic simulation of phase transitions and structure transitions under irradiation in u-mo alloys	168
I-833.	<i>Neugebauer J., Zhu L., Körmann F., Grabowski B., Hickel T.</i> Employing ab initio thermodynamics to design structurally complex materials	169
I-845.	<i>Stepanov E.A., Lichtenstein A.I., Katsnelson M.I.</i> Effective bosonic models for collective electronic fluctuations	169
I-834.	<i>Rubtsov A.</i> Fluctuating local field approach to strong correlations	170
I-831.	<i>Abrikosov I.A.</i> Theoretical physics approaches for understanding of materials: lessons from Yu. Kh. Vekilov	170
O-778.	<i>Sinyova S., Starykh R., Vasil'eva A., Boduen A.</i> Determination of temperature and composition areas of solid solution in Fe-Ni-Co-(Cu,Cr) system	170
P-830.	<i>Abrikosova N.A., Brommesson C., Larsson E., Eriksson P., Zhangjun H., Uvdal K.</i> Optimization of the cell uptake of gadolinium oxide nanoparticles by capping with sorbitol for cell tracking in MRI	171
P-531.	<i>Skripnyak N.V., Ponomareva A.V., Belov M.P., Abrikosov I.A.</i> Elastic consants for alloys with mechanical instability: ab initio investigation of bcc Ti	172
P-558.	<i>Belov M.P., Syzdykova A.B., Ponomareva A.V., Smirnova E.A., Abrikosov I.A.</i> The importance of the lattice dynamic in the magnetic phase transition in ferh .	172
P-609.	<i>Ponomareva A.V., Mukhamedov B.O., Abrikosov I.A.</i> Calculation of solution enthalpy of carbon impurity in fe – mn paramagnetic alloys	173
P-637.	<i>Smirnova E.A., Mosyagin I.Yu., Vorobuev D.A.</i> Data driven design of al alloys .	173
AUTHOR INDEX		175

**ENTROPIC PHASE TRANSITIONS AND ACCOMPANYING ANOMALOUS
THERMODYNAMICS REGIONS IN NONIDEAL PLASMAS**

Iosilevskiy I.L.

¹*JIHT RAS, Moscow, Russia,* ²*MIPT, Dolgoprudny, Russia*

iosilevskiy@gmail.com

Remarkable features of *entropic* 1st-order phase transitions (*S*-PT) [1,2] are under discussion in comparison with well-known ordinary *enthalpic* (VdW-like) phase transitions (*H*-PT) [3]. The basic “driving” mechanism for the 1st-order *S*-transitions is forced decomposition of any bound complexes in a system: atoms, molecules, clusters etc. [4,5] up to the forced deconfinement of hadrons onto constituent quarks in far and exotic state of ultrahigh density and ultrahigh temperature matter in interiors of neutron stars [6,7]. The key feature of 1st-order *S*-transition is opposite (negative) sign of latent heat of transition and consequently falling character of $P(T)$ dependence for *S*-PT. It results in appearance of anomalous thermodynamics regions both inside and outside of the two-phase region of *S*-PT. This anomalous thermodynamics, accompanying *S*-PT, manifests itself [2,6] in simultaneous loss of positiveness for great number of second cross derivatives for Helmholtz free energy. The most important of them are Gruneisen parameter, thermal expansion coefficient and (isochoric) thermal pressure coefficient. Tight connections of thermodynamic and hydrodynamic anomalies are under discussion for shock and isentropic compression and expansion [2,6], for convective instability [7], mutual intersections for most of iso-lined, e.g. isotherms, isoentropes, shock adiabats (Hugoniot) curves etc. Remarkably complicated structure of stable and metastable domains within two-phase region of *S*-transitions is under discussions [4,5,6] in comparison with well-known simple topology of these domains for (VdW-like) *H*-transitions. Discussed anomalies are illustrated on the base of *S*-transitions revealed in last years via modeling calculations, e.g. [5], and in experiments both numerical and real. It is valid for the so-called dissociation- and ionization-driven phase transitions in WDM of hydrogen, nitrogen and other WDM fluids.

-
1. Iosilevskiy I., Krasnikov Yu., Son E., Fortov V. Thermodynamics and Transport in Non-Ideal Plasmas, /MIPT Publ. 2000.
 2. Iosilevskiy I. Entropic phase transitions and accompanying anomalous thermodynamics of matter, J. Phys.: Conf. Series (IOP Publishing) 653, 012077 (2015).
 3. Iosilevskiy I.L. and Starostin A.N. Thermodynamic stability problem and phase transitions in low-temperature plasmas, in: “Encyclopedia of Low-Temperature Plasma”, vol. I, Ch. III-1.6, Ed. by V. Fortov (Moscow: Nauka, 2000) p.327-339
 4. Iosilevskiy I. Non-Ideality and Phase Transitions in Coulomb Systems, Lambert Academic Publishing, Germany, ISBN 978-3-8454-2137-7, PP. 235 (2011)
 5. Gryaznov V., Iosilevskiy I. // J. Phys. A: Math. Theor. 2009, 42, 214007.
 6. Iosilevskiy I., IV Int. Conference "Compact Stars in the QCD Phase Diagram Prerow, Germany, Ed. D. Blaschke, // eConf C140926 (2015) [arXiv:1504.05850]
 7. Hempel M., Heinemann O., Yudin A., Iosilevskiy I., Liebendoerfer M. and Thielemann F-K., Phys. Rev. D 94, 103001 (2016) [arXiv:1511.0655]

EXPERIMENTAL STUDY OF THERMOPHYSICAL PROPERTIES AND PHASE TRANSITIONS OF METALS AND ALLOYS IN SOLID AND LIQUID STATES

Stankus S.V., Abdullaev R.N., Agazhanov A.Sh., Kozlovskii Yu.M., Savchenko I.V., Samoshkin D.A., Khairulin R.A., Yatsuk O.S.*

ITP SB RAS, Novosibirsk-90, Russia

**stankus@itp.nsc.ru*

In this report, we present the results of experimental study of thermophysical properties and phase transitions of solid and liquid metals and alloys based on alkaline and rare-earth elements over wide temperature ranges. Measurements of the density and coefficient of mutual diffusion (293–2000 K) were performed by the gamma-method, thermal expansion (110–1800 K) by the dilatometer method, heat capacity (200–1200 K) by the DSC method, increment of enthalpy (420–1300 K) by the mixing method, thermal conductivity and thermal diffusivity (293–1770 K) by the laser flash method. The description of experimental installations and measurement procedures is given. The properties of pure Li, Na, K, Rb, Cs, Mg, Pb, Bi, Sn, In, Ni, La, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er; magnetic materials based on Nd–Fe–B and Sm–Co; liquid systems of Li–Pb, Na–Pb, K–Pb, Rb–Bi, Cs–Bi, Li–Mg, Li–La, Mg–Pb were investigated.

For all the materials studied, the temperature dependences of the properties were obtained, changes of the properties in the regions of phase transitions were determined, references tables were developed and their errors were estimated. The phase diagrams of binary systems were refined. It was shown that the critical exponents of the thermal coefficient of linear expansion are positive, they have different values above and below the points of magnetic transformations and substantially exceed the critical heat capacity exponents in absolute value. It was found that the concentration dependences of the properties for certain component ratios deviate strongly (up to 50%) from the laws of the ideal solution. This indirectly confirms the presence of associated complexes (with a partially ionic character of the interatomic bond) in the liquid state, which gradually break down with increasing temperature.

The study was supported by the grants of the Russian Science Foundation No. 16–19–10023 (Rb–Bi, Cs–Bi), No. 17–79–10237 (liquid REM) and the Russian Foundation for Basic Research No. 15–08–00275 (Li–Pb), No. 12–08–00192 (Na–Pb), No. 16–38–00669 (Li–Mg), No. 15–38–20223 (magnets), No. 14–08–00602 (solid REM).

SPECTRAL AND TEMPERATURE DEPENDENCE OF ABSORPTION COEFFICIENT OF MOLTEN ALUMINUM OXIDE

Petrov V.A.

MIREA, Moscow, Russia

vapetrov@mirea.ru

A critical compilation and analysis of all the available experimental data and approximation formulas for the wavelength and temperature dependences of the absorption coefficient of molten aluminum oxide in semitransparent spectral range from 0.3 to 8 micrometers and temperature region from melting to 3000 K are presented. The main factors and the influence of physicochemical processes on the value of the absorption coefficient are considered.

It is shown that the available data can be divided into two groups, according to the level of absorption. The first group includes the results of the research of optical properties of solid propellant combustion products, and the second group – the results of the research of single crystal melts and some other high-purity molten aluminum oxides. Discrepancies in the results

of different authors in each of these groups are quite big. The explanation lies in the influence of initial material or external conditions, or experimental errors.

On the base of realized analysis, it is shown that the common feature of change of the absorption coefficient with temperature and wavelength in molten alumina tends rather to a semiconductor than to a dielectric. High absorption on Urbach tail, as temperature increases, takes place not only in visible, but also in short infrared region. High multiphonon absorption takes place at wavelength longer than 4.0 micrometers. Between these two regions, absorption is due to free carriers, which are formed by presence of contaminations, impurities, and defects in the local order of atom arrangement.

The abrupt increase of the absorption coefficient of aluminum oxide takes place at melting. The level of this increase is about two orders of magnitude. The results of comprehensive experimental investigations of this effect are presented. Analysis of the most novel investigations of atomic structure of molten alumina shows that molten alumina has gamma-phase-like atom coordination with many defects. This can be the reason of higher value of the absorption coefficient of the melt in comparison with the single crystal. However, the kinetics of restructuring of the alumina has not been investigated to date.

STATE OF IRON IN THE EARTH CORE: PARADIGM CHANGE

Belonoshko A. B.

KTH, Stockholm, Sweden

anatoly@kth.se

There is a ball of solid (Inge Lehmann, 1934) iron (Altshuller et al., 1960) in the center of the Earth. This ball is called the Inner Core. Any theory trying to describe the past of the Earth, explain the present state of the Earth, and predict its future, has to accommodate and explain a number of enigmatic features that the Core possess. The Inner Core drives the geodynamo in the liquid Outer Core that protects the life on Earth from cosmic radiation. There is a possibility that the core-mantle boundary might be the place where heavy hydrocarbons are synthesized. The Inner Core possess low shear modulus, sound waves traveling through the Core are highly attenuated, the Core is elastically anisotropic, and there is an indication that the Inner and Outer Cores rotate with different pace. The properties of the Core are tightly connected to the way in which atoms in the iron phase are packed. The current paradigm is that the stable phase of iron in the Core is hexagonal close packed. I will demonstrate that the first principles molecular dynamics supports another phase, namely body-centered cubic phase of iron. Quite remarkable, this phase has already been observed in experiments but its signature was misinterpreted. I will demonstrate that the stability of the bcc phase allows to resolve all the existing controversies and provide explanation of all above-mentioned enigmatic features.

PREDICTION OF THERMODYNAMIC PROPERTIES AND PHASE EQUILIBRIA OF OIL HYDROCARBONS AND PETROLEUM PRODUCTS BASED ON THE MULTIPARAMETER FUNDAMENTAL EQUATIONS OF STATE

*Grigoriev B.A.,¹ Gerasimov A.A.,² Alexandrov I.S.*²*

¹GAZPROM VNIIGAZ, Moscow, Russia, ²KSTU, Kaliningrad, Russia

*alexandrov_kgrd@mail.ru

Prediction of the thermodynamic properties and phase behavior of oil hydrocarbons and multicomponent hydrocarbon mixtures is a complex and not fully resolved problem. Information on the thermodynamic properties of hydrocarbon systems is necessary for the development of technology for the extraction, transport and processing of hydrocarbon raw materials. A wide range of operating parameters and hydrocarbon composition does not allow providing the needs of technological practice in information on the thermodynamic properties using only the experimental data. One of the ways to solve this problem is the development of analytical models based on fundamental equations of state, which on the one hand reliably reproduce the state surface, and on the other hand they allow calculating all thermodynamic properties with high accuracy. The report summarizes and presents the result of the work of the authors devoted to the development of fundamental equations of state of oil and gas condensates hydrocarbons. These individual and generalized equations of state formed the basis for the author's method for calculating the thermodynamic properties of complex hydrocarbon systems - oil and gas condensates of various fields, their fractions and different commodity products. The method is constructed within the framework of a single-fluid model with the use of minimal initial information about the physicochemical properties of the substance and its composition determined by standard laboratory methods. The authors also developed a procedure for transition from a single-fluid model to an ideal mixture model for predicting the phase behavior of complex hydrocarbon mixtures. Other mixture models that take into account the interactions of components or pseudo-components are considered. The report also discusses an alternative approach based on the application of the generalized equation of state obtained within the framework of the statistical associated fluid theory (SAFT) and provides high accuracy in calculating the thermodynamic properties and phase equilibria of hydrocarbon systems.

SURFACE TENSION OF SOLUTIONS OF LIQUEFIED GASES: EXPERIMENT, THEORY, AND SIMULATION

Bidakov V.G., Kaverin A.M., Andbaeva V.N., Khotienkova M.N.*

ITP UB RAS, Ekaterinburg, Russia

*bidakov@itp.uran.ru

The differential capillary method has been used to measure the capillary constant a^2 and determine the surface tension σ of binary solutions of liquefied gases with complete ($\text{CH}_4\text{-N}_2$, $\text{O}_2\text{-N}_2$) and partial ($\text{CH}_4\text{-He}$, $\text{C}_2\text{H}_6\text{-He}$, $\text{C}_3\text{H}_8\text{-He}$, $\text{CH}_4\text{-H}_2$, $\text{C}_2\text{H}_6\text{-H}_2$) solubility of the components. Experiments were conducted in the temperature range from the triple point to temperatures close to the critical point of the solvent at pressures from that of saturation of the pure solvent to 4 MPa. The error of the data obtained was 0.5-2.0 percent, where the upper value refers to the vicinity of the critical point. The temperature, baric and concentration dependences of a^2 and σ are presented in analytical form.

Experimental data are interpreted in the framework of the finite thickness layer method and the van der Waals capillarity theory. The results of molecular dynamics simulation have been

used to determine the excess free energy of a homogeneous fluid. Equations of state have been set up for solutions of the liquefied gases under investigation with the use of a one-liquid model. The influence coefficient in the functional of the free energy of an inhomogeneous system has been determined from data on the surface tension at a plane interface and an equation of state describing stable and metastable solution regions. The adsorption and the effective thickness of the surface layer have been calculated, the positions of the dividing surfaces in the interfacial layer have been determined.

The possibility of describing the surface properties of gas-saturated solutions in the framework of the generalized law of corresponding states is considered. It is shown that the saturation of hydrocarbons of the methane series with helium leads to changes in the character of the temperature dependence of the solution surface tension. If for solutions of helium in methane the derivative $(d\sigma/dp)_T$ is negative in the whole temperature range from the triple point to temperatures close to the critical point, for a propane-helium system the derivative $(d\sigma/dp)_T$ changes its sign from negative to positive even at a temperature close to that of the solvent normal boiling.

The work has been performed with a support of the RFBR (project 18-08-00403) and the Programme of Fundamental Investigations of the Ural Branch of the Russian Academy of Sciences (project 18-2-2-13).

**RESENT ADVANCES IN INVESTIGATION OF THERMOPHYSICAL
PROPERTIES OF ULTRA HIGH TEMPERATURE CERAMICS (UHTCS)
WITH THE AID OF LASER HEATING**

Sheindlin M.A.

JIHT RAS, Moscow, Russia

sheindlin@yandex.ru

The presentation is a review of novel original methods of high-temperature materials properties measurements developed recently at High Temperature Institute of RAS (Moscow, Russia). The scope of the developments and investigations is related to the extension of the temperature/pressure range of the co-called conventional thermophysics towards vicinity of the melting points of the most refractory substances such as graphite, carbides, diborides and some high-temperature oxides. Various methods of laser heating experiments are performed covering pressure range from vacuum up to high static pressures of a few kilobars. It is shown that different properties of UHTCs as well as graphite materials can be measured with a precision comparable with that of conventional methods. Laser heating methods are applied for measurements of different properties of both non-metal and metal-like substances in the condensed state and for vaporisation studies at temperatures up to ca. 4500 K. One must acknowledge high importance of modern methods of high-speed optical diagnostics and especially polychromatic optical pyrometry. This important issue is discussed in detail with a presentation of a range of high-speed pyrometers. Some experimental results on solidus and liquidus lines in the Zr-C, Zr-U-C, Ta-C and Hf-C systems are presented along with the data on spectral emissivity of liquid and solid phases in the vicinity of the melting points. Modern methods of the thermal conductivity and the thermal expansion measurements up to extremely high temperatures and some measurement results up to 3500 K are presented. Some data on behaviour of a few very high-melted oxides in the domain of their melting points are presented as well.

**THERMODYNAMIC DATABASE FOR PURE SUBSTANCES
IVTANTHERMO-ONLINE**

**Belov G.V.,^{1,2} Dyachkov S.A.,^{1,3} Levashov P.R.,^{1,3} Mezinov N.S.,⁴ Minakov D.V.,^{1,3}
Morozov I.V.,^{*1,3} Smirnov V.N.^{1,3}**

¹JIHT RAS, Moscow, Russia, ²MSU, Moscow, Russia, ³MIPT, Dolgoprudny, Russia, ⁴MIEM
HSE, Moscow, Russia

*morozov@ihed.ras.ru

Thermodynamic databases play essential role in a wide range of applications such as rocket engine engineering, nuclear power, chemical technology, metallurgy, resource usage, waste recycling, etc. The IVTANTHERMO information system has made a significant contribution to the accumulation of thermodynamic data. It has been developed since 1966 in the Institute of High Temperatures of the Academy of Sciences of the USSR. Nowadays the development is continued in the Department for Thermophysical Data of JIHT RAS.

The IVTANTHERMO system includes the database which contains more than 3400 substances, formed of 96 chemical elements, as well as supplementary software for analysis of experimental results, data fitting, calculation and estimation of thermodynamical functions and thermochemistry quantities. In this report we present the next version called "IVTANTHERMO-Online" [1]. It has a new extensible database design, user-friendly web interface with client-server architecture and a number of features for online and offline data processing. The new system enables to handle multiple versions of each block of data, to store additional information for users and experts (such as comments, bibliography, experimental data, molecular structure, etc.), to present data in multiple forms, to attach calculation services and link with other databases. The substances can be searched using their names, formula, atomic composition or CAS numbers. The supplemented software includes modules for calculation of chemical composition and data fitting.

-
1. Belov G.V., Dyachkov S.A., Levashov P.R., Lomonosov I.V., Minakov D.V., Morozov I.V., Sineva M.A., Smirnov V.N. // J. Phys. Conf. Ser. 2018. V. 946. P. 012120

**ESTIMATION OF CRITICAL PARAMETERS OF REFRACTORY METALS
BASED UPON FIRST-PRINCIPLE SIMULATION**

Levashov P.R.,^{*1,2} Minakov D.V.^{1,2}

¹JIHT RAS, Moscow, Russia, ²MIPT, Dolgoprudny, Russia

*pasha@ihed.ras.ru

Critical points of the majority of metals are currently unknown. An experimental measurement of critical parameters of metals is very difficult to carry out owing to extremely high temperatures (higher than 3000 K) and pressures (from kilobars to tens of kilobar). A theoretical calculation of near-critical metallic fluid causes significant difficulties because of the degeneration of the electronic subsystem and strong interaction. Only model estimations exist having a particularly big scatter for refractory metals [1]. Meanwhile, the position of the binodal and critical point on a phase diagram of metals is necessary to know for the creation of adequate equations of state at densities below normal. Moreover, in the near-critical region of metals interesting phenomena have been predicted, in particular, the metal-non-metal transition and the cluster formation.

Only pulsed experiments can give some information about the position of critical points, in particular, on isentropic [2] and isobaric [3] expansion. In experiments on isentropic expansion with porous samples it is possible to observe the evaporation of a metal under its expansion

into different anvils. Isobaric expansion under the action of powerful current pulses allows one to investigate properties of matter near the liquid–vapor equilibrium curve. However, until recently there were no models able to consistently describe both these types of experiment, in particular, for tungsten and molybdenum. In this work we will present a review of approaches for a determination of critical parameters of refractory metals. Also we are going to discuss our results of quantum molecular dynamics simulation for the interpretation of experimental data and the estimation of critical parameters of tantalum, tungsten and molybdenum.

1. Minakov D. V., Paramonov M. A., Levashov P. R. // Phys. Rev. B. 2018. V. 97. P. 024205.
2. Gudarenko L.F. , Gushchina O.N. , Zhernokletov M. Yu., Medvedev A.B. and Simakov G.V. // High Temp. 2000. V. 38. P. 413.
3. Gathers G.R. // Rep. Prog. Phys. 1986. V. 49. P. 341.

THERMOPHYSICAL PROPERTIES OF THERMAL INTERFACE NANOMATERIALS FOR THERMAL STABILIZATION OF ENERGY AND ELECTRONIC DEVICES

Dmitriev A.S.

MPEI, Moscow, Russia

asdmiriev@mail.ru

In recent years, interest in the creation of new nanomaterials for the promising tasks of electronics, optoelectronics and energy has increased. The emergence of new functional materials for low-current and high-current electronics and energy are dictated by the active development of nanoelectronics and nanoenergetics. Of special interest are the thermophysical properties of the surfaces of new functional nanomaterials, since numerous applications and new trends in the development of promising technological directions depend on them. The paper presents the results of research in the field of development, creation and research of thermophysical properties of new hybrid nanocomposites based on metal monodisperse microspheres, polymers and graphene flakes. The results of the technology of creating such hybrid composites, studying the properties of wetting and spreading of droplets of various working fluids on the surfaces of hybrid composites are presented. Experimental and theoretical results on the study of heat transfer (thermal conductivity) in such hybrid nanocomposites are considered. Particular attention is paid to the results of studying thermophysics and hydrodynamics during the evaporation and boiling of droplets on superheated surfaces of hybrid graphene nanocomposites, maps of regimes, conditions for existence and suppression of the Leidenfrost effect were constructed. The variety of properties of new nanocomposites based on graphene flakes allows in the future to create functional energy materials with controlled thermophysical properties both on the surface and in the volume of the material. The work is supported by the Russian Science Foundation (Grant No. 17-19-01757).

**EQUATION OF STATE AND METALLIZATION IN METAL VAPORS AND
INERT GASES**

*Khomkin A.L., Shumikhin A.S.**

JIHT RAS, Moscow, Russia

**shum_ac@mail.ru*

The effect of metallization of dense metal vapors [1], inert and molecular gases (see [2]), discovered experimentally, has been long discussed in the literature [3]. Metallization of vapors shows itself in the growth of conductivity up to a minimum metallic value. An unusual explanation of the effect of metallization in metal vapors was proposed in [4] using the chemical model "3+". The increase in vapor conductivity at compression is due to the manifestation of a new component – jellium. Given the presence of jellium, we named this model the "3+" model. Jellium is constituted by tails of wave functions of bound electrons. In this work, using the "3+" model, we calculated the thermophysical and transport properties of plasma of both metal vapors and dense inert gases. Comparison with the available experimental data and theoretical calculations is made [1, 2]. The comparative analysis of the role of the jellium, interchange and interatomic interactions in dense plasma of inert gases and metal vapors is made. The proposed simple model of plasma fluid is quite successfully used in the near-critical region of metal vapors, and now for dense plasma of inert gases. Introduction to the model of a new component – jellium, made it possible to understand and solve a number of problems of physics of nonideal plasma.

This work was supported by Presidium RAS program No. 13 "Condensed Matter and Plasma at High Energy Densities".

-
1. DeSilva A. W., Rakhel A. D. // Contrib. Plasma Phys. 2005. V. 45. P. 236.
 2. Fortov V. E., Ternovoi V. Ya., Zhernokletov M. V. et al // J. Exp. Theor. Phys. 2003. V. 97. P. 259.
 3. Fortov V. E., Khrapak A. G., Yakubov I. T. Physics of Nonideal Plasma. Moscow: Fizmatlit, 2010.
 4. Khomkin A. L., Shumikhin A. S. // J. Exp. Theor. Phys. 2017. V. 124. P. 1001.

PLASMA PHASE TRANSITION IN HYDROGEN AT HIGH PRESSURES.

*Norman G.E., Saitov I.M.**

JIHT RAS, Moscow, Russia

**saitovilnur@gmail.com*

The assumption of the existence of metallic hydrogen was suggested by Wigner and Huntington in 1935. An estimate of the metallization pressure at zero temperature at 25 GPa was obtained. However, a sharp increase in the reflection coefficient of hydrogen was observed at a pressure of 495 GPa and a temperature of 5.5 K, which was interpreted as the transition of solid hydrogen to the conducting phase. The work reviews theoretical and experimental works, as well as proposals on practical applications of metallic hydrogen. The emphasis is on the latest theoretical and experimental research and the original results of the authors of the report. Within the framework of the density functional theory and quantum molecular dynamics, the dependences of pressure, electrical conductivity, and proton-proton pair correlation functions (PCF) on the density in the range 1.14-2.0 g/cm³ at temperatures 50 and 100 K were calculated. The pressure range is 300-1200 GPa, i.e. solid phase is considered. The calculations are carried

out using the VASP package. The monoclinic lattice of the C2/c group is used as the initial configuration, since this structure is the most stable in the pressure region above 260 GPa. A structural transition was observed at a pressure of 607 GPa, characterized by a marked jump in the electrical conductivity and a sharp decrease in the number of H₂ molecules. At a density of 1.563 g/cm³ and a pressure of 607 GPa, the PCF peak disappears at a distance of 0.74 Å corresponding to the interatomic distance in the H₂ molecule, which is an indication of the decay of the H₂ molecules. At the same time, the electrical conductivity value sharply increases to 85300 (Ohm·cm)⁻¹ and the PCF peak appears at a distance of 0.92 Å. This distance is equal to the interproton distance in the molecular ion H₃⁺. This position of the first maximum remains unchanged in the pressure range of 607-832 GPa. This indicates the implicit appearance of H₃⁺ ions in the structure of solid hydrogen upon its transition to a conducting state. Thus, the nature of the transition combines ionization with structural changes. With further compression, the first maximum of the PCF begins to correspond to the average distance between protons at a given density, which indicates the complete dissociation of hydrogen ions. Strong ionization during the phase transition in dense solid hydrogen/deuterium brings this transition closer to the plasma phase transition in the fluid hydrogen.

EXTENDED DESCRIPTION THERMAL PROPERTIES OF CARBON DIOXIDE USING EQUATION OF STATE WITH A SMALL NUMBER OF PARAMETERS

*Bezverkhii P. P.,¹ Martynets V. G.,^{*1} Kaplun A. B.,² Meshalkin A. B.²*

¹*IIC SB RAS, Novosibirsk, Russia, ²ITP SB RAS, Novosibirsk-90, Russia*

**mart@niic.nsc.ru*

A new combined thermal equation of state (EoS) with a small number of adjustable parameters is proposed, which describes both the regular and critical areas. This equation approximates experimental p, V, T -data of CO₂ in the intervals of their measurements ($0 < V_c/V < 2, 217K < T < 430K, 0 < p \leq 25MPa$). The array of p, V, T -data consisted of 731 points. The proposed EoS is an explicit function of V, T and is written in the form of:

$$p/p_c = (1 - Y)p_{reg}/p_c + Yp_{scal}/p_c.$$

The EoS includes a new regular part of p_{reg} for approximation of p, V, T -data outside the critical region, a singular scaling part of p_{scal} for the critical region, and a transitional (crossover) function Y . Comparison of the calculating results of pressures using this EoS with experimental and reference table data, even outside the approximation intervals up to 200 MPa, showed that they coincide within the data error. The high accuracy of approximation of CO₂ thermal data by the proposed equation made it possible to calculate the behavior of other properties, using the coefficients of this EoS, including caloric values in the specified regions of system state by the known thermodynamic relations. It was calculated the isochoric heat capacity, enthalpy and adiabatic speed of sound. The comparison of the obtained values with the known experimental data has shown their good coincidence. Thus, the proposed combined EoS makes it possible to develop reference tables on thermodynamic properties of CO₂ in a wide range of states, including the critical area. It is possible to calculate the calorific properties and sound velocity also for other liquids using a new equation of state, including regular and scaling parts with a relatively small number of adjusting parameters (up to 20).

NUMERICAL MODELING OF THERMODYNAMIC PARAMETERS FOR MIXTURES WITH A SMALL PARAMETRIC EQUATION OF STATE OF THEIR COMPONENTS

Maevskii K.K.

LIH SB RAS, Novosibirsk, Russia

konstantin@hydro.nsc.ru

The results of numerical experiments on modeling of shock-wave loading of porous and solid heterogeneous mixtures, including tungsten as a component, are presented. The model is based on the assumption that all components of the mixture, including gas, under shock-wave loading are in thermodynamic equilibrium (model TEC - thermodynamic equilibrium components). Condensed components are described by a small parametric equation of state of Mie–Grüneisen type [1, 2].

Interest in the investigating of the compressibility of powder mixtures with tungsten as a component is associated with the possibility of creating materials with the desired properties, and the properties of tungsten. The equation of state used for components contains only one free parameter, which allows one to describe the data obtained on the basis of experiments at maximum compressions. The parameters of the model, which allows one to describe reliably thermodynamic parameters of shock-wave loading of pure materials, are used for modeling mixtures, including tungsten as a component. It is shown that this model allows us to describe reliably shock-wave loading of mixtures of different compositions [3].

1. Kinelovskii S.A. and Maevskii K.K. Model of the behavior of aluminum and aluminum based mixtures under shock wave loading // High Temperature 2014. V. 52. P. 821.
2. Kinelovskii S.A. and Maevskii K.K. Modeling shock loading of multicomponent materials including bismuth // High Temperature 2016. V. 54. P. 675.
3. Maevskii K.K and S.A. Kinelovskii Thermodynamic parameters of mixtures with epoxy as a component under shock wave loading // Journal of Physics: Conf. Series 2018. V. 946. P. 012113.

CALCULATION OF THERMOPHYSICAL PROPERTIES OF CRYPTON AND XENON BASED ON FRACTAL EQUATION OF STATE

*Magomedov R.A.,*¹ Akhmedov E.N.,¹ Meilanov R.R.,¹ Beybalaev V.D.,^{1,2}*

Aliverdiev A.A.^{1,2}

¹*IGR DSC RAS, Makhachkala, Russia,* ²*DSU, Makhachkala, Russia*

**ramazan_magomedov@rambler.ru*

The actuality of the study of new materials and substances (determination of thermophysical properties) in connection with the development of new technologies in industry, resulted in appearance of a new state equations and development of substance thermophysical properties calculation methods, including methods with the application of the integro-differentiation of fractional order.

The need of computational data for the thermophysical properties of substances at high temperatures and pressures close to the extremes arises in connection with the complexity of the experimental study of such states.

Transition from the ordinary derivatives to derivatives of fractional order is connected with the principles of the physics of many-particle systems and realized on the basis of generalization of thermodynamics. From the derived “fractal” state equation:

$$P = \rho T \frac{R}{M} \left\{ 1 + \rho B + (1 - \alpha) \left[\ln \left(\frac{eM}{\rho N_A} \left[\frac{mkT}{2\pi h} \right]^{3/2} \right) + \psi(1) - \psi(2 - \alpha) - \rho B \right] \right\}$$

we can define the rate of the fractional order derivative α and further calculate thermodynamic

properties, using the obtained analytical expressions for entropy and isochoric heat capacity [1]. The transition to classical thermodynamics is obtained in the particular case when the rate of the fractional order derivative is equal to unity.

On the basis of the “fractal” state equation, with account of second virial coefficient B , the thermophysical properties of krypton Kr and xenon Xe: entropy S and isochoric heat capacity C_V have been calculated. Obtained results are in good agreement with the reference data. Deviation for the entropy is $\sim 0.03\%$, and for the heat capacity is $\sim 2.4\%$, which indicates the promise of the proposed method.

This paper has been supported by Russian Foundation for Basic Research (Grant No. 16-08-00067a).

-
1. Magomedov R.A., et al.//JTAC, 2018. P. 1-6. doi:10.1007/s10973-018-7024-2

CALCULATION OF THERMODYNAMIC FUNCTIONS BASED ON THE JOINT THERMAL AND ACOUSTIC MEASUREMENTS

Kuznetsov K.I., Sukhikh A.A., Granchenko P.P., Skorodumov S.V.*

MPEI (TU), Moscow, Russia

**granchenkop@gmail.com*

The use of new working fluids for steam turbine units that are able to compete with the traditional water vapor is one of the promising directions in expanding the fundamental foundations of heat power engineering [1]. Such fluorocarbons as e.g. octafluoropropane (C₃F₈), decafluorobutane (C₄F₁₀) and octafluorocyclobutane (c-C₄F₈) need to have cumulative databases on thermophysical properties in the range of parameters of the operation of power plants [2,6], since the listed substances were previously used primarily as refrigerants. A comprehensive study of thermodynamic properties, including measurements of the density of the working fluid and the sound speed as a function of pressure and temperature, as properties most accurately studied, allows to calculate other thermodynamic functions using the mathematical apparatus of thermodynamics [4,5]. The report presents the conclusions of the formulas for calculating the isobaric and isochoric heat capacities based on the mathematical apparatus of thermodynamics [3]. An example of calculation based on new experimental data on the thermal and acoustic properties of octafluorocyclobutane in the liquid phase is given.

1. Sukhikh A. A., Miljutin V. A., Antanenkova I. S. // Thermodynamic efficiency of carbon fluorines as working bodies in thermal cycles of the atomic power station // Power plants. 2010. V. 415. No. 10. P. 2-8.
2. Granchenko P. P., Sukhikh A. A., Kuznetsov K. I. // Thermodynamic analysis of use of fluorocarbon working fluids in power generating units of small scale power plants // Safety and Reliability of Power Industry. 2017. V. 10. No. 4. P. 310-315.
3. Sychev V. V. Differential equations of thermodynamics. Publ. 3. P. 161-165.
4. Granchenko P. P., Kuznetsov K. I., Sukhikh A. A., Skorodumov S. V. // Experimental measurements of the density of octafluorocyclobutane in the field of operation parameters of thermal power plants // Safety and Reliability of Power Industry. 2016. No. 3(34). P. 35-38.
5. Kuznetsov K. I. Sukhikh A. A., Skorodumov S. V., Granchenko P. P. Proceedings of the VII All-Russian Scientific and Technical Conference : Power: Condition, Problems, Prospects Orenburg, 2014, p. 66-70.
6. REFPROP 9.0: Reference Fluid Thermodynamic and Transport properties: Copyright 2010 by the U.S. Secretary of Commerce on behalf of the USA.

DETERMINATION OF SATURATED VAPOR PRESSURE OF AROMATIC HYDROCARBONS ON EXPERIMENTAL DATA OF THEIR SOLUBILITY IN SUPERCRITICAL CARBON DIOXIDE

Bilalov T.R., Gumerov F.M.*

KNRTU, Kazan, Russia

**t.bilalov@yandex.ru*

The paper presents a method for describing the solubility of various substances in supercritical carbon dioxide, based on the equation of state of real gases Peng-Robinson, as well as the one-parameter mixing law Muhopadhyaya and Rao. The calculation algorithm includes an unknown binary interaction coefficient determined by the method of iteration and minimization of the root mean square deviation of the calculated solubility values from the experimental ones on the described isotherm, as well as the saturated vapor pressure of the soluble substance at the process temperature. In the presence of experimental data of saturated vapor pressure, the accuracy of the description is primarily affected by the correctness of the experiment methodology and its accuracy. In the absence of reliable experimental data, this value is determined by different calculation methods [1]. Most of the calculation methods are based on the Clausius-Clapeyron equation, and use the critical parameters of the test substance as the initial data, as well as the normal boiling point. Different authors have proposed unique calculation methods for determining the pressure of saturated vapors. Results of calculations with the use of these methods sometimes differ by several orders for one and the same substance. The paper presents the results of a study of the influence of the method for determining the pressure of saturated vapors of a substance dissolved in supercritical carbon dioxide on the accuracy of the description of solubility. The list of calculation methods for establishing the value of the saturated vapor pressure includes methods: Clapeyron, Lee-Kesler, Riedel, Frost-Kalkwarf-Todos and Riedel-Plank-Miller. It is shown that in most cases these methods do not allow describing experimental data on substance solubility in supercritical carbon dioxide with acceptable (up to 10-12%) accuracy. The paper also suggests the use of saturated vapor pressure as a second adjustable parameter in the description of solubility in addition to the traditionally accepted binary interaction coefficient. This significantly increases the accuracy of the description of the solubility of substances in supercritical carbon dioxide. The substantially greater convergence of the saturated vapor pressure values established in this way with the values obtained in the framework of the experimental methods is shown. Experimental data on solubility of various substances used in the work were taken from [2].

-
1. R. Reid Properties of Gases and Liquids, McGraw-Hill publisher, New York, (1987). Khimiya publisher, Leningrad, (1982) 592 p.
 2. Solubility in Supercritical Carbon Dioxide, Ram B. Gupta, Jae-Jin Shim, CRC press, ISBN: 0849342406, 960p.

THE FUNDAMENTAL EQUATION OF STATE FOR R1234yf

Rykov V.A., Rykov S.V., Sverdlov A.V.*

SPbSU ITMO, Saint-Petersburg, Russia

**togg1@yandex.ru*

On the basis of the phenomenological theory of the critical point and the Benedek hypothesis, the fundamental equation of state for R1234yf was developed in the form of the following expression for the Helmholtz free energy F :

$$F(\rho, T) = F^0(\rho, T) + RT\omega \sum_{i=0} \sum_{j=0} C_{ij} \tau_1^j (\Delta\rho)^i + F_{nreg}(\rho, T), \quad (1)$$

where $F^0(\rho, T)$ is the ideal gas component of F ; $\Delta\rho = \omega - 1$; $\omega = \rho/\rho_c$; ρ_c is the critical density; T_c is the critical temperature; R is the gas constant; C_{ij} are constant coefficients.

The function $F_{nreg}(\rho, T)$ is the irregular component of the Helmholtz free energy:

$$F_{nreg}(\rho, T) = \frac{p_c}{\rho} \phi(\omega) |\Delta\rho|^{\delta+1} a(x), \quad (2)$$

where $a(x)$ is the scale function; $x = \tau/|\Delta\rho|^{1/\beta}$; $\tau = T/T_c - 1$; β and δ are critical indices; $\phi(\omega)$ is the regular function; p_c is the critical pressure.

To calculate the parameters of the function (2), the results of [1] are used. Two variants of the choice of the scale function $a(x)$ are considered: (i) on the basis of Migdal phenomenological theory of the critical point [2]; (ii) on the basis of a new presentation of the scale hypothesis [3]. As a result, the equation of state for R1234yf has been developed, which has the following working area: for temperature 230–400 K and for pressure up to 20 MPa. A comparison is made with the known experimental data on the equilibrium properties of R1234yf and the fundamental equation of state [4].

-
1. Lysenkov V.F., Rykov V.A. // High Temp. 1991. V. 29. P. 1236.
 2. Kudryavtseva I.V., Rykov S.V. // Russ. J. Phys. Chem. A. 2016. V. 90. P. 1493.
 3. Rykov S.V., Rykov V.A., Kudryavtseva I.V. // XXXI International Conference on Equations of State for Matter. 2016. P. 62.
 4. Richter M., McLinden M.O., Lemmon E.W. // J. Chem. Eng. Data. 2011. V. 56. P. 3254.

ABOUT ROUND DATES, ACUTE QUESTIONS AND SOLVING PROBLEMS OF LOW-PARAMETRIC EQUATIONS OF STATE BY LOGICAL ABDUCTION

Petrik G.G.

IGR DSC RAS, Makhachkala, Russia

galina_petrik@mail.ru

It is generally recognized that the ancestor of one of the two directions in the construction of the equations of state (ES) – low-parametric and multi-constant – is the work, model and the ES of Van der Waals. The famous ES (his author got a Nobel Prize) in five years will “hit” 150. During this time hundreds of modifications of the Van der Waals ES were proposed, but Redlich-Kwong ES stands out among them (in 2019 he will be 70 years old). Restoring the extinct interest in the work of Van der Waals, their ES created a lot of important modifications (Soave-Redlich-Kwong, Peng-Robinson, Schmidt-Wenzel, Usdin, McAuliffe), which age is also significant: 45 – 40 years. However, despite the known successes, the problem of creating the optimal low-parametric ES does not solved yet.

There are many questions to such low-parametric ES. One of the first are about number of parameters in the famous “two-parametric” ES, about the meaning of the parameter b of different ES, the meaning of the third parameter and the molecular model that customary associated with these ES. The undefined meaning of the parameters leads to the main disadvantage of the ES vdW-type, which is their weak connection with the microlevel. Making a conclusion the advantages of the new ES (thermodynamic-level model), authors usually do not touch upon the reasons and do not link it with changes of the molecular-level model.

The situation responds to the method of logical abduction. There are questions that cannot be resolved within the framework of the current model. If problems within the framework of the new model can be solved, this means its adequacy. The new molecular-thermodynamic model built by us. It based on the simplest micromodel – the interacting point centers. Families of low-parameter physically grounded realistic thermal equations of state (PGRTEs) were obtained. Within the framework of this model, it is possible to receive answers to many questions that are available in the ES of vdw-type that means the adequacy of the new ES. It should be noted that the ES of the interacting point centers will be 10 years next year (see our work at www.csmos.ru).

ISOPLERE EQUATIONS OF A BINARY MIXTURE IN THE VICINITY OF VAPOR-LIQUID CRITICAL POINT IN THE FRAMEWORK OF SCALING THEORY

Kulikov V.D., Belyakov M. Yu.*

OGRI RAS, Moscow, Russia

**sl-kulikov@ogri.ru*

An analytical expression of liquid phase (or gas phase) volume of a binary mixture in the vicinity of liquid-vapor critical point have been obtained in the framework of scaling theory and isomorphism concept of critical phenomena in mixtures [1,2]. The behavior of liquid phase volume was studied along the lines of fixed average densities ρ (isochores), lines of constant temperatures T or pressures P . It has been shown that the liquid phase volume reveals nonmonotonic behavior resulting in the appearance of specific maximums. The equations which determine the locations of such maximums have been derived. In particular, it was demonstrated that the maximum of liquid phase v_L arising at variation of the temperature T on the isochore exists only for densities less than critical density ρ_c whereas the value of this maximum does not exceed the half of system volume. The analytical equations of isopleths in the vicinity of liquid-vapor critical point for pressure-temperature and temperature-density variables have been obtained. The expressions for the temperature derivatives of pressure and mixture density along the isopleths were also derived. It was shown that the equations which determine the positions of the so-called special points of dew-bubble curves, namely, the points of maximal pressure and temperature (cricondenbar and cricondentherm) result directly from these derivative expressions.

-
1. Belyakov M.Yu., Gorodetskii E.E., Voronov V.P., Kulikov V.D. // Chem. Phys. 2014. V. 445. P. 53.
 2. Belyakov M.Yu., Voronov V.P., Gorodetskii E.E., Kulikov V.D. // JETP Lett. 2008. V. 88. P. 302.

THE FUNDAMENTAL EQUATION OF STATE FOR ARGON SATISFYING THE SCALE HYPOTHESIS FOR THE REGION OF HIGH TEMPERATURES AND PRESSURES

*Rykov V.A., Kudryavtseva I.V., Rykov S.V.**

SPbSU ITMO, Saint-Petersburg, Russia

**togg1@yandex.ru*

In this report, the fundamental equation of state of matter (FEoS) is considered that satisfies the scale hypothesis of the critical point. When constructing FEoS, the method of pseudocritical points (PCP) is used [1–3]. The PCP method is based on the Benedek hypothesis [4]. At present,

the PCP method has been physically justified on the basis of Migdal phenomenological theory of the critical point [5, 6] and a new representation of the scale hypothesis of the critical point [7]. We have shown that, based on the PCP method, it is possible to construct FEOs of argon, which has the following characteristics: (i) in the region of small densities, it is transformed into the virial equation of state; (ii) in the region of the critical point FEOs is transformed into the Widom equation; (iii) the working area of FEOs is according to pressure ($0 \leq p/p_c \leq 740$), density ($0 \leq \rho/\rho_c \leq 3.2$) and ($83.8058 \leq T \leq 2300$ K) in temperature. We have compared FEOs with some known equations of argon state and discussed the results.

-
1. Rykov V.A. // J. Eng. Phys. Thermophys. 1985. V. 48. P. 476.
 2. Kozlov A.D., Lysenkov V.F., Popov P.V., Rykov V.A. // J. Eng. Phys. Thermophys. 1992. V. 62. P. 611.
 3. Kudryavtseva I.V., Rykov V.A., Rykov S.V., Ustyuzhanin E.E. // J. Phys.: Conf. Ser. 2018. V. 946. P. 012118.
 4. Benedek G.B. // Polarization Matiere et Rayonnement, Livre de Jubile en l'Honneur du Professeur A. Kastler. 1968. P. 71.
 5. Migdal A.A. // Zh. Eksp. Teor. Fiz. 1972. V. 62. P. 1559.
 6. Kudryavtseva I.V., Rykov S.V. // Russ. J. Phys. Chem. A. 2016. V. 90. P. 1493.
 7. Rykov S.V., Kudryavtseva I.V., Rykov V.A. // Scientific and Technical Bulletin of Povolzhie. 2014. No 2. P. 44.

EFFECT OF NON-LINEAR SCREENING ON COMPLEX PLASMA THERMODYNAMIC STABILITY REGIONS

Martynova I.A.,^{*1,2} *Iosilevskiy I.L.*^{1,2}

¹*JIHT RAS, Moscow, Russia,* ²*MIPT, Dolgoprudny, Russia*

**martina1204@yandex.ru*

Thermodynamic stability of complex plasma is under discussion. We obtained huge negative total pressure and compressibility areas in the initial phase diagram [1] of complex plasma using the equations of state [1, 2]. Questions of thermodynamic stability and an existence of an additional phase transition of gas–liquid and (or) gas–crystal types in two-component systems are discussed. The present work is devoted to the analysis of the applicability range of a basic assumption in the phase diagram [1], i.e., linearized (Debye) screening of macroions by microions, which leads to the Yukawa form for effective interactions between macroions. Parameters of non-linear screening of macroions were calculated within the direct Poisson–Boltzmann approximation. Two effects were revealed as a result of such calculations: (1) decomposition of all microions onto two subclasses, free and bound ones, and (2) significant reduction of effective charge Z^* of initial bare macroion Z . The corresponding thermodynamic effects based on the non-linear screening and the resulting reduction of the negative total pressure and negative total compressibility regions are discussed. The work is supported by the Presidium RAS Scientific Program of Fundamental Research "Condensed matted and plasma under high energy density".

-
1. Hamaguchi S., Farouki R.T., Dubin D. // Phys. Rev. E. 1997. V. 56. P. 4671.
 2. Khrapak S.A., Khrapak A.G., Ivlev A.V., Morfill G.E. // Phys. Rev. E. 2014. V. 89. P. 023102.
 3. Martynova I.A., Iosilevskiy I.L., Shagayda A.A. // IEEE Trans. Plasma Phys. 2018. V. 46. No. 1. P. 14.

THE SINGULARITY OF THE TWO-PARTICLE CORRELATOR IN THE VICINITY OF THE PHASE TRANSITION POINT OF THE PURE METAL MELT

Fleyta D.Iu.,^{*1,2} *Norman G.E.*,^{1,2} *Pisarev V.V.*^{1,2}

¹JIHT RAS, Moscow, Russia, ²MIPT, Dolgoprudny, Russia

**fleyta.du@phystech.edu*

The phase transition point of the substance, in spite of its exclusive effect on the behavior of a substance, is not special for its thermodynamic functions [1, 2].

It is shown that certain two-particle motion correlators have singularities in the neighborhood of the phase transition point. Correlators similar to those described in the paper [3], were calculated for systems of pure metal melt, modeled by the molecular dynamics method. The time behavior of the motion correlators is different in the liquid stable and supercooled metastable melt phase for a variety of metals. A physical interpretation of such spatial correlations of long-range order in metastable systems is also given. Dependences of correlation functions on the rate of cooling, as well as on the sort and number of atoms in the system are shown.

This work was supported by the grant of the President of Russian Federation for young scientists MK-1404.2017.8.

-
1. Andreev A. F., // JETP 1963, V. 64. No. 6. P. 2064.
 2. Landau L. D., Lifshitz E. M., Statistical physics, Moscow (1976), P. 284.
 3. Voloshin V. P., Malenkov G. G., Naberukhin Yu. I., //J. Struct. Chem. 2013, V. 54, Sup. 2. P. 233–51.

ESTIMATION OF CRITICAL POINT PARAMETERS OF TUNGSTEN AND COPPER FROM EXPERIMENTS ON ISENTROPIC EXPANSION OF SHOCK-COMPRESSED POROUS METALS

Emelyanov A.N.

IPCP RAS, Chernogolovka, Russia

emelyanov@fcp.ac.ru

Experimental data on thermodynamic properties of expanded metals by the isentropic expansion of shock-compressed porous tungsten and copper are presented. The metals reached the near-critical region of the liquid-vapor phase transition at the expansion. High temperatures at the expansion of shock-compressed porous tungsten into two-phase liquid-vapor regions was recorded. This led to the conclusion that local overheating is accompanied by shock compression. That is, there is uneven heating of the shock-compressed porous metal after shock-compressed and expansion. This can introduce errors at the estimation of the critical point parameters obtained from experiments on isentropic expansion of shock-compressed porous samples. The critical point parameters of tungsten and copper were estimated.

INVESTIGATION OF THE LIQUID DENSITY, THE GAS DENSITY AND THE PRESSURE: SOME MODERN MODELS AND NUMERICAL DATA ON THE SATURATION LINE OF H₂O

Ochkov V.F.,^{*1} *Ustyuzhanin E.E.*,¹ *Znamensky B.E.*,¹ *Rykov S.V.*,² *Rykov V.A.*²

¹*MPEI (TU), Moscow, Russia,* ²*SPbSU ITMO, Saint-Petersburg, Russia*

**evgust@gmail.com*

An analysis of some literary sources is made in the report. They contain tabulated data on the liquid density (ρ_l), the gas density (ρ_g) and the pressure (P) on the saturation line of H₂O. We have considered also a work of Alexandrov et. al. (1998) and a work of Anisimov et. al. (1990). It is shown that the accurate calculated ρ_l , ρ_g , T data are based on scaling models of Anisimov et. al. (1990). Among them there is a form, $\rho_g(\tau, D, C)$, which is associated with ρ_g , here $\tau = (T_c - T)/T_c$ is the relative temperature, $D = (\alpha, \beta, T_c \dots)$ are critical characteristics, (α , β) are critical indexes, C are adjustable coefficients. An Abdulagatov scaling model, $P(\tau, D, C)$, is considered too. These models meet the scale theory of critical phenomena (ST), work in the interval, $\tau = 0.002 - 0.012$, and reflects properties (ρ_l , ρ_g , P , T) data accumulated before 1990.

We have considered a model, $f_d(\tau, D, C)$, which is intended to describe the mean diameter, $f_d = (\rho_l + \rho_g)(2\rho_c)^{-1} - 1$. The model, $f_d(\tau, D, C)$, is adapted to H₂O (Anisimov, 1990) and has contained a scaling component with $(1 - \alpha)$ index and a linear component. Another type of $f_d(\tau, D, C)$ is developed in this work and referred to as a combined scaling model. Its structure contains several components, among them: (i) component with 2β index, (ii) a component with $(1 - \alpha)$ index. A similar combined scaling models have been developed for other properties (the order parameter, ρ_l , ρ_g , P).

A nonlinear methods are proposed to calculate characteristics, $D = (\alpha, \beta, T_c, \rho_c \dots)$, and adjustable coefficients, C . For example, this statistical procedure is oriented on $f_d(\tau, D, C)$ uses input ρ_l , ρ_g , T data, which are placed in a wide temperature range including the critical region. There are got numerical estimates of parameters those are related to functions ($f_d(\tau, D, C)$, $\rho_g(\tau, D, C)$, $P(\tau, D, B)$ et. al.) and based on tabulated ρ_l , ρ_g , P , T data related to IAPWS-IF 97 of H₂O. These functions have been used to calculate (ρ_l , ρ_g , P , T) values in the interval $10^{-5} < \tau < 0.01$. We have considered an equation of state (EOS), which is included in the formulation (IF-95) and recommended by IAPWS. We have compared our (ρ_l , ρ_g , P , T) data with results those are determined on the basis of this EOS.

THE SOUND VELOCITY MEASUREMENTS FOR FLUID IRON IN THE VICINITY OF THE METAL-NONMETAL TRANSITION

Kaptilnyi A.G., *Kondratyev A.M.*, *Pletnev A.E.*, *Rakhel A.D.*^{*}

JIHT RAS, Moscow, Russia

**rakhel@oivtran.ru*

Phase diagram of fluid iron is different from that for the dielectric fluids. There is some evidence that this fluid has two critical points and an extra triple point [1]. However, for a reliable detection of the metal-nonmetal transition of the first kind a direct diagnostics of the transition is required. It is known from hydrodynamics that in a transition from the liquid state to the two-phase state (the liquid with the fine dispersed vapor bubbles distributed in it) the speed of sound decreases discontinuously to very small values. This property of the two-phase state will be used here to determine the boiling curve and the metal-nonmetal transition equilibrium line for fluid iron.

To measure the sound velocity a sample in the form of a foil strip, sandwiched between two sapphire plates is uniformly heated by an electric current pulse. During the heating process the

volume of the sample, specific enthalpy, pressure and electrical conductivity are measured by means of the experimental technique [2]. To measure the sound velocity an acoustic disturbance is excited by a laser pulse at the back side of the sample. The emergence of the acoustic wave on the frontal surface is detected by the laser interferometer [3]. The sound velocity is determined as the ratio of the thickness of the sample to the time needed for the acoustic disturbance to traverse the sample. These quantities are directly measured in these experiments.

Preliminary results on the sound velocity measurements for solid and liquid iron are reported in this work. The results are compared with literature data. Based on the comparison an assessment of the measurements accuracy is made.

-
1. Korobenko V.N., and Rakhel A.D. // Phys. Rev. B. 2012. V. 85. P. 014208.
 2. Kondratyev A.M., Korobenko V.N., and Rakhel A.D. // J. Phys.: Condens. Matter. 2016. V. 28. P. 265501.
 3. Kondratyev A.M., Korobenko V.N., and Rakhel A.D. // Carbon. 2016. V. 100. P. 537.

DETERMINATION OF THE CRITICAL POINT PARAMETERS OF LIQUID-GAS TRANSITION FOR BORON.

Ternovoi V. Ya., Nikolaev D.N., Ostriuk A. V.*

IPCP RAS, Chernogolovka, Russia

**ternovoi@ficp.ac.ru*

The expanded final states with pressures 0.004-1,55 GPa of porous ($m=5-8$) of boron (amorphous phase) from a shock compressed state with pressures 20-30 GPa and the heating of the sample surface layer particles in the process of expansion were observed. The fast heating and vaporization of the boron particles in the atmosphere of shock-compressed helium at shock wave velocity 9-16 km/s was registered. The position of the critical point of liquid-gas transition in p-T coordinates for boron was determined as: $p=1,05$ GPa, $T=8100$ K with error bars estimated as 0,14 GPa and 400 K.

Project was done under support by RFBR grant 18-08-00964 A.

EXPERIMENTAL STUDY OF THE DENSITY OF THE GAS SYSTEM HELIUM-NITROGEN-NEON AT LOW TEMPERATURES.

Milyutin V.A.

MPEI (TU), Moscow, Russia

mva.z@yandex.ru

At the Department of TOT (Department of Theoretical Foundations of Heat Engineering) was created an experimental installation to measure the density of the ternary gas system helium-nitrogen-neon at temperatures of 100 – 300 K and pressures up to 16 MPa. The installation implemented a method of a piezometer of constant volume. The mixtures were prepared from pure gases-components. The purity of nitrogen to 99.999 vol.%, helium – not less than 99,993 vol.%, neon – 99,999 vol.%. The unit consists of three main components – a mixer, a piezometric cell and a gasometer. The amount of substance in the piezometer was determined by the volumetric method – with the help of the gasometer. The temperature in the main units of the plant was measured using platinum thermometers of the TSPN-1 and PTS-10 types and potentiometer of the R-348 and R-363-2 types. Pressure – with the help of pressure transducers type IPDC and a set of U-shaped pressure gauge and catheter type B-630. The

piezometer has a ballast volume at variable temperature. The temperature field of this volume was measured using copper-constantane thermocouples. Cryostatization of the piezometric cell is carried out with gaseous nitrogen, obtained by boiling liquid nitrogen in the Dewar-flask. The temperature control system in the piezometer is based on the temperature controller of the type VRT-3, the sensing element in it uses a copper resistance thermometer. The quality of regulation was $\pm 0,005$ K. The vessels of the mixer and the gasometer were thermostated in two liquid thermostats at room temperatures. The accuracy of the measurement of the density of the mixture, the facility assessed: a maximum of 0,3 – 0,6%; probability of 0.1 – 0.2% (with confidence interval of 0.95).

In the experiment, three mixtures with molar concentrations (xHe/xNe) were prepared): 0,33/0,33; 0,16/0,24; 0,24/0,59. A series of experimental isotherms was obtained: 100 K, 115 K, 125 K, 140 K, 190 K, 250 K, 294 K.

For this ternary system, the only experimental work was found in the open access [1].

-
1. Robert J. Burch, Low Temperature Phase Equilibria of the Gas-Liquid System Helium-Neon-Nitrogen. J. Chem. Eng. Data, 1964, 9 (1), pp 19–24.

CALCULATION OF THERMODYNAMIC PROPERTIES OF WATER+ALIPHATIC ALCOHOL SYSTEM USING EXPERIMENTAL VALUES OF

Osmanova B.K., Bazaev E.A., Bazaev A.R.*

IGR DSC RAS, Makhachkala, Russia

**badji@mail.ru*

Experimental data of relations for water—alcohol binary systems (methanol, ethanol, n-propanol) for values of composition x (0.2, 0.5, 0.8 mol.fraction of alcohol) among the phase equilibrium line in onephase (liquid, vapor) and in supercritical regions are described by polynomial equation of state, represented by expansion of the compressibility factor into a power series of density and temperature: and (1) where is a molar density (mol/m³),

ANOMALIES OF SPATIAL IONS DISTRIBUTION IN TRAP IN LOCAL EQUATION OF STATE APPROXIMATION

*Chigvintsev A. Yu,*¹ Iosilevskiy I.L.,¹ Noginova L. Yu.²*

¹MIPT, Dolgoprudny, Russia, ²RSAU-TMAA, Moscow, Russia

**iosilevskiy@gmail.com*

Impressive appearance of discontinuities in equilibrium spatial charge profiles in non-uniform Coulomb systems is under discussions in wide number of thermo-electrostatics problems. Such discontinuities are considered as peculiar micro-level manifestation of phase transitions and of intrinsic macro-level non-ideality effects in local equation of state (EOS), which should be used for description of non-ideal ionic subsystem in frames of local-density approximation (LDA or "pseudo fluid or "jellium" etc) [1, 2]. Such discontinuities were discussed already by the authors for electronic subsystems [3]. Special emphasis is made in present paper on the mentioned above non-ideality effects in non-uniform ionic subsystems, such as micro-ions profile within screening "cloud" around macro-ion in complex plasmas (dusty, colloid etc), in equilibrium ion distributions in ionic traps or/and in the neighborhood vicinity of "charged wall" etc. Multiphase EOS for simplified ionic model of classical charged hard spheres on uniformly compressible

electrostatic compensating background (HS-OCP) was constructed in present work and several illustrative examples of discussed discontinuous ionic profiles in traps with different external potential were calculated with the use of this EOS in LDA approximation.

-
1. Iosilevski I 1985 High Temperature 23 807
 2. Chigvintsev A and Iosilevskiy I 2012 Contrib. Plasma Phys. 52 22
 3. I. Iosilevski and A. Chigvintsev, in: Physics of Strongly Coupled Plasmas, edited by W. Kraeft and M. Schlages, (World Scientific, Singapore-London, 1996) pp. 145; arXiv:0902.2353.

PHASE TRANSITIONS AND BULK PROPERTIES OF THE TERNARY SYSTEM WATER-1-PROPANOL-n-HEXANE NEAR THE CRITICAL POINT

Abdulagatov I.M., Bazaev A.R., Bazaev E.A., Osmanova B.K.*

IGR DSC RAS, Makhachkala, Russia

**emilbazaev@gmail.com*

The phase equilibrium of observed ternary system at low temperatures is investigated by authors [1–3] and at high temperatures by authors [4]. In this work by the method of free-ballast constant volume piezometer [5] the data on p, ρ, T relations of water-1-propanol-hexane system (0.3333 mol.fractions) is obtained in the wide diapason of state parameters.

Isochoric P-T break point technique was applied to accurately determine phase transition p_s, ρ_s, T_s and the critical point p_k, ρ_k, T_k parameters. The measured p, ρ, T properties in the one-phase region including phase transition curve and supercritical conditions were used to develop multiparametric polynomial type equation of state in the form of expansion of the pressure into series in powers of the reduced density $\omega = \rho/\rho_k$ and the reduced temperature $\tau = T/T_k$: $p = RT\rho_m \left[1 + \sum_{i=1}^m \sum_{j=0}^n a_{ij} \omega^i / \tau^j \right]$. Average relative deviation between the measured and calculated values of pressure is less than 1.3% in the whole measured temperature and pressure ranges. The results of the present work showed that volumetric behavior of the ternary system in the critical regions just like one-component system.

The work was supported by RBSF Grant N18-08-00124 A.

-
1. Jones J.H., Hopson W.H. Ternary Solubility Data for Systems Involving 1-Propanol and Water // J.F.Ind. and Eng.Chemistry. 1953. V.45. N.2. P.454-456.
 2. Vorob'eva, A. I. Karapet'yants, M. Kh. Miscibility in systems water+aliphatic alcohol+n-alkane: II water+propan-1-ol+n-alkane (c(6)-c(9)) systems // Zh. Fiz. Khim., 1967, 41, 1144-9
 3. Hiroshi S., Takashi K. Liquid-Liquid Equilibrium Data for Three Ternary Systems of Aqueous Alcohol Solutions and Applicability of the Analytical Solutions of Groups // J. of Chem. Eng. of Japan. 1977. V.10. N5. P.400-402.
 4. Rasulov S.M., Rasulov A.R. Phase equilibrium and PVT-properties of 0.7223 H_2O +0.1242 C_6H_{14} +0.1535 C_3H_7OH ternary system // High Temp. High Press. 2005, V.43. N.1. pp.45-50.
 5. Bazaev. A.R. p,v,T,x - measurements and thermodynamic properties of aqueous solutions of hydrocarbons at supercritical conditions. Doctoral dissert. 1997. P. 264.

THERMAL EFFECTS DURING PROCESSING OF THE MAIN COMPONENTS OF NATURAL BIOSYSTEMS IN THE ENVIRONMENT OF SUPERCRITICAL CARBON DIOXIDE

Yarullin L.Y., Zaripov Z.I., Gumerov F.M.*

KNRTU, Kazan, Russia

**yarul.lenar@gmail.com*

On the example of pretreatment of tea leaves with supercritical carbon dioxide, a significant increase in the extraction of physiologically active substances of a natural material during their subsequent liquid extraction is shown. In the interaction of polymeric materials with sub and supercritical fluid media, as a rule, their swelling occurs, as a result of which the molecular structure, local dynamics and free volume of these polymers can and undergo very significant changes. This is of great theoretical and practical interest, since the types of molecular motion that exist in the polymer significantly depend on its mechanical, thermal, dielectric and diffusion properties. The results of the measurement of thermal effects as a function of pressure and various temperatures arising during processing of the main components of tea (caffeine, cellulose, tea leaf) with supercritical carbon dioxide are given. Comparison of the heat of dissolution in supercritical carbon dioxide of the main components of the tea leaves is shown, from which it can be seen that the values of the enthalpy of caffeine and cellulose have practically the same values.

The research was carried out at the expense of a grant from the Russian Science Foundation (project No.18-19-00478).

1. L.Y. Yarullin, F.M. Gumerov, Truong Nam Hung, I.I. Gilmutdinov, Z.I. Zaripov, F.R. Gabitov, and A.B. Remizov. *Butlerov Communications*. 2016. Vol.48. No.11. P.88-100.
2. Z.I. Zaripov, S.A. Burtsev, A.V. Gavrilov, G.Kh. Mukhamedzyanov. *Theoretical Foundations of Chemical Engineering*. 2002. Vol.36. No.4. P.400-405.
3. Z.I. Zaripov, S.A. Burtsev, A.V. Gavrilov, G.Kh. Mukhamedzyanov. *High Temperature*. 2004. Vol.42. No.2. P.282-289.
4. Z.I. Zaripov, S.A. Burtsev, S.A. Bulaev, G.Kh. Mukhamedzyanov. *J. Phys. Chem.* 2004. Vol.78. No.5. P.697-700.

ADIABATIC CALORIMETRY INVESTIGATION OF SUPERCOOLED STATE OF LIQUID WATER

*Voronov V.P., Podnek V.P.**

OGRI RAS, Moscow, Russia

**podnek77@gmail.com*

Using adiabatic calorimeter we have measured the temperature dependence of isobaric (at pressure 0.1 MPa) heat capacity of supercooled bulk water contained in sealed 1 ml glass ampoules up to temperature of 244 K. The measurements were carried out on heating from the low-temperature region with a rate of 0.4 K/hour. The anomalous increase in the isobaric heat capacity of supercooled water observed by us with lowering in temperature turned out to be very close to the data obtained using the analogous method by E. Tombari et al. [1]. Under the assumption of a power-law growth of the singular part of the heat capacity of the supercooled water with the critical index $3/2$, corresponding to the initial fluctuation regime within the Landau-Brazovskii weak crystallization theory [2], the apparent temperature of the heat capacity divergence is of the order of 228.8 K. The latter value is just below the temperature of homogenous ice nucleation and is very close to temperatures of second critical

point of water and the Widom line of the supercooled water heat capacity maximum at ambient pressure, predicted within the framework of the hypothesis of polyamorphism of liquid water [3]. Note however that above mentioned critical index of the heat capacity anomaly of supercooled water contradicts to the Ising universality class of the expected second critical point of water. We found a sharp increase in the relaxation time in supercooled water with a decrease in temperature, which did not allow us to conduct adiabatic measurements of the heat capacity at lower temperatures because of spontaneous freezing of bulk water. Our data on the isobaric heat capacity of bulk supercooled water in the temperature interval studied, like the analogous data of E. Tombari et al., lie above the data on the heat capacity of emulsified water obtained by C.A. Angell et al. [4] that until now are considered as the only true.

1. Tombari E., Ferrari C., Salvetti G., Chem. Phys. Lett. **300**, 749 (1999)
2. Brazovskii S.A., JETP **41**, 85 (1975)
3. Holten V., Bertrand C.E., Anisimov M.A., Sengers J.V., J. Chem. Phys. **136**, 094507 (2012)
4. Angell C.A., Oguni M., Sichina W.J., J. Phys. Chem. **86**, 998 (1982)

ANALYSIS OF DIMERIZATION EQUILIBRIUM DEVIATIONS FROM IDEALITY IN MIXTURES WITH INTERACTION IN THE FORM OF THE SQUARE WELL

Davydov A.G., Tkachev N.K.*

IHTE UB RAS, Ekaterinburg, Russia

**A.Davydov@ihte.uran.ru*

The analysis of chemical equilibrium in nonideal associated liquids is a sufficiently complex problem in statistical thermodynamics, since the interaction of associates and monomers in a dense liquid must lead to a certain shift in chemical equilibrium. The result depends on the nature of the intermolecular forces acting between the particles in the mixture.

The purpose of the present work was to analyze the influence of short-range attraction on the deviations of chemical equilibrium from ideality in a liquid mixture of monomers and dimers.

The attraction in the dimerizing mixture is accounted for by the pair potential of the square well. Moreover, the spontaneous dimerization reaction proceeds together a change in volume, depending on the degree of fusion of the monomers in the dimer.

To determine the equilibrium position of such liquid mixture, it is necessary to find the minimum of the Gibbs free energy with respect to two independent variables: the volume and dimer concentration. Moreover, it is reasonable to use the mean activity coefficient (in the equation of the mass action law), namely, in which (not in the equilibrium constant) all intermolecular interactions should be taken into account.

As a result, it was shown that an increase in attraction between monomers leads to a shift in equilibrium towards dissociation, while an increase in attraction between dimers plays an inverse role. Accounting attraction leads to an increase in the packing fraction, particularly in the case of greater attraction between dimers and smaller bond lengths. Under these conditions, the maximum tendency to ordering the liquid is observed.

The reported study was funded by RFBR according to the research project No. 15-03-01588.

EQUATION OF STATE OF DENSE NON-ISOTHERMAL PLASMA

*Ismagambetova T.N.,*¹ Gabdullin M.T.,^{1,2} Ramazanov T.S.¹*

¹*IETP, al-Farabi KazNU, Almaty, Kazakhstan, ²KBTU, Almaty, Kazakhstan*

**ismagambetova@physics.kz*

In this work interaction potentials considering Pauli exclusion principle were used [1, 2]. Pauli principle prohibits the simultaneous presence of two electrons in the same state, hence taking into account different directions of spin. The influence created by difference between temperatures of electrons and ions was also considered [3]. Thermodynamic properties, including equation of state, were calculated using these potentials and obtained on their basis radial distribution functions (RDFs).

-
1. Ramazanov T.S., Moldabekov Zh.A. and Gabdullin M.T. // Phys. Rev. E 2015. V. 92. P. 023104.
 2. Moldabekov Zh.A., Ramazanov T.S., Dzhumagulova K.N. // Contrib. Plasma Phys. 2012. V. 52. P. 207-210.
 3. Bredow R., Bornath Th., Kraeft W.-D., Redmer R. // Contrib. Plasma Phys. 2013. V. 53. P. 276-284.

INVESTIGATION OF PHASE EQUILIBRIUM OF BINARY SYSTEM “NAPHTHALINE-SCF-SOLVENT”

Ahmetzyanov T.R., Khayrutdinov V.F., Gabitov F.R., Gumerov F.M.*

Kazan, Kazan, Russia

**ahmetzyanov1992@bk.ru*

To simulate, optimize and scale the processes of deep processing of hydrocarbon feedstock using GFR media, reliable phase behavior data of high-pressure mixtures of interest are required, in particular solubility of low-volatile liquid and solid components in the GFR medium. These facts point to the need for reliable data on the phase equilibrium of the systems "GFR medium-hydrocarbon raw materials components".

In this paper, a hydrocarbon of naphthalene was chosen as an oil component. Naphthalene refers to aromatic hydrocarbons. The content of aromatic hydrocarbons in oil varies from 10-15 to 30% (by weight). These hydrocarbons form the basis of heavy oil residues. This involves the choice of naphthalene as an object of research in this work. To study the solubility of naphthalene in the GFR media, an experimental setup has been developed that implements the dynamic method. To test the installation, pilot experiments were conducted to study the solubility of naphthalene in GFR CO₂ [1, 2]. A good convergence of the data obtained in this work with literature data was obtained.

The solubility of naphthalene in a GFR propane-butane mixture containing 75% propane and 25% butane [3] was investigated in the pressure range of 5–20 MPa and in the temperature range 373–423 K. The effect on the solubility of the thermodynamic parameters of the process was analyzed.

The study was carried out through a grant from the Russian Science Foundation (project No. 18-19-00478).

-
1. Amirkhanov D.G. Solubility of substances in supercritical fluid media. / Amirkhanov D.G., Gumerov F.M., Sagdeev A.A., Galimova A.T. // Ed. Fatherland. Kazan 2014. p.264.
 2. Mark McHugh and Michael E. Paulaiti . Solid Solubilities of Naphthalene and Biphenyl in Supercritical Carbon Dioxide. J. Chem. Eng. Data 1980, 25, 326-329.

- Gumerov FM, Farakhov MI, Khairutdinov VF, Gabitov RF, Zaripov ZI, Khabriev I.Sh., Ahmetzyanov TR Increase in the functionality of carbonate rubble by supercritical fluid impregnation with bituminous compounds // *Supercritical Fluids: Theory and Practice*. -2015. -T.10. - 2.-C. 4-16.

THE SOLUBILITY OF ANTHRACENE IN SUPERCRITICAL CARBON DIOXIDE

*Hazipov M.R.,*² Galimova A.T.,¹ Gatin R.S.,¹ Sagdeev A.A.¹*

¹NCHTI KNRTU, Nizhnekamsk, Russia, ²KNRTU, Kazan, Russia

**2351092@mail.ru*

In the study of phase equilibria, a special place is occupied by such a concept as the solubility of substances, including in supercritical fluids. Knowledge of phase equilibria in systems in a supercritical fluid state is necessary for understanding the broad spectra of processes that form the basis of an innovative technological direction called “supercritical fluid technologies” (SCFT).

Anthracene is one of the main deactivating catalysts of compounds. The subject of this study is the measurement of solubility of anthracene under isotherms 423 K, 435 K, 448 K in the pressure range 9.6 — 22 MPa. The solubility study was carried out on an experimental setup protected by the patent for a utility model [1].

The results of the study showed that the more temperature and pressure increases the more increases the solubility of anthracene. This is due to the fact that an increase in temperature leads to an increase in the pressure of saturated vapors of the dissolvable substance, in consequence of which its concentration in the solvent phase increases. Thus the solubility also increases.

In addition, the solubility of anthracene was described using the Peng — Robinson equation of state and three fitting parameters [2]. Measurement error in describing the solubility results was 7 %.

The solubility results of compounds which deactivate the catalyst determine in a large extent the optimum energy- and resource-saving regimes of catalyst regeneration processes.

-
- The patent for the utility model of the Russian Federation No. 163707 publ. 08/10/2015.
 - The certificate of the official registration of the computer program No. 2016613119 publ. 03/17/2016.

ANALYSIS OF METHODS FOR CONSTRUCTING A PHASE EQUILIBRIUM LINE FOR DIFFERENT MODELS OF MEAN DIAMETER

Kudryavtseva I. V., Rykov S. V., Rykov V. A.*

SPbSU ITMO, Saint-Petersburg, Russia

**togg1@yandex.ru*

We analyzed various models of the phase equilibrium line in the range from the triple point to the critical point. For this we used a system of mutually consistent equations. This system includes: the equation of the elasticity line $p = p_s(T)$ in the form used in [1], the equation for the saturated liquid density, the singular component of which has the following form:

$$\rho^+(T) = \rho_c \left(1 + \sum_{n=1} D_n^* |\tau|^{n\beta} + D_2 |\tau|^{\beta+\Delta} + D_2 |\tau|^{1-\alpha} + \dots \right); \quad (1)$$

the equation for the saturated vapor density ρ^- :

$$\rho^-(T) = T p'_s(T) (1 - \rho^-/\rho^+) [r(T)]^{-1} = T p'_s(T) [r^*(T)]^{-1}, \quad (2)$$

where $r^* = r/(1 - \rho^-/\rho^+)$ is the "apparent" heat of vaporization; the singular component of which has the following form:

$$r^*(T) = \left(\frac{p_c}{\rho_c}\right) \left(d_0 + \sum_{n=1} d_n^* |\tau|^{n\beta} + d_2 |\tau|^{\beta+\Delta} + d_3 |\tau|^{1-\alpha} + \dots\right). \quad (3)$$

Here p_c is the critical pressure; $\tau = t - 1$; $t = T/T_c$; T_c is the critical temperature; α , β , Δ are critical indices; ρ_c is the critical density; r is the heat of vaporization.

On the basis of this system of equations $p = p_s(T)$ [1] and (1)–(3), an analysis of a number of mean diameter models has been performed. In doing so we used the same array of data on the pressure of p_s and the density ρ^+ and ρ^- a number of substances (argon, sulfur hexafluoride, DEE, etc). The results obtained for different models of mean diameter are discussed.

-
1. Kozlov A.D., Lysenkov V.F., Popov P.V., Rykov V.A. // J. Eng. Phys. Thermophys. 1992. V. 62. P. 611.

STATISTICAL THERMODYNAMIC ANALYSIS OF COMPLEX FORMATION IN SALT MELTS

*Peshkina K.G., Tkachev N.K.**

IHTE UB RAS, Ekaterinburg, Russia

**N.Tkachev@ihte.uran.ru*

The report will present the results of theoretical calculations of dissociation equilibria for anion complexes of the $(MX_4)^{2-} = M^{2+} + 4X^-$ type in halogenide melts based on MX_2 . A simplified model of a mixture of charged hard spheres of differing diameters is considered, when only electrostatic interactions and the final dimensions of ions are taken into account, and the contribution of the complexes to the thermodynamics of the melt is additionally contributed by its energy of formation. Such a model is a natural starting point for this problem and sheds light on the mechanism of the spontaneous (in the thermodynamic sense) appearance of charged complex groupings. The core of the problem is a system of equations of equilibrium, which contains both the law of effective masses and the equation of state, which allows one to self-consistently calculate the equilibrium concentration of complexes and the density of the melt. By the example of approximation of the diameter of a complex as a tripled diameter of simple ions, it is shown that this can lead to a significant overestimation of the effects of the change in the molar volume when considering its temperature dependence. Allowance for the overlap of atoms within the complex allows us to describe a smoother change in volume with temperature. A generalization of the developed model to the case of binary melts of multivalent metal halides with alkali metal halides is carried out. Examples of typical concentration dependencies of complexes from the composition of these binary melts and thermodynamic characteristics are given. In conclusion, problems and prospects for describing real salt melts containing two- and three-valence cations are discussed. This work was supported by Russian Foundation for Basic Research 18-03-00606

THERMOPHYSICAL PROPERTIES OF THE BORON CARBIDE MELT AT THE MEGABAR SHOCK PRESSURES

Molodets A.M.

ICPC RAS, Chernogolovka, Russia

molodets@icp.ac.ru

Boron carbide (B_4C) combines a number of high performance characteristics, which leads to its successful use in the important applications- armored structures, nuclear power, etc.. Therefore, an extensive research literature (see [1-3] and references in them) is devoted to the study of various properties of boron carbide in the field of high pressures and temperatures, including extreme conditions of shock compression. In the context of the proposed report, it should be noted that taking into account the new experimental data [1] for the region of 200-800 GPa suggests the existence of a pronounced kink of the B_4C Hugoniot caused by melting of boron carbide under shock compression in the pressure range of 95-125 GPa. This hypothesis, its rationale and development are presented in [2]. At the same time, the free energy of boron carbide and its melt is constructed as a function of its variables in the megabar range of shock pressures.

The report shows that some results of [2] can be used as the equation of state of Mie-Gruneisen. This equation of state is known to be widely used in mathematical modeling of shock wave processes and a number of thermophysical properties of the shocked materials. In the report, the key components of the Mi-Gruneisen equation for boron carbide melt are discussed. These are the volume dependences of Gruneisen coefficient, as well as potential pressure and energy functions. Calculations of the shock velocity-mass velocity, temperature, heat capacity and sound velocity along the melt of boron carbide Hugoniot are considered. The obtained results are compared with the latest publications of other authors [3] with quantitative results on thermophysical properties of boron carbide melt obtained on the basis of first-principle molecular dynamics calculations.

The work was supported by the fundamental research program of the RAS Presidium "Condensed matter and plasma at high energy densities".

-
1. Sterne P.A. et al., // Journ. Phys. Conf. Ser., 2016. V. 717. P. 012082.
 2. Molodets A.M. et al., // JETP. 2017. V 124. No. 3. P. 469.
 3. Shamp A. et al., // Phys. Rev. B. 2017. V. 95. P. 184111.

METHOD OF CONSTRUCTION OF THE FUNDAMENTAL EQUATION OF STATE FOR SF_6

Rykov S. V., Kudryavtseva I. V., Rykov V. A.*

SPbSU ITMO, Saint-Petersburg, Russia

**togg1@yandex.ru*

A method for constructing a fundamental state equation (FEOS) based on the Schofield linear model, the Benedek hypothesis, and the representation of the scale hypothesis of the critical point in the following form is considered [1]

$$\Delta S \cdot X^{\frac{1-\alpha}{\chi}} = \varphi_0 + \varphi_1 \cdot m^2, \quad m = \Delta\rho \cdot X^{\frac{\beta}{\chi}}, \quad (1)$$

where $\Delta S = (\rho_c T_c / p_c) [S(\rho, T) - S_0(\rho, T)] / \phi(\omega)$; S is the entropy; $\phi(\omega)$ is the crossover function; $\Delta\rho = \omega - 1$; $\omega = \rho / \rho_c$; α , β , χ and Δ are the critical indices; X is the thermodynamic function that has a singularity at the critical point, which is characterized by a critical index χ (for example, if $X = K_T$, then $\chi = \gamma$).

On the basis of the system of equations (1) the structure of FEOS and the scale function of the Helmholtz free energy are calculated:

$$a(x) = A \left[(x + x_1)^{2-\alpha} - \frac{x_1}{x_2} (x + x_2)^{2-\alpha} \right] + B(x + x_3)^\gamma + C. \quad (2)$$

FEOS with the scale function (2) was tested on sulfur hexafluoride. The analysis of the obtained results is carried out. The tables of the equilibrium properties of SF₆ in the range of the state parameters have been calculated: for temperature from 223.555 to 625 K and for pressure up to 150 MPa. Detailed thermodynamic tables for a wide neighborhood of the critical point are also calculated. It is shown that the accuracy of calculating the equilibrium properties in the regular part of the thermodynamic surface suggests that the proposed equation R1234yf is not inferior to the fundamental equations of state [2, 3].

-
1. Rykov V.A., Rykov S.V., Kudryavtseva I.V., Sverdlov A.V. // J. Phys.: Conf. Ser. 2017. V. 891. P. 012334.
 2. Scalabrin G., Bettio L., Marchi P., Stringari P. // J. Phys. Chem. Ref. Data. 2007. V. 36. P. 617.
 3. Guder C., Wagner W. // J. Phys. Chem. Ref. Data. 2009. V. 38. P. 33.

EQUATIONS FOR CALCULATIONS LIQUID-VAPOR EQUILIBRIUM IN BINARY MIXTURES CONTAINING METHANE

Vasserman A.A., Halkin V.N.*

ONMU, Odessa, Ukraine

**avas@paco.net*

Some authors investigated experimentally the liquid-vapor phase equilibrium in binary mixtures containing methane, but did not describe analytically obtained data. Therefore we fulfilled the analytical description of experimental data on phase equilibrium in binary mixtures helium-methane, argon-methane and carbon dioxide-methane. The compiled equations represent the pressure of liquid or vapor as a function of temperature and composition and contain from 4 to 6 coefficients.

At compiling equations the program was used that provides optimization of coefficients of equations number without significant reducing the accuracy of experimental data approximation. The program provides the selection of the most significant coefficients from the bank, which contains 30 coefficients.

For the mixture helium-methane 305 experimental values of pressure for liquid and vapor from 4 sources were used in the intervals of temperature 93...191 K and pressure 0,48...26,22 MPa. For the mixture argon-methane 168 values of pressure for liquid and vapor from 4 sources were used in the intervals of temperature 90...126 K and pressure 0.016...3.87 MPa. For the mixture carbon dioxide-methane 184 values of pressure from 4 sources were used in the intervals of temperature 219...293 K and pressure 0,58...8,52 MPa. For liquid and vapor, almost equal quantity of data is obtained.

The standard deviations of the experimental values of pressure from the calculated values are from 1.8 to 5.3%. The greatest deviation is observed for the mixture helium-methane due to a sharp increase of pressure on the isotherms depending on the composition. Constructed histograms of deviations indicate that the distribution of deviations is close to normal.

Equations allow to determine the composition or temperature of phases at given values of the remaining parameters of phase equilibrium. Calculations of the composition and temperature of the coexisting phases showed quite satisfactory agreement of the calculated values with the experimental data.

**ISOCHORIC HEAT CAPACITY AND PHASE EQUILIBRIUM LINES IN THE
BINARY SYSTEM N-HEXANE + WATER IN THE CONCENTRATION
RANGE 0-0.2566 M.F. H₂O**

Bezgomonova E.I., Saidov S.M.*

IP DSC RAS, Makhachkala, Russia

**bezgomonova_lena@mail.ru*

Experimental investigation of the C_v , V , T properties in the n-hexane + water system with the different compositions (x) 0.1195; 0.1662; 0.1998; 0.2566 molar fraction (m.f.) H₂O in the temperature range 312 - 503K and pressures up to 6 MPa, were made with the high-temperature adiabatic calorimeter designed by Kh.I. Amirkhanov [1].

For our investigations we used adiabatic calorimeter with the volume 432.611 cm³ at temperature $T = 298.15$ K and atmosphere pressure 0.1 MPa.

For each measured isochore, two jumps of the isochoric heat capacity were observed. A sharp jump of isochoric heat capacity at the intersection of the boundaries of the three and two-phase regions is associated with the phase transitions liquid-liquid-gas in liquid-gas in the binary mixture n-hexane + water, the phase transition associated with the dissolution of the components (liquid-liquid), more smooth and occurs in a certain temperature range.

According to the measurements of the heat capacity C_v , phase equilibrium curves liquid-liquid-gas, liquid-liquid and liquid-gas are plotted as a function of density and composition. The form of the phase equilibrium curve of liquid (less volatile component) - gas (more volatile component) for the composition of 0.2566 mole fractions of H₂O has a parabolic shape and differs from all compositions. For this concentration, the liquid-liquid phase and liquid-gas phase curves intersect at one point - the critical point of the three-phase equilibrium or the upper critical end point (UCEP).

Using the experimental data on the critical line for the mixture and the vapor pressure of the pure solvent (n-hexane), the Krichevsky parameter was calculated. Based on the Krichevsky parameter, the thermodynamic and structural properties of the dilute n-hexane + water mixture near the critical point of n-hexane were also calculated.

1. Amirkhanov Kh.I., Alibekov B.G., Vikhrov D.I., Mirskaya V.A. Isochoric heat capacity and other caloric properties of methane hydrocarbons. Makhachkala: Dagestan book publishing, 1981.

**THERMODYNAMIC CHARACTERISTICS OF MOLTEN SALTS
CONSIDERING POLARIZATION EFFECTS**

Davydov A.G., Tkachev N.K.*

IHTE UB RAS, Ekaterinburg, Russia

**A.Davydov@ihte.uran.ru*

The study of thermodynamic characteristics and phase equilibria in various systems is an important part of most of the studies related to materials science, since in considering particular properties of the material, it is first necessary to have information about the stability boundaries of each phase in the system. There are various theoretical approaches to solving this problem, based on ab initio methods, molecular modeling, thermodynamic modeling and their combination, while the statistical-thermodynamic theory applied to these problems is less developed.

One of the directions in this field is the study of thermodynamic properties and interphase boundaries in molten salts. Therefore, a theoretical description of the various effects observed in these systems is an important issue. This investigation is related to the study of the influence

of polarization effects between ions on the thermodynamic properties and the melting process of halide melts of alkali metals. The difficulty here is that polarization effects always arise not only between neighboring particles, but also in subsequent coordination spheres. Therefore, to consider the polarization effects, it is necessary to introduce a dielectric constant.

In this report, we will present a simple statistical-thermodynamic model to take into account the polarization contribution to the pair potential of the ion interaction in a molten salt. Such a model is realized using thermodynamic perturbation theory, where the reference system is the potential of charged hard spheres. Thus, the weaker polarization effect of ions can be considered as a perturbation.

The reported study was funded by RFBR according to the research project No. 18-33-01234.

VISCOSITY OF LIQUID ALLOYS OF COBALT WITH SILICON AND BORON

Olyanina N.V., Beltyukov A.L., Ladyanov V.I.*

UdmFRC UB RAS, Izhevsk, Russia

**albeltyukov@mail.ru*

In the present work, the temperature (polytherm) and concentration (isotherm) dependences of the kinematic viscosity of melts of Co-Si, Co-B and Co-Si-B systems have been studied.

Viscosity studies were carried out by the method of torsional vibrations using an automated installation [1] in a protective atmosphere of helium in the crucibles of Al_2O_3 in the presence of two end surfaces of friction [2].

Polytherms of the viscosity of Co-Si and Co-B melts (up to 54 at.% metalloid), as well as melts of $\text{Co}_{89}\text{B}_x\text{Si}_{11-x}$, $\text{Co}_{81}\text{B}_x\text{Si}_{19-x}$ and $\text{Co}_{75}\text{B}_x\text{Si}_{25-x}$ systems have a monotonic character and are well described by the Arrhenius equation. This indicates that a sharp change in the structure of the melts does not occur upon heating.

The viscosity isotherms of Co-Si melts have a domed shape with maximum values in the range of 30-40 at.% silicon. The viscosity of the Co-B melts at a boron content up to 15 at.% and in the range from 36 to 50 at.% practically does not depend on the concentration. The values of the melt viscosity increase rapidly in the concentration range from 20 to 36 at.% boron. The nonmonotonic nature of the viscosity isotherms indicates a change in the type of short-range ordering in the melt with a change in composition.

The viscosity isotherms of quasi-binary Co-Si-B systems are monotonic. The replacement of silicon atoms by boron atoms in these systems has practically no effect on the viscosity of the melts.

The work was carried out within the framework of the state task of the FASO Russia (state registration number AAAA-A17-117022250039-4)

1. Beltyukov A.L., Ladyanov V.I. // Instrum. Exp. Tech. 2008. V. 51. P. 304.
2. Olyanina N.V., Beltyukov A.L., Goncharov O.Yu., Ladyanov V.I. // Rasplavy. 2012. No. 2. P. 83. (In Russ.)

SHEAR VISCOSITY CALCULATION FOR LIQUID HYDROCARBONS
USING MOLECULAR DYNAMICS METHODS

Kondratyuk N.D., Pisarev V.V.*

JIHT RAS, Moscow, Russia

**kondratyuk@phystech.edu*

Modern industry is strongly interested in research of liquid hydrocarbon properties since they are parts of lubricants, insulators and fuels. One of the main properties of such liquids are transport coefficients (diffusivity, viscosity and thermal conductivity).

The calculations of the viscosity of liquid hydrocarbons have demonstrated the applicability of the Green-Kubo method [1] in the case of single-component systems. The obtained values of the viscosity coefficients for the hydrocarbons under study coincide with the experimental data within 10%. The experimental dependence of viscosity on temperature is reproduced using the methods used.

The contributions of various components of the stress tensor to the viscosity integral is analyzed. An approach is proposed for the convenient presentation of data in the form of tables. It is shown that the contributions of individual components can exceed by an order of magnitude the total value of the integral. It was also found that the correlation times increase with the increase of the number of atoms in the hydrocarbon molecule. In this connection, in further calculations, the authors of the project consider it most effective to use the method of nonequilibrium molecular dynamics, since it requires less computational time.

Comparison of the results obtained by the Green-Kubo method with the results of nonequilibrium molecular dynamics [2] is performed. The values coincide within the limits of the computational error for the entire series of n-alkanes under study at different temperatures and pressures.

Three interaction potentials are used: TraPPE-EH, OPLS-AA and COMPASS, unlike TraPPE-EH and OPLS-AA, which takes into account the anharmonicity of bonds and angles. In the case of viscosity, all three potentials give similar results. This can be explained by the calibration of the interatomic interaction potentials during their development.

The work is supported by the grant No. 17-79-20391 of the Russian Science Foundation.

1. Zhang Y., Otani A., Maginn E.J. // *J. Chem. Theory Comput.* 2015. V. 11. No. 8. P. 3537.

2. Bordat P., Müller-Plathe F. // *J. Chem. Phys.* 2002. V. 116. No. 8. P. 3362.

VISCOSITIES OF ACETIC ACID, BUTYRIC ACID AND THEIR AQUEOUS SOLUTIONS

Gabitov I.R., Zaripov Z.I.*

KNRTU, Kazan, Russia

**gabitov.ilgiz@gmail.com*

The problem of industrial wastes disposal is extremely important. According to the last report of the Ministry of natural resources of Russian Federation [1], about half a billion tons of waste belonging to I-IV hazard classes have been accumulated in Russia. And this number increases every year. In this connection, the task of developing and introducing new progressive methods of utilization, capable of solving existing problems, is still relevant. The process of supercritical water oxidation SCWO [2] could be such a method. It is highly effective, ecologically safe, and still economically viable.

A large number of papers have been devoted to investigation of the SCWO process, including those carried out at the Heat engineering department of KNRTU [3, 4], where the present stage of the research is aimed at constructing a mathematical model of the water oxidation process. One of the most important conditions for obtaining such a model is the availability of reliable data on thermophysical properties of the participating thermodynamic systems.

This report is devoted to the investigation of the viscosity of acetic and butyric acids, as well as their aqueous solutions in the temperature range 298.15 - 473.15 K at pressures up to 30 MPa. The experimental values of the dynamic viscosity are obtained on the approved experimental setup [5]. The experimental curves are described by mathematical models using the Arrhenius-Andrade and Redlich-Kister equations.

1. Report of the Russian Ministry of natural resources // Moscow: NIA-Priroda 2017. 760 p.;

2. Galkin A.A., Lounin V.V. // *Uspehi Chimii.* 2005. Vol. 74. No. 1, p. 24-40;

3. Zakharov A.A., Usmanov R.A. // *Vestnik Kazanskogo technologicheskogo univesiteta.* 2012. Vol. 15. No. 11, p. 194-196;

4. Aetov A.U., Gumerov F.M. et al. // *Butlerovskiye soobsheniya.* 2017. Vol. 50. No. 4, p. 67-75;

5. Shamsetdinov F.N., Gabitov I.R., Zaripov Z.I. et al. // Vestnik Kazanskogo technologicheskogo univesiteta. 2012. Vol. 16. No. 18, p. 112-114.

**THE SOLUTION OF THE INVERSE COEFFICIENT PROBLEM FOR THE
SEARCH FOR REFLECTIVE-RADIATIVE CHARACTERISTICS BY
TIKHONOV'S REGULARIZATION METHOD**

Borshev N.O., Antonov V.A., Belavskiy A.E.*

MAI, Moscow, Russia

**www.moriarty93@mail.ru*

When carrying out a thermophysical experiment, it is difficult to determine the various characteristics of the material at any point in space, it is necessary to install a huge number of thermocouples, accurately know the error of the measured equipment, the method of modeling the temperature field, etc. The aim of this paper is to create a stable algorithm for determining the radiative-reflective characteristics in the region under consideration using the Tikhonov regularizing algorithm [1].

The first stage of the study is to determine the theoretical fields by the method of finite elements, where the step in space is chosen in such a way that the experimental and theoretical temperatures are in one node.

The second stage is the assignment of basis functions to time and coordinates, thus allowing calculation with respect to some constant value of the flow. The third step is the formulation of the residual functional between the theoretical and calculated temperature values. The minimum of the functional is equated to the zero vector and the system of linear algebraic equations, from which the constant values of effective flows on the boundary are found, the required heat fluxes are added to the corresponding basis functions.

The fourth step is to determine the effective degree of blackness and the diffuse reflectance of the material, solving the classical Stefan-Boltzmann equation for a gray body.

Thus, the dependences of the temperature nonstationary field on the degree of blackness [2] and the coefficient of diffuse reflection of the material in diffuse high-intensity radiant heating, the sensitivity coefficients on the characteristics of space are constructed.

-
1. Tikhonov AN, Goncharovsky AV Numerical methods for solving ill-posed problems. Ed. M. 2012.
 2. AG Bloch, Yu.A. Zhuravlev, LN Ryzhov. Heat exchange by radiation. Ed. Moscow: Energoatomizdat. 1991.

THERMAL RESISTANCE OF SUPERHEATED AQUEOUS SOLUTIONS

Povolotskiy I.I., Volosnikov D.V., Skripov P.V.*

ITP UB RAS, Ekaterinburg, Russia

**iliyapov@rambler.ru*

The report is dealt with an experimental verification of the hypothesis of L. P. Filippov on the relationship between the additional thermal resistance of solutions (with respect to the additive law) and their excess volume. Earlier, the fact of such relationship was confirmed for solutions with a positive value excess volume. In this study, solutions with a negative excess volume are considered.

The technique consists in recording the parameters of the response to pulse heat release for the given parameters of the heating function and their subsequent comparison with the additive

values. The source of heat and a sensitive element is a wire probe — resistance thermometer. According to the primary data measured in the experiment, the values of the weight-average temperature of the probe $T(t)$, the power of its heating $P(t)$, the density of the heat flux through its surface $q(t)$, and the thermal resistance of the substance $R_\lambda = \Delta T(t)/q$ are calculated for a given timing t .

According to the presented technique, experiments were carried out with pure substances and water–glycol solutions (ethylene glycol, diethylene glycol, triethylene glycol) at atmospheric pressure and temperatures of 90°C, 120°C, 150°C. The last two temperatures are in the region of superheated states of solutions with a significant water content.

It is found that the heat transfer characteristics of solutions with negative excess volume have negative deviations from additive values. This circumstance indicates the existence of additional thermal resistance in solutions of this type. A qualitative correlation was also found between the value of the additional thermal resistance and the value of the excess volume of the solutions.

INVESTIGATION OF THE SPECTRA OF HIGHLY ORIENTED PYROLYTIC GRAPHITE

Senchenko V.N., Belikov R.S.*

JIHT RAS, Moscow, Russia

**pyrolab@ihed.ras.ru*

Today the knowledge of the thermoradiation properties of pyrolytic graphite at high temperatures is of great interest. The main reason for the lack of experimental data on these properties is the impossibility of carrying out stationary experimental studies of graphite at the temperatures above 3300 K, as well as the typical features of the material under study.

This work represents the results of the pulsed millisecond electrical heating experiments, such as radiation spectra of HOPG at the temperatures close to the melting point. The experiments were carried out at a static gas pressure of about 1 kbar, the spectral range of the obtained spectra was 0.25–0.8 μm . The spectra of thermal radiation of the heated samples allow obtaining the values of the thermoradiation properties of the sample surfaces parallel and perpendicular to the basal plane of pyrographite, such as the spectral emissivity at given temperatures.

CORRELATION OF ELECTRICAL RESISTANCE AND THERMAL EXPANSION OF INTERMETALLIDE Ti_3Al

Murlieva Zh.Kh.,^{1,2} Palchayev D.K.,¹ Iskhakov M.E.,¹ Rabadanov M.Kh.¹*

¹DSU, Makhachkala, Russia, ²DSUNE, Makhachkala, Russia

**zhariyat@mail.ru*

The anomalous behavior of the electrical resistivity of the intermetallide Ti_3Al is studied, which consists in the fact that its temperature coefficient (TCR) is of a semiconductor nature. This behavior of TCR for conductors is associated with high static disorder. To determine the nature of the features of the properties of this intermetallide compound, we investigated the temperature dependences of the electrical resistivity and the of thermal expansion coefficient (TEC). The sample was obtained by induction melting of pure titanium and aluminum, cooling was carried out in the same furnace after it was turned off. Precision measurements of the electrical resistivity by a four-probe method were performed with current switching from room

temperature to 1000°C. Simultaneously, on the same sample, under the same conditions, was measured its thermal expansion by the quartz dilatometer method.

We made four cycles of heating and cooling the sample. In the first heating, the temperature dependence of the resistance exhibits a hysteresis, which was significantly reduced in subsequent cycles. The disappearance of the hysteresis effect indicates that the system has reached a stabilized state. Features on the temperature dependences, both TEC and electrical resistance are manifested. They are most clearly visible for the electrical resistivity. This is due to competition and the dominance of the metallic and semiconductor conductivity characters at each of the temperature intervals.

It is established that the anomalies in the temperature dependences of the resistance and the TEC correlate, and this correlation is direct, as for traditional metals. This indicates the decisive role of the change in the interatomic distance associated with the anharmonicity of lattice vibrations, not only in the formation of the scattering potential of elementary charge excitations, but also in the formation of charge excitations themselves. Local disordering of atoms in the unit cell Ti_3Al after the corresponding heat treatment makes it possible to control the absolute values of the electrical resistivity of this intermetallic compound and its temperature coefficient.

The work was carried out with the financial support of the State Budget No. 3.5982.2017/8.9

SPECIFIC ELECTRICAL CONDUCTIVITY OF SAPPHIRE AT SHOCK COMPRESSION UP TO 750 GPa

Nikolaev D.N., Ternovoi V.Ya., Shutov A.V., Ostriuk A.V.*

IPCP RAS, Chernogolovka, Russia

**nik@ficp.ac.ru*

Monocrystalline sapphire is widely used as insulator in experiments on measurements of the electrical conductivity of single and multiple shock compressed matter. However, direct measurements of electrical resistance of shock-compressed sapphire were performed only up to 220 GPa [1], where extrapolated data indicated metallic level of conductance at pressure over

270 GPa. In this talk the new data on electrical conductivity of monocrystalline m-cut sapphire under shock compression up to 750 GPa will be presented. The Mach cumulative generators of shock wave, analogous to [2], in single- and double- staged configurations, were used for shock loading of measuring cell. 3-electrodes scheme of resistance measurements was used. Optical multi-channel pyrometry and fast optical detectors were used to measure shock velocity and brightness temperatures in sapphire sample. Also a reflectance was measured at 810 nm channel. The data obtained was compared with calculations [3]. At pressure 550 GPa the measured electrical conductivity of sapphire didnt exceed 60 S / cm, that opens possibility to use it as an electric insulator for measurement of electrical properties of compressed Hydrogen. Work performed under RFBR 18-08-00964 A project, using facilities of Moscow regional center for collective use of RAS.

1. Weir S.T., Mitchell A.C., Nellis W.J. // J. Appl. Phys. 1996. V. 80. No. 3. P. 1522 - 1525.
2. Nikolaev D., Ternovoi V., Kim V., Shutov A. // Journal of Physics: Conference Series. 2014. V. 500. No. 14. P. 1-5.
3. H. Liu, J.S.Tse, W.J.Nellis. // Scientific Reports. 2015. V. 5. P. 12823.

THE NATURE OF THE FORMATION OF THE TEMPERATURE DEPENDENCE OF THE RESISTIVITY IN CONDUCTORS

Palchaev D.K.

DSU, Makhachkala, Russia

dairpalchaev@mail.ru

The modern theory of electrical resistivity of conductors undergoes a crisis in solving such questions as: a quantitative description of the temperature dependence of the phonon resistivity, even for pure, normal metals; a quantitative description of the temperature dependences of the resistivity at magnetic and atomic ordering and disordering; the nature of the conductivity of high-temperature superconductors, in which free and non-localized charge carriers are absent; interpretation of the negative temperature coefficient of electrical resistance for conductors with high static disorder. Moreover, there is a contradiction connected with the direct and inverse dependence of the conductivity of materials on the relaxation times in the expressions of Bloch and Maxwell, respectively. In both cases, it is expected that the system relaxes to the initial state as a result of its linear reaction to a deviation from the charge homogeneity when an electric potential gradient satisfying Ohm's law is established.

The development of technologies similar to those observed in nature for obtaining materials and products from them requires fundamental knowledge, including on conductivity and its connection with the structure and other properties of these materials, based on reliable empirical data. A reliable source of data on the temperature dependence of the properties of materials is still the experimental results.

Based on the experimental data on the temperature dependences of the electrical resistivity and thermal expansion obtained in situ for metals and alloys, a close relationship has been found between the electrical resistivity and the of the coefficient of thermal expansion multiplied by temperature. This connection does not contradict the recognized positions of the theory of conductivity and is empirically justified. It indicates the determining role of the thermal deformation of the lattice of atoms in the formation of the temperature dependence of the electrical resistivity of conductors. The presence of such a connection allows us to establish the nature of the conductivity of materials from the first principles of the first level.

The work was carried out with the financial support of the State Budget No. 3.5982.2017 / 8.9

TRANSPORT PROPERTIES OF DILUTE GASES AND GAS MIXTURES. DIFFUSION

*Bogatyrev A.F.,*¹ Kucherenko M.A.,¹ Makeenkova O.A.²*

¹MPEI (TU), Moscow, Russia, ²Smolensk State University, Smolensk, Russia

**tfs209@yandex.ru*

Mixtures of dilute gases are widely spread in nature and are often used in many technological processes. To calculate and generalize the transport properties of dilute gases and their mixtures, methods of kinetic theories and semiempirical methods based on them are used [1]. These methods allow calculating viscosity in a sufficiently wide temperature range within the experimental error.

Calculation of the binary diffusion coefficients (BDCs) usually gives a deviation of 3–10%, with a tendency to increase in the areas of high and low temperatures. In [2], we proposed a method for calculating BDCs in moderately dense gases at different temperatures. The error in calculation according to this method depends on BDCs of dilute gases significantly.

In [3], we proposed a method for calculating the viscosity and BDCs for binary gas mixtures basing on the data on the pure gases viscosity. We calculated the viscosity and BDCs for three gas systems and obtained a coincidence with experimental values within the experimental error.

This work presents the results of calculating BDCs for four gas systems: H₂-N₂, H₂-CO₂, H₂-Ar, CO₂-Ar, using the proposed method. Experimental data and calculation methods, proposed by various authors, are available for these systems in a wide range of temperatures.

As our calculations show, the proposed method of calculating BDCs, basing on viscosity of pure gases, is simpler and more reliable and does not require a large amount of computation for most natural gases.

-
1. Fokin L. R., Kalashnikov A. N. Transport properties of a rarefied CH₄-N₂ gas mixture // J Eng Phys Thermophy, 2016. Vol. 89. No. 1. Pp. 249–259.
 2. Bogatyrev A. F., Belalov V. R., Nezovitina M. A. Thermal diffusion in binary mixtures of moderately dense gases // J Eng Phys Thermophy, 2013. Vol. 86. No. 5. Pp. 1225–1231.
 3. Bogatyrev A. F., Makeenkova O. A., Belalov V. R., Kucherenko M. A. Calculation of viscosity and diffusion coefficients in binary mixtures of dilute gases // Advanced Studies in Theoretical Physics, 2017. Vol. 11. No. 6. Pp. 283–296.

INVESTIGATION OF THERMAL CONDUCTIVITY OF OILS

Galkin D.A., Povolotsky I.I., Skripov P.V.*

ITP UB RAS, Ekaterinburg, Russia

**dmitry.gal10@gmail.com*

For reliable operation of equipment involved in heat transfer processes, special technological media are being developed - lubricating and cooling and quenching liquids, coolants, binders, etc. There is a problem of a reasonable choice of such media, primarily in thermally stressed processes. The basis for solving the problem is the knowledge of the thermophysical properties of the substance under conditions of a significant and rapid change in temperature. In the case of liquid media, such data can be obtained predominantly by experiment.

The report will present the results on the measurement of the thermal conductivity of a number of motor oils at an unique set-up [1], [2], which realizes the method of nonstationary heating of a wre probe (in the English-language literature - THW-method). The main attention is paid to the agreement of the experimental conditions with the requirements of the model used to calculate the thermal conductivity from the primary data of the experiment.

The study was partially supported by the Russian Foundation for Basic Research under Grant No. 18-38-00206 and by the Presidium of UB RAS Complex Program (grant No. 18-2-2-3).

-
1. Rutin S.B., Galkin D.A., Skripov P.V. // Int. J. Heat Mass Transfer. 2017. V. 115, P. 769-773.
 2. Rutin S.B., Galkin D.A., Skripov P.V. // Applied Thermal Engineering. 2018. V. 129, P. 145-147.

HEAT CONDUCTION OF SOLUTIONS: SUPERHEATED AND UNSTABLE STATES

Skripov P. V.

ITP UB RAS, Ekaterinburg, Russia

pavel-skripov@bk.ru

The phenomenon of superheating attracts the attention of researchers in connection with the substantial extent of the region of superheated states on the phase diagram of substance. Its key features have found application in high-speed technical applications. At the same time, rigid limitations are imposed on the system with respect to the volume of the superheated substance and the time of observation of the superheated state.

The report is devoted to the study of the heat conduction of solutions under high-power heat release. Objects of study were solutions that were impulsively superheated with respect to the liquid-vapor or liquid-liquid equilibrium temperature at a given pressure. A separate series of experiments was performed under superheat with respect to the diffusion spinodal of the solution. Specificity of the study is due to the variety of types of phase diagrams, as well as the possibility of concentration supersaturation of the solution. The elucidation of the influence of the double metastability factor (and instability one), which has its own characteristic times, on the processes of heat transfer and spontaneous boiling-up of solutions with different degrees of compatibility of components is a priority task of the study. The range of the heating pulse length was chosen on the basis of a compromise between the achievement of a sufficient thickness of the heated layer and the guaranteed absence of macroscopic liquid-liquid phase separation and/or convection.

This study was supported by the Russian Foundation for Basic Research (grant no. 16-08-00381-a).

INFLUENCE OF FAST RADIATION PROCESSES ON COOLING OF A METAL TARGET AFTER IRRADIATION BY A POWERFUL ION BEAM

*Prima A.I.,^{*1} Ding L.,² Zhang Q.,² Zhang Z.C.²*

¹TPU, Tomsk, Russia, ²DUT, Dalian, China

**artyom.prima@yandex.kz*

Results of an experimental research and modeling of cooling of a target after irradiation by powerful ion beam with energy density 1-10 J/cm^2 are presented. Researchers are executed on accelerator TEMP-6 (200-250kV with 120 ns duration). Experiments with stainless steel, titanium, brass, copper and tungsten target (thickness 75-200 μm) were carried out. The original estimation method of a thermal conductivity contribution in cooling of a heated target area of the target is presented. It is found that radiation defects formed in the target have a significant impact on the cooling dynamics of the target, which depends on the ratio of the target size and the ion beam. The cooling of a small target (the size of the target is smaller than the transverse dimensions of the ion beam) is satisfactorily described by two processes - the removal of thermal energy from the target due to thermal radiation and the release of energy at fast thermal annealing of radiation-induced defects. The cooling of the heated area of a large target, whose dimensions are much larger than the transverse dimensions of the powerful ion beam, occurs faster than it should be when cooled due to thermal radiation and thermal conductivity. It is shown that this can be caused by suppression of annealing of radiation defects due to migration of interstitial atoms from the irradiation area.

This work was supported by Russian Science Foundation, project no. 17-79-10140

METHOD FOR INVESTIGATION OF THERMAL CONDUCTIVITY OF METAL MATERIALS AT ACTION OF ULTRASONIC OSCILLATIONS

Lepeshkin A.R.

CIAM, Moscow, Russia

lepeshkin.ar@gmail.com

The investigation of the thermal conductivity in the field of action of ultrasonic oscillations is a new and complex problem and the solution of this problem is of current importance for ultrasonic equipment operating at elevated temperatures in various technological processes used in power engineering and industry. The technological processes intensified by ultrasonic oscillations in the gaseous medium are included combustion processes, gasification of solid fuels, processes of mass exchange and coagulation of aerosols, cleaning of flue gases and others. In this paper we propose the method for nonstationary investigation of the thermal conductivity in the field of ultrasonic waves at a frequency 20 kHz. A device for determining these characteristics has been developed, which is a design with an ultrasonic transducer and a rod-shaped waveguide. A thermograph was used for investigation of the nonstationary thermal state of a conical rod and contactless measurements of its surface temperatures. The investigations of the heating curves of the tip of the conical rod and the time of heat transfer from the electric heater to the tip of the rod in experiments with an ultrasonic transducer turned on and without it were carried out. According to the results of the research it was obtained that the thermal conductivity of a metal rod made of carbon steel is increased by 1.5 times.

THE SOLUTION OF THE INVERSE COEFFICIENT PROBLEM FOR THE SEARCH FOR THE HEAT CONDUCTIVITY TENSOR BY THE GRADIENT METHOD OF CONJUGATE DIRECTIONS

Borshchev N.O., Antonov V.A., Belyavsky E.A.*

MAI, Moscow, Russia

**www.moriarty93@mail.ru*

When conducting a thermophysical experiment, it is often difficult to determine the various characteristics of the material at any point in space, it is necessary to install a huge number of thermocouples, to accurately know the error of the measured equipment, method, etc.

The aim of this paper is to create a stable algorithm for determining the thermal conductivity tensor in the region under consideration using the conjugate gradient method while minimizing the mean-square residual functional of the theoretical and experimental temperature differences taking into account the measurement error.

This method of the first order of accuracy makes it possible to determine the required parameters of the object with a minimum number of iterations with a high accuracy with minimal a priori initial information.

The first stage of the study is to determine the theoretical fields of the considered region, taking into account the anisotropy [1] by the finite element method, where the step in space is chosen in such a way that the experimental and theoretical values of the temperatures are in the same nodes.

The second stage is the compilation of the mean-square residual functional or mean-square error, which is minimized in accordance with the method, and also the choice of the form of the corresponding basis functions of the thermal conductivity coefficients, which depend on temperature.

The third step is the iterative search for the required constant characteristics, using the conjugate gradient method, previously selecting the descent step and calculating its direction [2].

Multiplying the constant values of the tensor by their corresponding basis functions, we obtain the desired values.

Thus, the dependences of the temperature nonstationary field of the parameters of the heat conductivity tensor for diffuse high-intensity radiant heating, the sensitivity coefficients on the characteristics of space, and also the dependence of the tensor parameters on the number of iterations are constructed.

1. V. F. Formaliev. Heat transfer in anisotropic solids. M. Fizmatlit. 2015.
2. F.V. Vasiliev. Optimization methods. M. Fizmatlit. 2011.

THERMAL CONDUCTIVITY FOR THE CO₂+R1234YF AND CO₂+R1234ZE(Z) BINARY GASEOUS MIXTURES AT LOW PRESSURE

*Laptev Yu.A.,*¹ Tsvetkov O.B.,¹ Pyatakov G.L.,¹ Zainullina E.R.²*

¹SPbSU ITMO, Saint-Petersburg, Russia, ²SPbSPU, Saint-Petersburg, Russia

**laptev_yua@mail.ru*

Chlorofluorocarbons (CFCs) have been phased out under Montreal Protocol of 1987 as a result of ozone depleting potential (ODP). Carbon dioxide owing to the environmental benefits zero ODP, low global warming potential (GWP), no flammability was expected to replace the principal classes of refrigerants. The use of CO₂ may require a total redesign of refrigeration units. Hydrofluoroolefins (HFOs) especially R1234yf and R1234ze(Z) has recently proposed as new generation alternative refrigerants. Because of their mildly flammability the mixing of CO₂ and HFOs may offer a good alternative to meet the requirement of high cycle efficiency and not dangerous for human beings. A representation for the thermal conductivity of the mixtures of CO₂ and HFOs at atmospheric pressure is developed. The thermal conductivity concerning the mixtures was estimated by Sutherland equation type and by Wassiljeva relation modified by Lindsey and Bromley. To apply this procedure the viscosity and thermal conductivity of pure HFCs substances were established. To obtain these properties the theoretical approach by Mason, Monchick, Filippov and Golubev were used. The data were obtained at temperatures from 250 K to 360 K. The proposed technique was checked by the comparison with the experimental thermal conductivity data for the binary mixtures of R134a and R32 and for the triple zeotrop R407C. The agreement is satisfactory.

MECHANICAL PROPERTIES OF GLASSY CARBON UNDER SHOCK WAVE LOADING IN THE AREA OF ITS ABNORMAL COMPRESSIBILITY.

Molodets A.M., Savinykh A.S., Golyshev A.A.*

IPCP RAS, Chernogolovka, Russia

**molodets@icp.ac.ru*

The glassy carbon is the nano-structured metamaterial, which has anomalous compressibility (see [1]) under isothermal conditions by static compression.

Previously [2], we have established the formation of shock rarefaction waves in the glassy carbon, as well as the transformation of the shock wave front into a ramp compression wave. This generally means abnormal compressibility of glassy carbon not only in static loading conditions, but also in microsecond shock-wave compression-release cycle.

In the development of results [2] in this paper, we measured the evolution of the mass velocity in one-dimensional compression pulses propagating through the samples of glassy

carbon at its abnormal compression. Then, mathematical modeling of free surface velocity experimental profiles was performed within the hydrocode. Hydrocod based on itself upon the equation of state of the glassy carbon from 1. The results of mathematical modeling, together with the initial experimental information, allowed to determine the spall strength and the parameters of the fracture wave in the glassy carbon in the area of its abnormal compressibility.

Work is executed at financial support RFBR, research project No. 16-08-00237

-
1. Zhao Z., Wang E.F., Yan H., et al. // Nature Comm. 2015. V. 6. P. 1.
 2. Molodets A.M., Golyshev A.A., Savinykh A.S., Kim V.V. // JETP. 2016. V. 122. No. 2. P. 289.

CALCULATION OF TRANSPORT PROPERTIES OF HELIUM BASED GAS MIXTURES IN APPLICATION TO EXPERIMENTAL DETERMINATION OF THE TEMPERATURE RECOVERY FACTOR

Kochurov D.S., Eletskiy I.A., Kotova E.S.*

BMSTU, Moscow, Russia

**kochurov_ds@yahoo.com*

A great amount of experimental data for temperature recovery factor r [1] values is available for compressible air flows (Prandtl number $Pr \approx 0.7$), however, there is no such data in open sources for the cases of flows of binary helium He based gas mixtures with lower Pr values (from 0.2 up to 0.7). To carry out the experiments on determination of the r values, it is necessary to select or establish a reliable methodology for calculation of thermophysical and transport properties (and the Pr values) of the binary gas mixtures, and to verify this methodology against available experimental data for wide ranges of pressures and temperatures. The methodology can also be used in designing processes of gas-dynamic temperature stratification devices [2] as parts of space gas turbine energy systems [3], as well as other parts of such systems.

In this paper an analysis is being conducted of the known techniques of transport properties calculation (based on the intermolecular interaction potential parameters, quantum-mechanical ab initio calculations with known intermolecular interaction potentials, law of corresponding states, and empirical polynomials) of He based binary gas mixtures. The calculation results obtained with the techniques are compared against experimental data available in open sources for binary mixtures $He - Ar$, $He - N_2$, $He - Kr$, $He - Xe$ in the complete range of their composition and at pressures up to 10 MPa and temperatures up to 2000 K. Based on the results of the analysis a modified law-of-corresponding-states methodology is proposed with recent available quantum-mechanical calculations included. This work was financially supported by the Russian Science Foundation (RSF) under grant no. 14-19-00699.

-
1. Leontiev A.I. Gas-dynamic method of energy separation of gas flows // High Temperature, 1997. V.35. No.1. Pp. 155 – 157.
 2. Burtsev S.A., Leontiev A.I. Study of the influence of dissipative effects on the temperature stratification in gas flows (Review) // High Temperature, 2014. V.52. No.2. Pp. 297 – 307. DOI: 10.1134/S0018151X13060060.
 3. Leontiev A.I., Burtsev S.A. Cycle of a closed gas-turbine plant with a gas-dynamic energy-separation device // Doklady Physics, 2017. V.62. No.9. Pp. 443 – 445. DOI: 10.1134/S1028335817090099.

**THERMAL CONDUCTIVITY INVESTIGATION OF R-125/R-134a (39/61)
MIXTURE IN THE VAPOR PHASE**

Raschektaeva E.P., Stankus S.V., Verba O.I.*

ITP SB RAS, Novosibirsk-90, Russia

**raschektaevaep@gmail.com*

Ozone-friendly mixture of 39.2 mass % pentafluoroethane (R-125) and 60.8 mass % 1,1,1,2-tetrafluoroethane (R-134a) was investigated in the work. The relevance of developing new mixtures and studying their thermal conductivity is grounded by the continuous search for compositions with the optimal combination of high efficiency, availability, environmental safety and ease of use. This mixture was prepared in the laboratory by the weight method, the maximum weighing error being 0.1 g.

Thermal conductivity measurements were performed by the stationary method of coaxial cylinders in the temperature ranges from 320 to 415 K and pressures ranges from 0.1 MPa to 1.8 MPa. The measurement technique and the experiment procedure are described in detail in [1]. The measuring cell consisted of two vertical coaxial nickel cylinders: the external, 140 mm long, and the internal, 101.3 mm. The width of the annular gap between the cylinders was equal to 0.366 mm. We used copper-constantan thermocouples to measure the temperature of the cylinders and the temperature drop difference between them. The influence of the free ends on the thermal conductivity values was accounted by entering the respective corrections [1]. We filled the measurement cell with the investigated mixture from the liquid phase, thus avoiding the variations in the mixture composition. The error of the experimental data on the thermal conductivity was equal to 1.5–2.5%, while that on the temperature was 0.05 K and that on the pressure was within 4 kPa.

The measurement results were processed by an empirical dependence

$$\lambda(T, p) = a_0 + a_{10} \cdot \frac{T}{100} + a_{20} \cdot \frac{100}{T} + p \cdot (a_{11} \cdot \frac{T}{100} + a_{21} \cdot \frac{100}{T}) + p^2 \cdot (a_{12} \cdot \frac{T}{100} + a_{22} \cdot \frac{100}{T}), \quad (1)$$

where T in K, p in MPa, λ in $mW/(mK)$. It is shown that the dependence (1) can be applied in a wide range of parameters from atmospheric pressure to pressure on the condensation line. Reference tables for the temperature and pressure dependences of the mixture thermal conductivity are calculated using equation (1), and their errors are determined.

-
1. Verba, O.I. and Gruzdev, V.A. Thermophys. Aeromech. 2002. Vol.9. no.3. P. 445.

**THERMODYNAMIC ASSESSMENT OF LOW GLOBAL WARMING
POTENTIAL REFRIGERANT ALTERNATIVES**

*Mitropov V.V.,*¹ Tsvetkov O.B.,¹ Laptev Yu.A.,¹ Babich A.Yu²*

¹SPbSU ITMO, Saint-Petersburg, Russia, ²SPbSPU, Saint-Petersburg, Russia

**v_mit@mail.ru*

Global warming and ozone depletion are leading effects attaching the consideration of environmental organizations. Conversion to alternative hydrofluorocarbons (HFC) refrigerants without chlorine atoms progressed over the last two decades. However recently because of the significant global warming impact of HFCs the hydrofluoroolefins (HFOs) were proposed as new generation alternative refrigerants. This article discussed fluorinated propene based isomers, summarizes refrigerant numbering scheme, flammability, fundamental parameters

and thermodynamic properties of isomers containing five-, four- and three-fluorine atoms respectively, summarizes in T-s state diagrams the thermodynamic property estimates. In the present study evaluated the refrigerant performance in an idealized vapor compression refrigeration cycle for air-conditioning example and high temperature heat pumping. Presented HFC and HFO blends as non-flammable refrigerants with relatively low global warming potential values.

THE INFLUENCE OF SMALL ADDITIONS OF NI, CO, FE ON THE VISCOSITY OF LIQUID ALUMINUM

Beltyukov A.L., Menshikova S.G., Lad'yanov V.I., Korepanov A. Yu.*

UdmFRC UB RAS, Izhevsk, Russia

**albeltyukov@mail.ru*

Viscosity is one of the most structurally-sensitive properties of melt and measurements of its temperature and concentration dependences are often used in the study of the structure of liquid alloys and the analysis of interparticle interaction in them.

Temperature and concentration dependences of melts viscosity of Al-Ni, Al-Co and Al-Fe systems with the content of the second element up to 10 at.% have been studied in this work.

For liquid aluminium and melts of Al-Ni, Al-Co, Al-Fe systems with low content of alloying element (up to 1.0 at.% Ni and up to 1.4 at.% Co and Fe) the deviation of viscosity temperature dependences on Arrhenius dependence due to structural transformation in liquid aluminium was found.

An increase in the content of the alloying element leads to an increase in the melt viscosity for all three systems. For the Al-Ni system, the viscosity concentration dependence is nonmonotonic with a maximum near 1.5 at.% and a minimum in the range 2-2.7 at.% Ni. Isotherms of the viscosity of Al-Co and Al-Fe systems are monotonic.

The found features of temperature and concentration dependences of melt viscosity are explained by the formation of clusters from atoms of different sort and the dependence of their composition on the content of the alloying element. Clusters consisting of an atom of the alloying element (AE) and surrounding Al atoms (cluster Al(AE)) are formed in the melt at low concentrations of the alloying element. With an increase in the alloying element content, an increase takes place in the Al(AE) cluster quantity as well as a decrease of the volume part of the melt with the short range ordering characteristic for the liquid aluminum itself. With further alloying, after achieving a particular concentration of the AE atoms in a certain local melt domain, larger clusters occur with short range ordering close to the intermetallic compound. In the Al-Ni system, it can be an Al₃Ni compound.

The work was performed as part of the state task of FASO of Russia (state registration number AAA-A17-117022250039-4).

**MAXWELL FACTOR FOR GASEOUS 2.3.3.3-TETRAFLUOROPROPENE
AND ZIS-1.3.3.3-TETRAFLUOROPROPENE AT ZERO DENSITY**

*Tsvetkov O.B.,^{*1} Laptev Yu.A.,¹ Prostorova F.O.,² Vinzarevich A. V.²*

¹*SPbSU ITMO, Saint-Petersburg, Russia, ²SPbSPU, Saint-Petersburg, Russia*

**obereg@softrex.com*

In this study we focused on the Maxwell factor of fluorinated propene isomers - 2,3,3,3-tetrafluoropropene and zis-1,3,3,3-tetrafluoropropene last years receiving considerable attention as the next generation of refrigerants. Fluorinated propene isomers contain carbon-carbon double bond. The advantage of both refrigerants is a low global warming potential value of 4 and 6 respectively. This paper deals with the temperature dependence of thermal conductivity in the limit of zero density for dilute gases. A theoretically based correlation formalism has been examined according to the kinetic theory of Mason-Monchik-Parker using a set of trial functions and related to the translational and integral effective collisions that incorporate the information concerning intermolecular pair potential and binary collisions. The results have correlated using the Maxwell factor. The analysis of quantities for practical purposes which are related to the thermal conductivity and viscosity has been made.

**FISSION FRAGMENTS AND ENERGY SPECTRA OF PRIMARY
ELECTRONS IN A FISSIONING PLASMA**

*Shapiyeva A. Ye.,^{*1} Kunakov S.K.,² Son E. Ye.^{1,3}*

¹*MIPT, Dolgoprudny, Russia, ²KazNU, Almaty, Kazakhstan, ³JIHT RAS, Moscow, Russia*

**shapieva.ae@gmail.com*

Since the appearance of outstanding in its importance theory of non-uniform gases [1], sufficient number publications are released. Most of them are focused to adjust Boltzmann kinetic equation in different fields of applications. One of the most cited is [2], in which the high frequency gas discharges are studied for slightly ionized plasma within which the following limited conditions exist. The major this work [2] is devoted to the development of methods for calculating the energy distributions in a gas of low ion density under the influence of a high frequency a. c. field. The assumption that initial and final velocities are very close to each other leads to sufficient number of limitations in use for definite applications. Incident electrons interact with atoms not in the way like sphere with some rigid objects, but as with a complex system of charged particles moving in the state of dynamical equilibrium and actually interact initially with cycling electrons moving on the upper orbits. What is the source of primary electrons, this is very important problem also was not discussed and identified. The identification of fast electrons with energy around Mev's region (runaway electron) is not discussed or presented as well as the fact that where the radiation (bremsstrahlung) starts and ends, and how the formation of X-rays should be included in kinetic equation [3]. The X-rays [4] also might be treated like electrons (the de Broglie wave length) and the next coming question is that whether or not the absorption of X-ray by electrons leads to rise its kinetic energy lifting them to the MeV level, where usually neutrino oscillations connected with presence the beta electrons are existing. Boltzmann kinetic equations governing energy spectra of fast particles in nuclear induced plasma are defined and presented in detailed form for continuous plasma interacting with neutrons. Primary electrons spectra analytical expressions were derived on the bases of monochromatic energy spectra of helium-3 isotope fission products. The expressions for primary electrons born from tritium nuclei are also obtained in numerical and analytical way the proposed system of kinetic equation solution. The primary electrons in their own turn may also cause ionization processes. The energy distribution for the primary electrons,

created by fast electrons born from protons and tritium nucleuses are defined and compared with Monte–Carlo statistical approach.

1. Chapman S., Cowling T.G. The Mathematical Theory of Non-Uniform Gases. // Cambridge University Press. 1952. P. 431.
2. Holstein T. Energy distribution of Electrons in High Frequency Gas Discharges. // Phys. Rev. 1946. V. 70. P. 367.
3. Gurevich A. V., Zybin K. P. Runaway Breakdown and the Mysteries of Lightning. // Phys. Today. 2005. P. 37.
4. Loeb L. B. The Mechanisms of Stepped and Dart Leaders in Cloud- to-Ground Lightning Strokes. // J Geophys. Res. 1966. V. 71. No. 20. P. 4711.

=====

**THERMODYNAMIC PROPERTIES OF
SUBSTANCES IN THE CONDENSED STATE**

=====

**THERMOPHYSICAL PROPERTIES OF 1-BUTYL-3-METHYLIMIDAZOLIUM
TRIFLUOROMETHANESULFONATE**

*Guluzade A.,¹ Safarov J.,*² Hassel E.,² Abdulagatov I.³*

¹*AZTU, Baku, Azerbaijan,* ²*UNI Rostock, Rostock, Germany,* ³*DGU, Makhachkala, Russia*

*javid.safarov@uni-rostock.de

Ionic liquids are salts that are liquids at ambient temperatures and included to the green chemistry solvents. They have small vapor pressure, low melting point, high solvating capacity, high ionic conductivity and high thermal stability, which make them attractive for practical applications.

In this work, we will present the thermophysical properties of 1-butyl-3-methylimidazolium trifluoromethanesulfonate, [BMIM][TFO] at pressures up to $p = 140$ MPa and over a temperature range $T = (283.15$ to $413.15)$ K. These investigations covering such an extended p , T -range were performed the first time. The experiments were carried out using a specially adapted high pressure – high temperature Anton Paar DMA HPM vibration-tube densimeter with an estimated relative combined standard uncertainty up to $\Delta\rho/\rho = \pm 0.08$ % in density. The temperature T in the measuring cell is administrated with an error of ± 10 mK and is measured using the (ITS-90) Pt100 thermometer with an experimental error of ± 15 mK. Pressure p is measured with a relative uncertainty of 0.1 % (up to 100 MPa) and 0.5 % (up to 140 MPa), respectively, of the measured value.

The density values $\rho(p_0, T)/\text{kg}\cdot\text{m}^{-3}$ at ambient pressure and at $T = (283.15$ to $413.15)$ K were investigated using the combination of the Anton Paar DMA 5000M, DSA 5000M and DMA HPM vibration tube densimeters with an uncertainty of $\Delta\rho = \pm(5 \cdot 10^{-3}$ to $3 \cdot 10^{-1}) \text{ kg}\cdot\text{m}^{-3}$. The constant pressure specific heat capacity $c_p(p_0, T)/\text{J}\cdot\text{kg}^{-1}\text{K}^{-1}$ is measured at $T = (283.15$ to $413.15)$ K using the DSC differential scanning calorimetry. The speed of sound values $u(p_0, T)/\text{m}\cdot\text{s}^{-1}$ at ambient pressure and temperatures at $T = (283.15$ to $343.15)$ K are investigated using the Anton Paar DSA 5000M vibration tube densimeter and sound velocity meter.

The dynamic viscosity $\eta(p_0, T)/\text{mPa}\cdot\text{s}$ of [BMIM][TFO] at ambient pressures and at $T = (283.15$ to $413.15)$ K is measured using an Anton Paar SVM 3000 Stabinger Viscometer and Rheometer MCR 302.

The literature values available were subject to a consistency check with our data. An equation of state was established using parameters based on the new results to calculate the isothermal compressibility κ_T , isobaric thermal expansibility α_p , thermal pressure coefficient γ , internal pressure p_{int} , specific heat capacities at constant pressure c_p and at constant volume c_v , speed of sound u , and isentropic exponent κ_s of this IL.

**STRUCTURAL FEATURES OF AROMATIC HYDROCARBONS CLUSTERS
IN A WIDE RANGE OF STATE PARAMETERS**

Vervevko V.N., Vervevko M.V.*

KSU, Kursk, Russia

*vervevkovn@mail.ru

The cluster formations in liquids define structural features and thermophysic properties of liquids. Earlier the authors proposed the relation for clusters distribution function in liquid on

number of the particles contained in cluster [1]: $f(Z) = \frac{\lambda^m}{6} \cdot Z^{m-1} \cdot e^{-\lambda Z}$, $Z \geq 0$, where Z is the number of particles in cluster, $\lambda > 0$ ($\lambda = 1/\theta$) is the scale parameter determined by physical properties of the liquid, $m = 4$ is the distribution order.

The parameter θ is the function of the molecular packing factor η : $\theta = a_1\eta + a_2\eta^2 + \dots + a_n\eta^n \approx (5/2)\eta e^\eta \approx (5/2)(1 + \eta)$, where a_i is the serial power expansion coefficients; $\eta \approx 0.22\rho^*$, where $\rho^* = \rho/\rho_c$ is the reduced density of a liquid.

Using the cluster size probability distribution on a number of particles and experimental data on the density of liquids, we have estimated and analyzed the most probable number of particles in cluster: $\hat{Z} = \frac{m-1}{\lambda} = (m-1)\theta = 3\theta$, the average number of particles in clusters:

$$\bar{Z} = \int_0^\infty Z \cdot f(Z) dZ = \frac{m!}{(m-1)! \lambda} = \frac{m}{\lambda} = m\theta = 4\theta$$

and the root-mean-square number of particles in clusters: $\overline{\overline{Z}} = \sqrt{\overline{Z^2}} = \frac{\sqrt{m(m+1)}}{\lambda} = \sqrt{m(m+1)} \cdot \theta = \sqrt{20} \cdot \theta$ of benzene, toluene and their halogen-substituted depending on the state parameters at temperatures 293–423 K and pressures 0.1–600 MPa.

This work is supported by the Russian Foundation for Basic Research (RFBR) (Project No. 16-08-01203).

-
1. Verveyko V.N., Verveyko M.V., Melnikov G.A. // Eur. Phys. J. D. 2016. V. 70. P. 47.

EXPERIMENTAL STUDY OF THE THERMAL EXPANSION COEFFICIENT OF HEAT-CONDUCTING GASKETS

Borisenko D.I., Kuznecov K.I., Sukhikh A.A., Shish A.I.*

MPEI (TU), Moscow, Russia

**dima-luxinzhi@mail.ru*

Thermal expansion coefficient is an important thermal characteristic. The object of research — heat conducting pads — domestic analogues of materials series SilPad, GapPad and Bond-Play foreign production, widely represented in the market of electronic equipment.

To perform this task, a thermal expansion measurement unit was developed and manufactured. The error of measurement of the coefficient of thermal expansion is determined by the accuracy of measurement of linear displacement of the indicator and the precision of the fixing temperature (the temperature measurement error of 0.5 percent). Maximum permissible error of the indicator in a vertical position on the plot scale does not exceed: in the range of 200 divisions 2 micron; in the range 1 mm — 2.5 micron and a sample thickness of 5 mm is not greater than 0, 1 percent.

With positive temperature values, the difference between the coefficient of thermal expansion of domestic samples and American analogues does not exceed 10 percent.

The studies were carried out in the temperature range from –140 to 150 Celsius degree. Conducted performance measurements on the samples of PTFE 4. The experimental data are compared with the known literature sources [1, 2].

The results of thermal expansion measurements of heat-conducting gaskets are obtained for the first time. The limits of thermal resistance of new materials are also fixed. The effect of "hysteresis" of the dependence of the height increment of the tested samples on the temperature during heating and cooling processes is found.

1. The fluoroplastics in machine building. Goryainov, A. V., Bozhkov, G. K. and Tikhonova M. S., — M: "mechanical engineering 1971, p. 233.
2. Aviation technical reference. Aleksandrov V. G., Mayorov V. A., Pamukov N. P. — Publisher "Transport"Ed. 2nd, 1975, 432 p.

HOT CRYSTALLIZATION CENTERS IN GAS-SATURATED LAYERS OF AMORPHOUS ICE

Faizullin M.Z., Vinogradov A.V., Tomin A.S., Koverda V.P.*

ITP of UB of RAS, Ekaterinburg, Russia

**faizullin@itp.uran.ru*

A distinctive feature of crystallization at intensive nucleation in amorphous solids is the possibility of spontaneous emergence of "hot" centers and explosive crystallization in places of local accumulation of fluctuation arising embryonic crystals. The condition for the emergence of "hot" centers and a spontaneous transition to an explosive crystallization regime in an amorphous medium with frozen crystals requires their locally high concentration, which can be achieved both as a result of the natural nucleation process and external influence at a nonequilibrium system.

In a series of experiments, the possibility of initiating explosive crystallization in layers of amorphous ice saturated with methane in the presence of artificially introduced embryonic crystals is shown. Nonequilibrium amorphous condensates were obtained by supersonic deposition of molecular beams of rarefied vapor and gas on a liquid nitrogen cooled substrate. Adiabatic expansion of the molecular steam flow at the outlet of the supersonic nozzle led to a decrease in temperature and the formation of crystal clusters of ice in the molecular flow. The presence of the crystal centers in the sample shifted the beginning of crystallization to the low temperature region, and the form of the thermal signal, consisting of several peaks, testified to crystallization from different centers.

The initiated explosive crystallization of gas-saturated layers of amorphous ice was also investigated by the influence of local thermal heating at temperatures below the temperature of spontaneous crystallization of the sample. Heating was carried out by a short-term thermal pulse using a wire electric probe or laser beam.

Crystallization of water-gas layers under deep metastable conditions leads to formation of gas hydrate. The avalanche-type initiation of crystallization centers captures gas molecules and does not lead to their displacement by the crystallization front.

The work was supported by the Russian Foundation for Basic Research (Grants No 18-08-00352-a, No 18-38-00443 mol-a) and the Program for Basic Research of the Ural Branch of the RAS (Grant No 18-2-2-3).

THERMODYNAMIC PROPERTIES OF AQUEOUS SOLUTIONS OF UREA AND ITS ALKYL DERIVATIVES IN A WIDE RANGE OF THE PARAMETERS OF STATE

Egorov G.I., Makarov D.M.*

ISC RAS, Ivanovo, Russia

**gie@isc-ras.ru*

The values for the volume change during the formation of a liquid-phase mixture depend upon the changes in its intermolecular and intramolecular interactions as well as upon the interaction energy, the presence of H-bonds, hydrophobic or hydrophilic groups etc. When

varying the external state parameters (pressure and temperature), the bulk properties of a mixture are dependent upon both its molecular geometry and packing of the molecules, as well as upon their ability to transform.

This report focuses on the bulk properties and structural organization of aqueous solutions of urea and its alkyl derivatives. Urea is known to act as a denaturing agent for proteins and to play a substantial role in many other biological processes. Alkyl derivatives of urea act similarly, all being protein destabilizers. The mechanism of urea denaturation of proteins in aqueous solutions has not yet been fully explained: whether urine molecules directly interact with the macromolecule or they affect the protein stability through the surrounding water by changing its properties. Research findings in this field have been contradictory thus far. Some findings show that urea can be incorporated into water structure as a "water-like" molecule, thus not affecting the water-water interaction at all, other findings consider urea as a "structure-breaker" of water structure, the third ones consider it to be a "structure-maker".

This report presents the results of an experimental research of the density of aqueous solutions of urea and its alkyl derivatives at atmospheric pressure and compression (relative volume variation) at pressures ranging between 0.101 and 100 MPa and at temperatures between 278.15 and 323.15 K. The report discusses the calculated values of molar isothermal compressibility and molar isobaric expansibility, isochoric thermal pressure coefficients and the internal pressure of the mixture. The report also addresses the partial molar volumes of components as well as the limiting partial molar volumes..

The work was financially supported by the Russian Foundation for Basic Researches (grant 18-43-370010-a).

CLUSTERS IN THE "SIMPLE" AND "NORMAL" FLUIDS

Radchenko A.K., Shakhov A.V., Neruchev Y.A.*

KSU, Kursk, Russia

**radchenko.antoshka@mail.ru*

It has been proposed relation for estimating the structural features of molecular liquids according to their thermophysical properties.

$$T \left(\frac{\partial p}{\partial T} \right)_V = B_0 \left(1 - \frac{\langle n \rangle - 4/3}{Z^*} \right) \rho^3 + \frac{1}{\langle n \rangle} \frac{RT}{M} \rho$$

It is shown that the origin of the liquid phase is accompanied by the dimer association of molecules.

In "simple" monoatomic liquids, when the temperature decreases, the number of particles in the associates (clusters) increases that leads to the formation of a "nearest order" in the liquid. This process is confirmed by x-ray investigation and measuring of isochoric heat capacity of argon, krypton, etc.

On the contrary, in liquids with polyatomic molecules, excluding liquids with hydrogen bonds, only dimeric association is observed practically on the entire equilibrium liquid-vapor curve of up to the crystallization region.

The obtained results indicate that, as in liquid hydrocarbons in "simple" liquids, in addition to dispersion forces (m=6) and repulsion forces (n=12) exhibit themselves the long-range weak chemical bonds of the "Coulomb" type causing association of particles. The character of association was determined by the symmetry of the molecules.

This work was supported by the Russian Foundation for Basic Research, project 16-08-01203A.

1. Hobza P., Muller-Dethlefs K. Non-covalent Interactions: Theory and Experiment. Cambridge: Royal Society of Chemistry, 2010.

THERMODYNAMIC PROPERTIES OF AQUEOUS SOLUTIONS OF SODIUM THIOSULFATUM

Sobol O. V.

DonNABA, Makeyevka, Ukraine

cluck@mail.ru

The analysis of literature [1,2] demonstrates that the choice of these or those materials for accumulation of heat (cold) is carried out rather by an a trial and error method, but not as a result of systematic targeted researches. There are no reliable experimental datas on heats of melting and crystallization, overcoolings, stability of thermal properties at multiply the alternating processes like "melting a – crystallization"etc.

In this work as the differential thermal analysis method thermograms of melting and a crystallization of exemplars in system water – sodium thiosulfatum pentahydrate are received. The "independent" character exo- effects is established. The steady regularity is observed: with increase in concentration of sodium thiosulfatum exo- effects decrease concerning the eutectic temperature and increase concerning temperature a liquidus. For all exemplars the enthalpy of a nonequilibrium crystallization was always 15-20% lower than enthalpy of fusion. The regularity of change of the common enthalpy of a crystallization, to an eutectic comes from a principal component under the U-shaped law.

-
1. Mozgovoy A. G. Thermal properties of heat-retaining materials. Crystallohydrates. Reviews on thermal properties of substances., 1990.
 2. Danilin V.N. Materials for accumulation of heat (cold). Physical and chemical analysis of properties of multicomponent systems., 2008.

MELTING CURVE OF TITANIUM. THERMODYNAMIC DATA CONSISTENCY ASSESSMENT

Kulyamina E. Yu., Zitserman V. Yu., Fokin L.R.*

JIHT RAS, Moscow, Russia

**kulyamina.elena@gmail.com*

The work continues to study the properties of Ti, carried out in the JIHT of the Russian Academy of sciences [1], extending them to the melting line at a pressure of up to 90 GPa. To date, the melting point is known $T_m^0 = 1944 \pm 3 K$, corresponding to the bcc phase, and the heat of fusion with an error of 5%; reliable data on the volume change are absent. For the first time, experimental data on the melting curve in the interval 15-80 GPa were obtained in 2001 [2] by the diamond anvil cell. Extrapolating them to a pressure of 1 atm, the authors obtained an anomalously low value of the melting curve slope $\sim 7 K/GPa$, not characteristic of refractory metals. After 14 years [3] these measurements were repeated using the same technique. This time the melting point was controlled by the loss of crystallinity of the sample.

Here, data processing [3] was performed, consistent with the estimate of the volume change at the melting point. Inaccuracy in its definition from the data on the density of both phases forced us to resort to the analysis of the dependence of the volume jump on the melting entropy for 3d elements, from Ti to Ni. For Ti, an estimate is obtained $\Delta V_m = 0.257 \pm 0.026 \text{ cm}^3/\text{mole}$, which gave the initial slope of the melting curve $(dT_m/dp)_{p \rightarrow 0} = 35 \pm 5 K/GPa$ [4]. Note that

without the data [3] the conclusion about almost invariable steepness of the melting line in the whole interval would follow. This conclusion is obtained in [5], where the Ti phase diagram is constructed without using the results of [3].

1. Chekhovskoi V.Ya., Fokin L.R., Peletskii V.E. et al. Handbook of Titanium Based Materials: Thermophysical Properties. Data and Studies. NY: Begell House, 2007. 275 p.
2. Errandonea D., Schwager B., Ditz R. et al. Systematics of transition metals melting // Phys. Rev. B. 2001. V. 63. pp. 131–134.
3. Stutzmann V., Devaele A., Bouchet J. et al. High-pressure melting curve of titanium // Phys. Rev. B. 2015. V. 92. 224110.
4. Kulyamina E.Yu., Zitserman V.Yu., and Fokin L.R. Titanium Melting Curve: Data Consistency Assessment, Problems and Achievements // Technical Physics. 2018. Vol. 63. No. 3., pp. 369 – 373.
5. Elkin V.M., Mihaylov V.N., Mihaylova T.Yu. Semiempirical equation of state for titanium solids α, ω, β and liquid phase with vaporization // VANT. Seriya "Teoreticheskaya i prikladnaya fizika" 1977. No 1. pp. 28 – 42.

ON THE POSSIBILITY OF THE EXISTENCE OF A DOUBLE MAXIMUM ON THE ADSORPTION ISOTHERM OF BINARY METALLIC SYSTEMS

*Lesev V.N.,^{*1} Alchagirov B.B.,¹ Dadashev R.Kh.,² Kyasova O.Kh.,¹
Uzdenova A.N.¹*

¹KBSU, Nalchik, Russia, ²ChSU, Grozny, Russia

^{*}lvn_kbsu@mail.ru

The study of adsorption phenomena in metallic melts has a great importance for the development of the theory of surface phenomena and the practice of developing new technological processes. But analysis of the literature shows, double maximum on the adsorption isotherms of a number of binary systems are found, for example, on the isotherm of potassium adsorption in alloys with sodium (P. Pugachevich and co-workers). It turned out that the value and position of the first maximum is consistent with the theory of surface phenomena V. Semenchenko, but the explanation of the second maximum in the framework of this theory is difficult. In this regard, we consider the possibility of the existence of a double maximum on the adsorption isotherms of surface-active components in binary liquid metal melts using an example of Pb based on In, in which Pb is a surface-active component. To that end, using our own experimental data on the surface tension (ST) isotherm of the In-Pb system, we calculated the adsorption of lead on the surface of alloys for $T = 573$ K.

From the results of Guggenheim-Adam in the "N variant, it follows that the adsorption isotherm does detect two maximum at a content of 0.12 and 0.17 atomic share of Pb in the alloys with indium. Moreover, the possibility of the appearance of a double maximum on the adsorption isotherm is inherently "laid by" in the calculation formula itself, which is the product of two factors: the parabola $(x_{In}x_{Pb}) = x_{Pb}(1 - x_{Pb})$ and the hyperbolas $(d\sigma/dx_{Pb})_T$, in which the concentration x_i are expressed in atomic fractions if the normalization $x_{Pb} + x_{In} = 1$. For alloys with a surface-active component, the isotherms $d\sigma/dx$ are usually the rapidly decreasing functions of the alloy compositions, i.e. hyperbole. As a result of multiplying the coordinates of the points of intersecting parabola and hyperbola in a plane " $d\sigma/dx$ –composition of alloys and the desired maximum appear on the adsorption curve.

Therefore, calculations of lead adsorption in alloys with indium and an analysis of the Guggenheim-Adam formula themselves show the possibility of the appearance of a double maximum on the adsorption isotherms of surface-active components in binary liquid metal solutions.

DEFECTIVE STRUCTURE OF CRYSTALLINE LATTICE OF ZIRCONIUM CARBIDE

Pakhomov E.P.

JIHT RAS, Moscow, Russia

evg-pakhomov@yandex.ru

When analyzing the nature of the ordered equilibrium distribution of carbon vacancies in the crystal lattice of nonstoichiometric zirconium carbide ZrC_x , attention is paid to the formation of a layered structure (alternating fully filled layers and layers with "chemical" vacancies in the lattice). This allowed us to establish the mechanism for the onset of the decay of the crystal lattice and, accordingly, determine the position of the boundaries of its homogeneity region, the dependence of the concentration of "thermal" vacancies on temperature, and also determine the composition of the second phases formed. It is obtained that, for $x = 0.5625$, the stability boundary is vertical to $T = 3000$ K, in the region $x = 0.75-0.875$ the melting point is maximal and constant, in the region $x = 0.125-2$ the melt probably has a molecular structure, and in the region $x = 0.75-0.875$ apparently formed dome of immiscibility

THE ENERGY OF INTERMOLECULAR FORCES IN LIQUID HALOALKANES AND THEIR BINARY MIXTURES

Neruchev Yu.A., Korotkovskii V.I., Ryshkova O.S.*

KSU, Kursk, Russia

**yuan2003@mail.ru*

Measurements of the sound speed (0.1%), the density (0.05%), and the isobaric heat capacity (2%) of liquid halogenated alkanes and their binary mixtures were evaluated in the temperature range (25-150) °C and used to calculate the energy of intermolecular forces in these liquid haloalkanes and their binary mixtures. It is shown that in these compounds in addition to the dispersion forces of attraction ($m = 6$) and repulsive forces ($n = 12$) manifest themselves the long-range bonding forces causing a dimer association of particles. The energy of the intermolecular forces is determined by the relation:

$$|E_p| = B\rho^2 + b\rho^{1/3} \left(1 - \left(\frac{\rho}{\rho_b} \right)^{11/3} \right),$$

where B and b are the dispersion and bounding force constants (determined by critical parameters), ρ is the density of a liquid, and ρ_b is the density at the normal boiling point. The expression in brackets takes into account the contribution of the energy of the repulsive forces.

On the base of the atom-atom interaction mechanism, a formula was obtained for predicting the value of the dispersion-force constant from the data on the individual properties of the atomic centers:

$$B = B_0 \left(\frac{(1 - \chi)\mu_l + \frac{l+1}{n+1}\chi\mu_n}{\mu_l} \right)^3 (\xi^2 + (1 - \xi)^2 a + 2\xi(1 - \xi)\sqrt{a}).$$

Here n – is the number of the n-alkane, l – is the number of n-alkyl present in the mixture, χ – the weight concentration of n-alkyl, ξ – is the value characterizing the concentration of hydrogen atoms in the mixture.

This work is supported by the RFBR project no. 16-08-01203.

1. Korotkovskii V.I. , Ryshkova O.S. , Neruchev Yu.A. , Goncharov A.L., Postnikov E.B. Isobaric Heat Capacity, Isothermal Compressibility and Fluctuational Properties of 1-Bromoalkanes // Int .J. Thermophys. 2016. V. 37:58.
2. Ryshkova O.S. , Bolotnikov M.F., Korotkovskiy V.I. , Neruchev Yu.A. Peculiarities of temperature dependence of liquid 1-chloroalkane viscosity // High Temperatures. 2016. V. 54. P. 872.

ENTHALPIES OF FORMATION OF MIXED OXIDES IN ZnO-BASED TRANSPARENT CONDUCTIVE OXIDE SYSTEMS BY KNUDSEN EFFUSION MASS SPECTROMETRY

Gribchenkova N.A., Smirnov A.S., Alikhanyan A.S.*

IGIC RAS, Moscow, Russia

**gribchenkova@igic.ras.ru*

The evaporation thermodynamics of three quasi-binary systems of Transparent Conductive Oxides (TCOs) Ga₂O₃, In₂O₃, SnO₂ with a common volatile component ZnO was studied by high temperature Knudsen effusion mass spectrometry.

Individual phases of mixed oxides ZnGa₂O₄, Zn₇In₂O₁₀, Zn₅In₂O₈, Zn₂SnO₄ as well as heterogeneous samples of the systems were investigated at the temperatures from 1360 to 1460 K. The systems exhibit the incongruent character of evaporation processes. The vapor above the systems was found to contain almost only ZnO evaporation products Zn(g) and O₂ for all phase fields under consideration. From isothermal effusion experiments the vapor species partial pressures were determined and principle p-x-sections of the systems phase diagrams were constructed. Energetic characteristics of sublimation and formation of the mixed oxides including the standard enthalpies of formation were obtained by the third-law calculations.

Acknowledgement: This study was supported by the Presidium of the Russian Academy of Sciences (program I.14P1).

METHODS AND DEVICES FOR MEASURING SURFACE ENERGY AND SURFACE TENSION OF METALS AND ALLOYS

Taova T.M., Khokonov Kh.B., Shebzukhova I.G., Alchagirov B.B.*

KBSU, Nalchik, Russia

**khb180532@mail.ru*

The important properties of the dividing surface between the phases are surface energy and tension, adsorption of components, structure and composition of the surface layer. The original theoretical and experimental methods to determine the structure and properties of the interphase boundaries were elaborated. The special attention is spared to studies of the specific free surface energy (f_ω) and surface tension (σ) of the dividing surfaces between the phases in heterogeneous systems when researching such processes as sintering and curing of solid's surface defects, heterogeneous catalysis and modifying metals and alloys, welding and soldering various materials, forming and growing a new phase, creation of the composite materials and so on.

Experimental measurement of f_ω and σ of solids is difficult problem. Analysis of the many experimental methods for determining f_ω and σ gives the measurement error by these methods was 10-50 %.

In this work a description of the developed by the authors new methods, allowing to measure f_ω and σ of solid metals and binary alloys are presented. The most perspective

method for measuring σ of solid metals and alloys is the compensation method of zero-creep (CMZC) elaborated in Kabardino-Balkaria State University. Basing on CMZC method the special schemes and devices were elaborated and more than 10 certificates and patents were obtained by authors. By this method the ST (σ) and its temperature coefficients for 22 metals and 4 binary alloys were measured with error about 2 %. It should be noted that ST of a several solid binary metallic systems was determined for the first time. It was revealed a mutual surface activity of the components in In-Pb and In-Tl binary systems

We consider that in physics of the interphase phenomena the actual problem is elaboration of new and more perfect methods of measuring f_ω and σ of solid metals and alloys.

THERMODYNAMIC STUDY OF SOME AZIDONITROCOMPOUNDS. ENERGIES OF REORGANIZATION OF RADICALS

Pashchenko L.L.,¹ *Miroshnichenko E.A.**²

¹*MSU, Moscow, Russia,* ²*ICP RAS, Moscow, Russia*

**eamir02@mail.ru*

THERMODYNAMIC STUDY OF SOME AZIDONITROCOMPOUNDS. ENERGIES OF REORGANIZATION OF RADICALS

Pashchenko L.L., Miroshnichenko E.A. Lomonosov Moscow State University, Leninskie Gory 1-3, 119991, Russia Semenov Institute of Chemical Physics RAS, Kosygin str. 4, Moscow, 119991, Russia

Azidonitro containing compounds are important industrial chemicals with a broad range of applications. This class of compounds is widely used in the synthesis of many diverse products. Some compounds are highly explosive. To investigate the stability and performance of these chemicals, knowledge of the enthalpy of formation is an essential requirement. Other thermo chemical properties, such as enthalpies of vaporization and energies of reorganization of azido-radicals are needed for the characterization of the chemical degradation pathways of their compounds. Despite the extensive studies of azidonitro containing compounds, available thermo chemical experimental information is often scarce and frequently shows significant discrepancy among published results. In this work the enthalpies of formation and vaporization of five azidonitro containing compounds are determined, Using experimentally obtained values, the standard enthalpies of formation in gas phase are calculated. The bond dissociation energies are calculated. Using fundamental equations of the chemical physics, the calculation scheme of the energies of reorganization of molecules fragments into radicals is offered. The new calculation method is offered to determine the energies of reorganization of molecule fragment into radical and the energies of reorganization of nitroazidoaromatic radicals. Reorganization energies of azido radicals and bond dissociation energies are calculated. The new calculation method for determination of the energy of reorganization of azido radical gives a way to calculate (kJ mol⁻¹): the enthalpy of formation of radicals, bond dissociation energy median thermo chemical bond energies. Reorganization energies of radicals are calculated, which is near to energy of reorganization of acetylene radicals. Bond dissociation energies for calculation process of reorganization energy of azidonitro radicals are obtained from the enthalpies of formation of compounds and literature data. Obtained ours data of reorganization energies of azidonitroradicals and bond dissociation energies are needed for energy calculations of the kinetics of the reactions involving azidonitro containing compounds.

A NEW CODE FOR JOINT APPROXIMATION OF ENTHALPY INCREMENTS AND HEAT CAPACITY DATA

Sineva M.A.,*¹ *Aristova N.M.*,¹ *Belov G.V.*,^{1,2} *Morozov I.V.*¹

¹*JIHT RAS, Moscow, Russia*, ²*MSU, Moscow, Russia*

**maria.a.sineva@gmail.com*

Original experimental data on thermodynamic properties of substances in the condensed phase are often presented as tables and need to be approximated with functions that reproduce them with an acceptable accuracy. These functions can be used then for thermodynamic modeling and other theoretical studies. There are various codes for processing thermodynamic data. Some of them are meant for low-temperature heat capacity [1], others for high temperature data measured by, for example, laser flash method. Moreover, there is a significant amount of methods for processing data on enthalpy increment obtained by classic calorimetry. Filling databases (IVTANTHERMO, NASA etc.) with new information on substances requires fitting data with preset polynomials [2].

A new computer program based on a combination of fitting algorithms is proposed for analyzing experimentally obtained enthalpy and heat capacity of substances in the condensed state. The program is supposed to unite all processing steps (low- and high- temperature heat capacity data, enthalpy increment data etc) to combine and analyze available data of several types simultaneously. The program has a friendly user interface. It comes in the forms of a standalone application and web application with limited functionality. The enthalpy increment data can be fitted by a polynomial of a chosen degree which can be used at the next step to process heat capacity dependence on temperature. Provided the user has high temperature heat capacity experimental data, it can be fitted by a polynomial combined of elementary functions picked manually or by preset combinations. The results can be exported in various database formats.

-
1. I. Roslyakova, B. Sundman, H. Dette, et al // Calphad 55 (2016) 165
 2. G.V. Belov, N.M. Aristova, I.V. Morozov, M.A. Sineva. // J. Math. Chem. 55 (2017) 1683

BEHAVIOR AND THERMODYNAMIC CHARACTERISTICS OF A GETE SEMICONDUCTOR IN A FERROUS AND PARAPHASE CONDITION

SOBIROV J.F., SAFAROV M.M.

Safarov M.M.,² *Sobirov J.F.**¹

¹*BEHAVIOR AND THERMODYNAMIC CHARACTERISTICS OF A Ge, kurgan-tyube, Tajikistan*, ²*12CSRI MOD RF, Sergiev Posad, Russia*

**mahmad1@list.ru*

The abstracts should not exceed one page if A5 format including the title, author list, affiliations, the abstract body and bibliography. The abstracts should be submitted using the forms at the web site [1].

Figures and tables are not allowed. The formulae and special symbols can be entered using \TeX commands. Below the basic rules of \TeX text formatting are given.

Extra spaces are ignored. The tilde symbol “~” denotes the non-breaking space. Use “ and ” as “quotation marks”. Celsius degree can be entered as: temperature 15°C, the expression “of the order of 10%”—as: ~10%. You can use formulas in the text, for example, to obtain “x1 to the 11th power”, type x_1^{11} .

One or more empty lines begin a new paragraph. There are three types of dashes in \TeX : hyphen (in words as mother-in-law), en-dash (used between digits: 1–3) and em-dash (—). You

shouldn't add spaces before and after the em-dash as you probably do in Russian: "yes—or no?".

You can also use displayed equations:

$$\int_0^1 x^2 dx = 1/3.$$

Please pay attention that the formula here ends a sentence and should be followed by a full stop. You can use cross-references in the abstract. For example, you can refer to the article like [2]. The symbols in braces stand for the reference identifier. The reference itself is defined at the end of text in the "thebibliography" environment. The T_EX system is described in the book [3].

-
1. RCTP-15 web site, <http://www.ihed.ras.ru/rctp2018/en/contribution>
 2. Fortov V. E., Khishchenko K. V., Levashov P. R., Lomonosov I. V. // Nucl. Instr. Meth. Phys. Res. A. 1998. V. 415. No. 3. P. 604.
 3. Knuth D. E. T_EX: The Program, volume B of Computers and Typesetting. Reading: Addison-Wesley, 1986.

THERMODYNAMIC PROPERTIES OF THE GRAY AND WHITE TIN

*Syzdykova A.B.,^{*1} Belov M.P.,¹ Abrikosov I.A.²*

¹MMDL NUST "MISIS Moscow, Russia, ²(IFM) LiU, Linkoping, Sweden

^{*}*syzdykova.aygerym@gmail.com*

Tin is commonly found in one of two allotropic forms: the stable phase at low temperature is alfa or gray tin which is a zero-gap semiconductor having the diamond structure; when the temperature is raised above $T \sim 13$ °C, the crystal transforms into the beta-phase or white tin which is a body-centered tetragonal metal [1]. There is a lack of data for the enthalpy of alfa→beta phase transformation. And there is a wide spread in the available results which do not very well converges between themselves [2], [3]. In this work we calculate mechanical and thermodynamic properties: equilibrium lattice parameters, bulk modulus, entropy and enthalpy of transformation, Gibbs free energy.

-
1. Pavone P., Baroni S., Gironcoli S. // Phys.Rev.B. 1998. V. 57. No. 17.
 2. Hultgren R., Desai P.D., Hawkins D.T., Gleiser M., Kelley K.K., Wagman D.D. // American Society For Metals, Metals Park, Ohio. 1973.
 3. Cohen E., van Eijk C. // Phys. Chem. 1899. V. 30. P. 601-622.

AB-INITIO MODELING AND EXPERIMENTAL INVESTIGATION OF THE PROPERTIES OF ULTRA-HIGH TEMPERATURE SOLID SOLUTIONS

Ta_xZr_{1-x}C

*Sidnov K.,^{*1,2} Vorotilo S.¹*

¹NUST MISiS, Moscow, Russia, ²ISMAN RAS, Chernogolovka, Russia

^{*}*sidnov@list.ru*

Due to their high melting temperature, resistance towards high-temperature oxidation and high mechanical properties, solid solutions Ta_xZr_{1-x}C are promising carbides for the application as the ultra-high temperature materials (UHTCs).

The absence of reliable data on the phase equilibria in the Ta–Zr–C system hinders the development and implementation of the related UHTCs. In particular, there are contradictory

reports regarding the existence of the miscibility gap in Ta–Zr–C system at the temperatures lower than 900 °C [1–3].

In this work, we carry out ab-initio calculation of the thermodynamic properties of $Ta_xZr_{1-x}C$ alloys and demonstrate that the decomposition of the solid solutions into TaC and ZrC should not occur.

Among the various methods that allow the synthesis of solid solution in Ta–Zr–C system, self-propagating high-temperature synthesis is widely considered one of the most prospective [4, 5].

We synthesize single-phase specimens with the composition $Ta_xZr_{1-x}C$ ($x=0.9, 0.8, 0.6, 0.3$) and anneal it for 40 hours. We do not observe any sign of the decomposition of the solid solution during the annealing, corroborating the conclusions obtained in theoretical simulations.

1. E.I. Gladyshevsky, T.F. Fedorov, L.V. Gorshkova. The zirconium–tantalum–carbon system. Russ. J. Inorg. Chem. 9 (1964), 639–642.
2. A.I. Gusev, Order–Disorder Transformations and Phase Equilibria in Strongly Nonstoichiometric Compounds, Phys.-Uspekhi, 43(1) (2000), 1–37.
3. P. Zhou, Y. Peng, Y. Du, S. Wang, G. Wen, W. Xie, K. Chang, A thermodynamic description of the C–Ta–Zr system. Int. J. Refract. Met. Hard Mater. 41 (2013), 408–415.
4. A.S. Rogachev, A.S. Mukasyan, Combustion for Material Synthesis. CRC Press, Boca Raton, 2014.
5. Concise Encyclopedia of Combustion Synthesis: History, Theory, Technology, and Products (Eds. I. Borovinskaya, A. Gromov, Yu. Maksimov, A. Rogachev, E. Levashov, A. Mukasyan), Elsevier, Toronto, 2017.

EXPERIMENTAL DEPENDENCE OF THE DENSITY OF LOCAL ENTROPY RATE OF PRODUCTION OF CHANGE OF THE TEMPERATURE IN TIME

Kostanovskiy A. V., Kostanovskaya M. E.*

JIHT RAS, Moscow, Russia

**kostanovskiy@gmail.com*

The paper reports on the analysis of experimental thermograms $T(\tau)$ of the tungsten solid-phase samples obtained in the process of instant cooling of a spherical by the method of electrostatic levitation, or heating the thin plate by a direct current in a circuit with the unloaded battery or heating the thin plate by a laser stream of radiation. The range of change of the temperature in time $dT/d\tau$ makes $10 \div 9 \cdot 10^7$ K/s in various experiments. The comparative analysis is lead - the density of a heat flux q shares on product of speed of change of a heat flux $dq/d\tau$ and relaxation time $\tau_q = 10^{-12} - 10^{-10}$ s. The analysis has shown that in all experiments the Fourier's law of heat conductivity which corresponds to a linear mode of thermodynamics is realized. Density of local entropy rate of production p counted under the known formula which is deduced in the assumption of constant value of an isobaric thermal capacity of substance. The assumption, that a thermal capacity is a constant, is executed as a result of small values of change of temperature which gets out at processing thermogram. Check of an opportunity of application of the specified formula for calculation of the density of local entropy rate of production is based on performance of the extremum principle for dependence $p = f(\tau)$ when the condition of system aspired to an equilibrium. It is shown, that in four various experiments the density of local entropy rate of production has uniform linear dependence from speed of change of temperature. The given result allows to assume, that linear dependence $p = f(dT/d\tau)$ can be considered as universal dependence for a linear mode of thermodynamics.

**ANALYTICAL DESCRIPTION OF EXPERIMENTAL ISOTHERMS FOR
SURFACE TENSION OF BINARY METAL SYSTEMS WHICH FORM
STABLE CHEMICAL COMPOUNDS**

Kalazhokov Z.K., Kalazhokov K.K., Sherieva E.K.*

KBSU, Nalchik, Russia

**z-kalazh@yandex.ru*

The analysis of the available in the literature experimental isotherms of surface tension (ST) for metal systems shows that they can be divided into two large groups:

1. Isotherms of ST with a monotonic variation of ST, depending on the composition (approximately half of the available).

2. Isotherms with some features on curves with corners, extrema, points of inflections, etc. These isotherms have a complex form. The main reason for the appearance of features on isotherms of ST is the appearance in the system of capillary-active molecular formations of type A_nB_m , stable at the temperature of ST measurement.

It is shown that four types of the simplest isotherms of ST can be distinguished from the isotherms of the first group, which are described by the equation proposed in [1]. The average deviation of the calculated PN from the experimental ones allowed by this equation is about 1%.

The paper also analyzes the isotherms of the second group of ST. It is found that a complex system $A - B$ with features can be represented in the form of combinations of simple systems of the first group of isotherms PN. This approach allows to describe complex isotherms ST for binary system equation [1] is quite satisfactory. Methods of calculations of isotherms of ST of binary systems with one and two stable chemical compounds are considered in detail. The paper shows for the first time the role of A_nB_m molecular formations in the formation of surface properties of binary system alloys.

-
1. Kalazhokov Zamir Kh., Zikhova K.V., Kalazhokov Z.Kh., Kalazhokov Kh.Kh., Taova T.M. Calculation of isotherms for surface tension of melts for multicomponent metal systems. // High Temperature. - 2012. - V.50 N3. - P.469-472.

THE STUDY OF BINARY ALLOY SYSTEMS Sn-Pb AND In-Pb BY XPS

***Kalazhokov Z.K.,* Dzugurova L.K., Zhanimova D.A., Karamurzov B.S.,
Kalazhokov K.K.***

KBSU, Nalchik, Russia

**z-kalazh@yandex.ru*

This report presents the results of studies of the surfaces of alloys $Sn + 8,96at.\%Pb$ and $In + 51at.\%Pb$ by x-ray photoelectron spectroscopy (XPS, K-Alpha systems, UK) at room temperature on a device available at the Kabardino-Balkar state University. From the obtained results it is seen that on the spectra the doublets of photoelectron peaks of the core levels of tin and lead ($Sn3d$ and $Pb4f$, $In3d$) are observed. The surface of the sample before etching is characterized by the presence of compounds of the main components of the alloy with oxygen. Observed components of hydrocarbon contamination, as evidenced by the visible peaks of $O1s$ and $C1s$ in the spectrum recorded before ion-etching.

Thus, tin on the surface of alloys of the $Sn - Pb$ system is mainly in the oxidized state in the form of tin dioxide SnO_2 (486.1 eV). But a significant part of the tin remains in the metal state (484.5 eV). Indium is also on the surface of the alloys of the $In - Pb$ system in the form of InO . These results are confirmed by the values of the Wagner parameter. If we compare these

results with the results for lead, we can see that almost all lead is on the surface in a metallic, non-oxidized state. The correction of the charge displacement of the binding energy along the $C1s$ line leads to the binding energy of the basic peak $Pb4f7/2$ equal to 137.2 eV, which is in good agreement with the literature data.

By methods of ion etching of the alloy surface and XPS, we have built the profiles of the components distribution in binary alloys $Sn + 8,96at.\%Pb$ and $In + 51at.\%Pb$.

The data obtained for both alloys show that lead is adsorbed positively, which is consistent with the position of thermodynamics on the surface activity of the component in binary metal systems: the component with a smaller ST is more surface-active.

-
1. Pokrovsky N. L., Pugachevich P. P., Golubev N. Ah. Study of the surface tension of the In-Pb system. //Reports of the Academy of Sciences. USSR. 1968,N1. P.80-83.
 2. Demeri M., Farag M., Heasley T..Surface tension of liguidy Pb-Sn alloys. -J.Mater.Sci. 1974,v9. N4. p.683-685.

GLASS-FORMING ABILITY AND CRYSTALLIZATION BEHAVIOR OF Al-Ni-Co-Nd (Sm) AMORPHOUS ALLOYS

*Rusanov B.A.,¹ Sidorov V.E.,¹ Moroz A.I.,*¹ Svec P.,² Janickovic D.²*

¹*USPU, Ekaterinburg, Russia,* ²*Institute of Physics SAS, Bratislava, Slovakia (Slovak Republic)*

**nastmoroz97@yandex.ru*

Amorphous ribbons based on aluminum with 3d-transition metals (PM) and rare-earth metals (REM) are actively studied due to their unique physical properties. They have a whole set of such properties: high corrosion resistance, ductility and strength. However, their low glass-forming ability limits their industrial application.

In present work, we investigated the effect of Nd and Sm on the glass-forming ability of Al-Ni-Co-REM alloys.

Amorphous ribbons were obtained from the alloys $Al_{86}Ni_4Co_4Nd(Sm)_6$ and $Al_{86}Ni_6Co_2Nd(Sm)_6$ by the spinning method.

X-ray diffraction studies has shown that the ribbons are completely amorphous. The kinetics of crystallization was studied by the DSC method in the Perkin Elmer device, and the electrical resistivity was measured by a standard four-probe method.

On the basis of the data obtained, the most popular criteria for the glass-forming ability are calculated, the temperatures of the thermal processes accompanying the crystallization process are determined, and the activation energy is calculated of the Kissinger method.

The studied tapes, in contrast to tapes obtained on the basis of ternary systems containing only Ni or Co, have a pronounced glass transition point, which is not typical for amorphous aluminum-based alloys. In addition, the replacement of 8 at.% Ni with 6 at.% Ni and 2 at.% Co increases the temperature of existence of the amorphous phase by almost 30 K, and a further increase in the cobalt content to 4 at.% At 80 K. The process of crystallization in the measurement of resistivity is accompanied by three phase transitions of the first kind.

Analysis of the results showed that the use of Nd and Sm in Al-Ni-Co-REM alloys is very promising from the point of view of increasing the region of existence of the amorphous phase.

MOLECULAR DYNAMICS STUDY OF ISOTHERMAL COMPRESSIBILITY OF BINARY MOLTEN POTASSIUM HALIDES

Tatarinov A.S.,¹ *Kobelev M.A.*,*² *Stepanov V.P.*²

¹*UrFU, Yekaterinburg, Russia,* ²*IHTE UB RAS, Yekaterinburg, Russia*

**coulomb76@mail.ru*

The calculation of the isothermal compressibility of binary molten potassium halides (KBr-KI, KCl-KI, KF-KI) in the entire concentration range at a temperature of 1200 K was carried out using the classical molecular dynamics simulation. The cubic cell, containing 3456 particles, was simulated in the NVT-ensemble under periodic boundary conditions. The interionic interactions used in this work were based on the simple Born-Mayer potentials derived by Fumi and Tosi. Long-range forces were calculated by the Ewald method. Experimental densities were used for the pure binary melts and the additivity of molar volumes was assumed for the mixtures. The simulations were typically 10^6 steps in length, with a timestep of 4 fs.

The isothermal compressibility is calculable as the infinite wavelength limit of the static structure factor. The results from proposed model would assign the patterns of variation of the isothermal compressibility observed in the experiment as a function of the concentration. Namely, an increase in the positive deviations of the isothermal compressibility from additivity upon replacement of the anion of the second component in the Br-Cl-F series.

Analysis of the structural characteristics of the binary mixtures as a function of the concentration of the components demonstrates that the local environment of the potassium cation significantly changes in the KF-KI system upon addition of the fluoride ion. In the bulk of the binary molten mixture KF-KI, regions predominantly containing cation-anionic pairs corresponding to the pure salts are formed. In contrast, in the binary mixtures KBr-KI and KCl-KI, a natural change in the composition of the nearest cation-anionic environment is observed with the addition of the second component.

EXPERIMENTAL STUDY OF THE ELASTIC PROPERTIES OF 1-CHLORO-SUBSTITUTED N-ALKANES AND THE POSSIBILITY OF THEIR PREDICTION

Melent'ev V. V.

Kursk State University, Kursk, Russia

mels@inbox.ru

The possibility of predicting the density under pressure was studied for 1-chloro-substituted n-paraffins using the parameter of inverse reduced fluctuations, which is directly related to isothermal compressibility. This parameter can be determined on the basis of liquid thermodynamic properties on the saturation line and consists of only two constant factors unchanged within a relatively wide temperature range starting from the melting point. It is confirmed by comparison with experimental data for different classes of liquids. Experimental data on density, ultrasonic velocity, and heat capacity at constant pressure were obtained for 1-chloropropane, 1-chlorobutane, 1-chlorohexane, 1-chloroheptane and 1-chlorononane in a wide range of temperatures and pressures in Condensed Matter Physics Research Center, Kursk State University [1,2].

-
1. Melent'ev, V. V.; Postnikov, E. B. Speed of Sound and Density of 1-Chloropropane in the Range of Temperatures 180–373 K and Pressures up to 196.1 MPa. *J. Chem. Eng. Data* 2017, 62, 3409.
 2. Melent'ev, V. V.; Bolotnikov, M. F.; Neruchev, Yu. A. Speeds of Sound, Densities, and Isentropic Compressibilities of 1-Chlorohexane at Temperatures from (293.15 to 413.15) K and Pressures up

to 200 MPa. J. Chem. Eng. Data 2006, 51, 181.

THERMODYNAMIC PROPERTIES OF SODIUM AND POTASSIUM METHANESULFONATES

Sulimov A.V., Kosova D.A., Druzhinina A.I., Tiflova L.A.*

MSU, Moscow, Russia

**sulimov.art@gmail.com*

Investigation of the properties of methansulfonic acid's salt and systems based on them is of interest, first of all, from the fundamental point of view. Information on properties of these salts in the literature is given partially, despite of widely using of methansulfonic acid and its inorganic derivatives in various fields of industry. From a practical point of view, investigation of the properties of sodium and potassium methanesulfonates is interesting because of geochemistry problems. Methansulfonic acid is a product of oxidation of dimethyl sulfide by oxygen, which is a product of phytoplankton activity. Not so long ago, sodium and potassium methanesulfonates were found in the ice cores of Antarctica. Knowledge of the properties and composition of ice cores could be applied to reconstruct the climatic changes or ocean composition during the cores formation, - this might be used to solve the problems of geothermobarometry.

The aim of this work was to study the thermodynamic properties of methanesulfonic acid salts - $\text{CH}_3\text{SO}_2\text{ONa}$ and $\text{CH}_3\text{SO}_2\text{OK}$. In this study measurements of isobaric heat capacities of the salts were conducted by differential scanning calorimetry (DSC) in a wide range of temperatures. The thermal effect of dissolving salts in water at 298.15 K was determined by dissolution calorimetry method. Temperature dependences of the thermodynamic functions - isobaric heat capacity, entropy, enthalpy - were calculated in the program "CpFit" (<http://td.chem.msu.ru/develop/cpfit/>) on the basis of DSC experimental data. The linear combination of Einstein-Planck functions was applied in the approximation. Standard enthalpy of salt's formation at 298.15 K was calculated on the basis of dissolution calorimetry data.

1. Gernon M. D., Wu M. Buzsta, T. Janney. *Environmental Benefits of Methanesulfonic Acid. Comparative Properties and Advantages*. Green Chemistry, 1999, 1.
2. Baker S. C., Kelly D. P., Murrell J. C. *Microbial Degradation of Methanesulphonic Acid: A Missing Link in the Biogeochemical Sulphur Cycle*. Nature, 1991, 350.
3. Hatakeyama S., Okuda M., Akimoto H. *Formation of Sulfur Dioxide and Methanesulfonic Acid in the Photooxidation of Dimethyl Sulfide in the Air*. Geophysical Research Letters, 1982, 9.

HEAT CAPACITY OF IONS CADMIUM AND BARIUM IN DIMETHYLSULFOXIDE AT 298,15 K

*Rakhmanova P.A.,¹ Vasilyov V.A.,¹ Solovyov S.N.,¹ Novikov A.N.,*²
Doronin Ya.I.,² Skorba V.R.²*

¹MUCTR, Moscow, Russia, ²NI MUCTR, Novomoskovsk, Russia

**anngic@yandex.ru*

The heat capacity reflect the energy and structural changes during the formation of solutions; the thermodynamic characteristics of electrolytes and ions calculated from these characteristics allow us to reveal the peculiarities of ion-molecular interactions and evaluate the solvation effects on the physicochemical properties of various liquid systems. In the present

work, the heat capacity of dimethylsulfoxide (DMSO) solutions of barium and cadmium iodides were studied for the first time with high accuracy. The heat capacity of the solutions was studied in a sealed calorimeter with an isothermal coating and a platinum thermometer, whose resistance was determined using a bridge circuit. The error of heat capacity was 0,001 J / (g K). The apparent molar heat capacities of barium and cadmium iodides in DMSO were calculated from the experimental data. To determine the standard partial molar quantities corresponding to an infinitely dilute solution, the concentration dependences of apparent molar heat capacities were approximated by the linear equation. The standard partial molar heat capacity of barium and cadmium iodides were separated into ionic components based on the additivity of the partial molar quantities and literature value of heat capacity for the iodide ion in DMSO. The standard values of heat capacity of barium and cadmium ions are equal respectively -133 and -126 J/(mole K). The standard partial molar heat capacity of ion can be represented as the sum of contributions of the intrinsic heat capacity of the ion in solution and changes in the heat capacity of the solvent due to solvation, rearrangement of the primary structure, and specific interactions with ions. The latter contribution is characteristic only for complexating ions, in particular, cadmium ion. The barium and cadmium ions, however, differ significantly in size, while having the same charge; that is why all other components of standard partial molar heat capacity also differ for these ions, and a comparison of these characteristics allows, in our opinion, only qualitative evaluation of the contribution of the specific interactions of the cadmium ion with DMSO molecules. As in N-methylpyrrolidone solutions, the specific interactions of the cadmium ion with the solvent molecules do not lead to any significant change in heat capacity.

THERMODYNAMIC CHARACTERISTICS OF AN AQUEOUS OLEIC ACID EMULSION

Aetov A. U., Zaripov Z. I., Usmanov R. A., Nakipov R. R.*

"KNITU Kazan, Russia

**aetovalmaz@mail.ru*

The oxidation technology realized in the supercritical water environment (SCWO) is one of the environmentally friendly ways of processing industrial and household waste [1-2]. Studies of chemical reactions in the GFR media have received considerable attention [3-5]. Within the framework of this direction, experimental studies have been performed and the results of some thermodynamic properties of aqueous solutions of fatty (oleic) acid included in the sewage waters of the food industry: the coefficient of thermal expansion and density in the temperature range 298-363K and pressures of 0.098-49.0 MPa, isobaric heat capacity at temperatures of 320K-570K and pressures of 9.8-29.4 MPa without and in the presence of hydrogen peroxide. In the presence of hydrogen peroxide, a negative thermal effect is established, the magnitude of which increases with increasing pressure from 70 kJ / kg to 100 kJ / kg.

1. Marrone Ph. A., Hong G. T., Spritzer M.N. J. *Adv. Oxid. Technol.* 2007. Vol. 10. No. 1. 157-168p.
2. Anikeev VI I. Ermakova A.A. *Jour. prikl. chemistry.* 2011. T. 84. 88-94.
3. Gumerov F.M., Kayumov R.A., Usmanov R.A., Sagdeev A.A., Abdullin I.Sh., Sharafiev R. F. .. *American J. Anal. Chem.* 2012, Vol. 3. 950-957p.
4. Vostrikov AA, Dubov D.Yu., Psarov SA. *Proceedings of the Academy of Sciences (Ser, Chem.)*. 2001. P. 1409-1412.
5. Gayazova E. S., Usmanov R. A., Gumerov F. M., Friedland S. V., Zaripov Z. I., Gabitov F. R., Musin R. Z. *International Journal of Analytical Mass Spectrometry and Chromatography.* 2013. 48-54p.

MODIFIED COMPOSITIONS FOR ENDOPROSTHESES

*Andrusova N.N.,*¹ Zhavoronok E.S.,¹ Legon'kova O.A.,² Kedik S.A.¹*

¹*M.V. Lomonosov ITHT, Moscow, Russia,* ²*Vishnevsky Institute of Surgery, Moscow, Russia*

**nrychneva@mail.ru*

Endoprostheses replacement is a surgery in the course of which the damaged joint is eliminated from the body and replaced by artificial implant. Nowadays the most promising method of fixing parts of endoprostheses is the cementless method. According the method parts of prosthesis have porous surface consists of hydroxyapatite that allows a bone to intergrow into the implant. In order to improve existing endoprostheses it is suggested to modify them by biocompatible polymers which extend the term of service of endoprostheses and increase their mechanical strength.

Biocompatible polymer solutions - cellulose acetate OPADRY CA 500F 190001 produced by Colorcon in biocompatible solvents - N-methylpyrrolidone and dimethylsulfoxide - were selected as objects of the study. Rheoviscometric study of the solutions was conducted in a wide range of concentrations from 90 to 230 g/l and a temperature range from 15 to 45 °C. The experiments were carried out on a Brookfield DV2TLV rotary viscometer with a system of coaxial cylinders.

As a result of the experiment, the relationships of shear stress and dynamic viscosity vs shear rate were obtained. It shows that all solutions have Newtonian behavior, that allows to characterize them by the Newtonian viscosity. The temperature dependence of the viscosity obeys the Arrhenius-Frenkel-Eyring equation, which makes it possible to calculate the viscous flow energy of activation, which is from 30 to 35 kJ/mol for solutions in methylpyrrolidone and from 20 to 35 kJ/mol for solutions in dimethylsulfoxide. The energy of activation vs polymer concentration relationships indicate that the viscous flow energy of activation not that much depends on the concentration with a slight tendency to increase with increasing concentration. That indicates that the flow becomes difficult while moving to more viscous solutions. Concentration dependences of viscosity have been constructed and they can be approximated by two tangent lines forming a critical point at 170 g/l for solutions in dimethylsulfoxide and at 165 g/l for solutions in methylpyrrolidone. The optimal concentration of solutions for the next disintegration of hydroxyapatite has been determined.

THEORETICAL AND EXPERIMENTAL STUDY ON THERMODYNAMIC PROPERTIES INTERMETALLIC COMPOUNDS IN THE Zr-Fe BINARY SYSTEM

*Mukhamedov B.O.,*¹ Saenko I.S.,² Fabrichnaya O.B.,² Abrikosov I.A.³*

¹*NUST "MISIS Moscow, Russia,* ²*TUFBA, Freiberg, Germany,* ³*LiU, Linköping, Sweden*

**m_bobur_1991@mail.ru*

Zr-Fe system is the subject of great interest in modern industry of composite and structural steels. Composite materials based on TRIP (transformation-induced plasticity) matrix reinforced by zirconia ceramics are of particular interest due to the wide range of their possible technological, especially, in the nuclear industry and automotive production as structural and functional materials. Development of such composite materials requires the knowledge of thermodynamic properties and phase relations. Thus, the main purpose of this work is the experimental and theoretical study of the thermodynamic properties of the Zr₃Fe and ZrFe₂ compounds. Density functional theory (DFT) calculations in combination with the quasi-harmonic approximation have been used to determine the enthalpies of formation, standard entropies as well as isochoric and isobaric heat capacities (CV, CP) for the Zr₃Fe and ZrFe₂ compounds from 0 K up to high temperatures. Experimentally, the heat capacities of both

compounds was been measured using differential scanning calorimetry (DSC) method. Heat capacity of the Zr_3Fe compound was measured for the first time in the range of temperatures between 100 K and 1023 K. Experimental data on the heat capacity of the $ZrFe_2$ were obtained in the wide temperature range from 100 K to 1473 K and compared with available literature data. By using the combination of theoretical and experimental data, the main thermodynamic properties of the Zr_3Fe and $ZrFe_2$ compounds were described from 0 K up to temperatures close to the upper limits of stability.

HEAT CAPACITY OF (ER, IN)-DOPED BARIUM CERATE IN THE TEMPERATURE RANGE OF 200-700 K

*Matskevich N.I.,*¹ Wolf T.A.,² Samoshkin D.A.,³ Stankus S.V.,³ Vyazovkin I.V.¹*

¹IIC SB RAS, Novosibirsk, Russia, ²KIT, Karlsruhe, Germany, ³ITP SB RAS, Novosibirsk-90, Russia

**nata.matskevich@yandex.ru*

Alkaline earth oxide cerates, in particular doped barium cerates, are perspective materials for using as pigments, fuel cells electrolytes, etc.

In the paper the heat capacity of doped barium cerate which has the composition $BaCe_{0.7}Er_{0.2}In_{0.1}O_{2.85}$ is presented.

The compound $BaCe_{0.7}Er_{0.2}In_{0.1}O_{2.85}$ was prepared by solid state reaction. Identification was carried out by X-ray diffraction and fluorescence spectroscopy. The compound was an individual phase with orthorhombic structure (space group Pmcn).

The heat capacity was measured in the temperature range of 200-700 K with DSC 404 F1 calorimeter using a platinum crucible with corundum insert at a constant heating rate of 6 K/min in an argon flow (20 ml/min). A sapphire was used as calibration sample.

The results of experimental measurements of heat capacity have shown that there are no phase transitions in the temperature range of 200-700 K for employed compound. The specific heat at standard conditions was: $C_p = 114.9 \pm 1.5$ J/(K mol). Earlier [1] we measured heat capacity of (Ho, In) -doped barium cerate where phase transition of second order was observed at 550 K.

This work is supported by RFBR 16-08-00226, Karlsruhe Institute of Technology and Federal Agency for Scientific Organizations of Russia.

-
1. Matskevich N.I., Wolf Th., Le Tacon M., Adelman P., Stankus S.V., Samoshkin D.A., Tkachev E.N. // J. Therm. Anal. Calorim. 2017. V. 130. P.1125.

THERMODYNAMIC PROPERTIES OF COPPER AND ZINC METHANESULFONATES

Kosova D.A., Sulimov A. V., Tiflova L.A., Monaenkova A.S.*

MSU, Moscow, Russia

**dakosova@gmail.com*

Methanesulfonic acid (CH_3SO_2OH) is the simplest representative of sulfonic acid's. Such properties as relatively low corrosiveness, high thermal stability, low toxicity and the possibility of biological decomposition, as well as high solubility of salts allow applying of this acid as a solvent or reagent. In addition, methanesulfonic acid is the main product of the dimethyl disulfide photochemical oxidation in the atmosphere and therefore in the environment's

biogeochemical cycle. Thus, methanesulfonates of transition metals could be applied in the chemical industry as coatings obtained by various electroplating methods, and also as a catalysts. Due to the high density of zinc-containing water solutions of salts, zinc methanesulfonate might be applied as a well-killing fluid.

The aim of this work was to study the thermodynamic properties of methanesulfonic acid salts $\text{Cu}(\text{SO}_3\text{CH}_3)_2 \cdot 4\text{H}_2\text{O}$ and $\text{Zn}(\text{SO}_3\text{CH}_3)_2 \cdot 4\text{H}_2\text{O}$. In this study measurements of isobaric heat capacities of the salts were conducted by differential scanning calorimetry (DSC) in a wide range of temperatures. The thermal effect of dissolving salts in water at 298.15 K was determined by dissolution calorimetry method. Temperature dependences of the thermodynamic functions - isobaric heat capacity, entropy, enthalpy - were calculated in the program CpFit¹ on the basis of DSC experimental data. The linear combination of Einstein-Planck functions was applied in the approximation. Standard enthalpy of salts formation at 298.15 K was calculate on the basis of dissolution calorimetry data.

¹<http://td.chem.msu.ru/develop/cpfit/>

MELTING CHARACTERISTICS OF SODIUM HALIDES: A MOLECULAR DYNAMICS SIMULATION

Zakiryanov D.O., Kobelev M.A., Tkachev N.K.*

IHTE UB RAS, Yekaterinburg, Russia

**dmitry.usu.ph@yandex.ru*

A theoretical study of the of melting and crystallization phase transitions characteristics in classical ionic systems was carried out using molecular dynamics. In order to trace the role of the Born-Mayer repulsion on temperature, entropy, and density jump during melting a primitive electrolyte model with charges of opposite sign and identical radii is considered. The main attention will be focused on the description of the characteristics of the melting and crystallization phase transitions as a function of the Born-Mayer pair potential parameters. The melting of crystal cell containing 512 particles is modeled with NPT ensemble with a timestep of 0.005 ps and the total number of steps $4 * 10^6$, which in our opinion is enough to achieve the equilibrium state of the system. The simulation results show that the pre-exponential factor of the Born repulsion influences only the density of the system under consideration, while the temperature of the phase transition remains constant. The decrease in the characteristic length of the pair potential leads to a decrease in the melting temperature of the model system. Estimations of the vacancies effect on the melting point on the example of sodium halides are carried out. The proposed theoretical approach to the description of the liquid-solid phase transition is applied to sodium halides. In particular, for sodium chloride, having an experimental melting point of 1074 K, it is shown that the simulated crystal overheats by about 50 K above the melting point. The calculated temperature and heat of fusion are 1112 K and 38.4 kJ / mol respectively, and the density jump was 0,44 g/cm³. The report will provide a comparison of the calculated and experimental melting characteristics for all sodium halides. The study was supported by the Russian Foundation for Basic Research, project no. 18-03-00606.

ANALYSIS OF THERMOCHEMICAL DATA OF FATTY ORGANIC ACIDS

Ovchinnikov V.V., Kulakov A.A., Maltseva S.A.*

KNITU-KAI, Kazan, Russia

**chem_vvo@mail.ru*

It is known that fatty acids can be included in the structure of lipides. Many fatty acids have one or several double C=C bonds. Such type of acids plays an important role in steel industry, in particular. On this reason is important to unite their thermochemical data on vaporization $\Delta_{vap}H^\circ$, combustion Δ_cH° , formation Δ_fH° and make on their base the equations, which can serve for the prediction of properties of new similar fatty acids. Analysis of the mentioned above thermodynamic functions of fatty acids: dodecanoic ($C_{12}H_{24}O_2$), meristic ($C_{14}H_{28}O_2$), palmitic ($C_{16}H_{32}O_2$), margaric ($C_{17}H_{34}O_2$), stearic ($C_{18}H_{36}O_2$) and arachidic ($C_{20}H_{40}O_2$), represented in the works [1, 2] allows to calculate the equations (1-3), in which the functions $\Delta_{vap}H^\circ$, Δ_cH° and Δ_fH° depended from the number of valence electrons N without of the number of lone electron pairs g of oxygen atoms (2 pairs) in the consistence of acids.

$$\Delta_{vap}H^\circ = (27.1 \pm 7.9) + (1.4 \pm 0.2) (N-g); r 0.974, So 7.3, n 6 \quad (1)$$

$$\Delta_cH^\circ = (5.7 \pm 80.5) - (108.7 \pm 0.8) (N-g); r 0.999, So 32.0, n 6 \quad (2)$$

$$\Delta_fH^\circ = (-433.5 \pm 50.1) - (4.9 \pm 0.5) (N-g); r 0.977, So 20.4, n 6 \quad (3)$$

The correlation parameters of calculated equations for fatty acids, having from 12 to 20 carbon atoms in their structures are practically equal to the same for simple carbon acids [3], but have a different errors at correlation coefficients.

1. Adriaanse N., Dekker H, Heats of combustion of normal saturated fatty acids and their methyl esters. J. Coops, Rec. Trav. Chim. Pays/Bas, 1965, 84, 393.

2. Stephenson R.M., Malanowski S., Handbook of the Thermodynamics of Organic Compounds 1987.

3. Ovchinnikov V.V. Thermochemistry of heteroatomic compounds. The analysis and calculation of thermodynamic functions of organic acids. Harold of Kazan technological university. 2014, 17, 144.

=====

**THERMOPHYSICAL PROPERTIES OF
SUBSTANCES AT HIGH TEMPERATURES**

=====

**COMPREHENSIVE STUDY OF EVAPORATION OF BMImBF₄ IONIC
LIQUID**

Dunaev A.M., Motalov V.B., Kudin L.S.*

ISUCT, Ivanovo, Russia

**amdunaev@ro.ru*

It is known that ionic liquids based on imidazolium with tetrafluoroborate anion have a complex composition of vapor. To determine the nature of the saturated vapor components and find their thermodynamic characteristics a comprehensive study of the ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate, comprising Knudsen mass spectrometry, IR spectroscopy, thermal analysis and NMR, gas chromatography and quantum chemical calculations is performed.

It is established that the composition of the condensed phase does not undergo appreciable changes in the process of heating and evaporation of the liquid. In the temperature range 424-514 K in the mass spectra of the object under study the ions of both the ionic liquid itself and its conversion products are detected. First of all it is necessary to note products of interaction of a cation with an anion - ylidenes, concentration of which reaches 70% from an ionic liquid. Another characteristic feature is the possible cyclization of the starting compound. Products of this conversion in electron ionization mass spectrum are dominating and their fraction (as the fraction ylidenes) increases with time and temperature.

The revealed features of evaporation indicate the impossibility of using integral methods for determining the pressure of saturated vapor to find thermodynamic characteristics. However, the slope of the temperature dependence of the ion current of the parent BMIm⁺ cation the enthalpy of vaporization of the ionic liquid was determined.

**CALCULATION OF THE TEMPERATURE IN 3D CARBON-CARBON
COMPOSITE MATERIAL.**

Brykin M. V.

JIHT RAS, Moscow, Russia

mbrykin@gmail.com

The dynamics of the temperature field in a three-dimensional carbon-carbon composite material heated from the surface by a uniformly distributed heat flux (laser radiation) is calculated. It is shown that when only the radiative mechanism of the surface cooling is taken into account a region with a highly inhomogeneous temperature distribution is formed near it. The temperature drop reaches hundreds of K at the initial stage of heating and tens of K in a steady state. This effect is due to the strong anisotropy of the fibers thermal conductivity which differs by almost 2 orders of magnitude in the longitudinal and transverse directions. Accounting for the evaporative cooling mechanism caused by the sublimation of the material into a vacuum or an external inert atmosphere somewhat reduces the inhomogeneity of the temperature field on the surface. The evaporation rate was calculated taking into account the difference between the individual evaporation coefficients of different carbon vapor components from unity and the so-called parameter jumps in the Knudsen layer [1, 2]. Its sharp dependence on temperature especially in the jet regime leads to a different rate of sublimation from different parts of the surface and the formation of its complex relief. In particular, the initial complete structure of

the material breaks down which can lead to its more rapid destruction in comparison with the sublimation mechanism as a result of cracking due to arising thermal stresses. It is shown that, although the rates of evaporation into vacuum and a medium at the same surface temperature differ very strongly, in the steady state this difference is practically leveled by the difference in the established average surface temperature.

-
1. Brykin M.V., Vorobev V.S., Shelyukhaev B.P. State of the vapor near an evaporating surface. High Temp., 1987, vol. 25, no. 3, p. 343.
 2. Brykin M.V., Sheindlin M.A. On particularities of the vapor pressure measurements of refractory substances at very high temperatures. High Temp., 2018, vol. 56, no. 4.

RECENT ADVANCES IN LASER-PULSE MELTING OF GRAPHITE AT PRESSURE UP TO 6 KBAR

Vervikishko P.S., Sheindlin M.A.*

JIHT RAS, Moscow, Russia

**pvervikishko@gmail.com*

Melting temperature of graphite and nature of liquid carbon remains a subject of permanent discussions in the literature for many decades. The main reason of this inconsistency is the extremely high melting temperature of graphite making it the most refractory material. The present study deals with a further improvement of the laser-heating technique first used in [1] with the aim to reach a higher reproducibility of the results, to improve and to broaden means of optical measurements and to better control the process of cooling and freezing of liquid carbon. The important aspect of this work is to study the nature of the inflection point on the thermogram ascending due to the formation of liquid carbon first reported in [1]. Since the nature of this inflection can be only attributed to the less thermal conductivity of liquid carbon in respect to the original solid, the study of the magnitude of the inflection with pressure can significantly contribute to the current knowledge of the nature of liquid carbon. In the present work, the changes in thermal conductivity of liquid carbon vs. pressure are studied in the domain of 0.15 to 6 kbar. It turns out that thermal conductivity increases steadily from the triple point pressure to ca.6 kbar. It means that if a certain correlation between the thermal and electrical conductivities is accepted the existing controversy between numerous studies of graphite melting can be successfully resolved. Moreover, through visualization of formation of liquid carbon by the ad-hoc developed system with a high-speed camera and the power diode laser used as a spotlight, the fact of graphite melting at high pressure is finally confirmed. _____

1. M.Musella, C.Ronchi, M.Brykin and M.Sheindlin. The molten state of graphite: An experimental study. //J. of Applied Physics, 84, No.5 (1998), p.2530-2537.

ZIRCONIUM CARBIDE PHASE DIAGRAM. EXPERIMENTAL RESEARCH AND MATHEMATICAL MODELING.

Falyakhov T.M., Brykin M.V., Petukhov S.V., Sheindlin M.A.*

JIHT RAS, Moscow, Russia

**tfalyakhov@gmail.com*

Experimental data on the phase diagram of zirconium carbide ZrC_x preceded by the results of numerical simulation of the experiment, are presented. The main problem of modeling was the absence in the literature of comprehensive data on the equation of state in a wide range of temperatures and compositions, including solid and liquid phases. An approximate method to calculate the ZrC_x enthalpy is proposed. Calculations of surface thermograms for conditions close to the experimental ones are carried out. In particular it is shown that for any compositions there are no any features on thermograms corresponding to the beginning of melting (solidus). Experimental data were obtained by laser heating, one of the most promising methods for the study of phase diagrams of high-temperature materials. Its effectiveness was demonstrated, in particular, in the study of non-stoichiometric uranium dioxide phase diagram [1]. Samples for the study were made using a one-way static pressing of powders followed by sintering in a vacuum furnace. Zirconium carbide powders of controlled composition were obtained by self-propagating high-temperature synthesis (SHS). The samples were heated by a powerful YAG laser. Different methods for the simultaneous surface state diagnosis during its heating and cooling were used: high speed filming in reflected light, the spectrum of radiation of multichannel spectrophotometers, registration of the nature of the reflection from the surface of radiation of the auxiliary laser. Simultaneous processing of all signals made it possible to reliably detect solidus, liquidus and high-temperature eutectic temperatures in a wide range of compositions, as well as to determine the spectral emissivity of solid and liquid phases. The obtained experimental data are qualitatively fully consistent with the results of calculations.

-
1. Manara D., Ronchi C., Sheindlin M., Lewis M., Brykin M. Melting of stoichiometric and hyperstoichiometric uranium dioxide. *J. of Nucl. Mat.* V. 342 (2005), Issue 1-3, pp. 148-163.

PHYSICAL PROPERTIES OF THE MOST REFRACTORY SUBSTANCES (GRAPHITE AND CARBIDES) IN THE TEMPERATURE RANGE 2000-7000 K

Savvatimskiy A.I.,^{1,2} Onufriev S.V.¹*

¹JIHT RAS, Moscow, Russia, ²LPI RAS, Moscow, Russia

**savva@iht.mpei.ac.ru*

Experimental studies on the melting of refractory substances (graphite and carbides) at high temperatures, in the solid phase near melting, during melting and in the liquid state (up to 7000 K) are considered. Method of heating- pulsed electric heating for units of microseconds. Specimens - in the form of thin plates (thickness from 1 micron to 200 microns). Pulse currents - from 1 kA to 30 kA, depending on the thickness of the specimens. The heating time is about 5 microseconds. It was measured: input energy, heat capacity, electrical resistance - depending on the measured temperature T. The latter was measured by a high-speed pyrometer based on the high-speed photodetector PDA-10A (Thorlabs).

Calibration of T was used with the help of the temperature lamp up to 2500 K. Above this value the temperature scale was based on the Planck formula with the known normal spectral emissivity of the substance (literature data). A melting model of the blackbody was also used, made of the studied substance in the form of two closed plates with a gap on one side (a

wedge-shaped model of the blackbody). The theory and practice of such measurements were published earlier (see books [1, 2]). The report covers the following issues:

1. The use of graphite specimens grade HOPG (Russian analogue UPV-1T) in the form of thin layers of purity 99.99%. Preparation of carbide specimens (ZrC, HfC, TaC) - by magnetron sputtering from a solid phase.

2. Measurement of temperature in a fast heating process (model of a blackbody or selection of normal spectral emissivity). The problem of the graphite melting.

3. Measurement of electrical resistance and heat capacity (including CP and CV).

4. The appearance of non-stationary pairs of Frenkel defects prior to melting.

The work was supported by the Russian Science Foundation (grant No. 14-22-00273-P).

-
1. Graphite melting and the properties of liquid carbon. Fizmatkniga, 2013 or 2014 (2nd edition), 257 pages.
 2. Savvatimskiy A.I. Carbon at high temperatures, Springer series in materials science, 2015, V. 134, P. 1-246.

HIGH-TEMPERATURE THERMOPHYSICAL PROPERTIES OF SOLID SOLUTIONS OF THE Y-Ho SYSTEM

Chernoskutov M. Yu., Ivliyev A. D., Meshkov V. V.*

RSVPU, Ekaterinburg, Russia

**ad_i48@mail.ru*

The thermal diffusivity of the Y-Ho system was studied by us earlier [1], and it was shown that the concentration and temperature dependences of thermal diffusivity exhibit a number of unusual features. To establish the concrete nature of the change in properties, we undertook a detailed study of the complex of thermophysical characteristics of twenty samples of different compositions of this system in the interval from 400 K to the melting point. The thermal diffusivity, relative heat capacity, thermal conductivity, specific electric resistance, and electronic thermal conductivity were studied. The thermal characteristics were investigated by the temperature wave method [2] in the helium atmosphere. The electrical resistance was studied by a four-probe method at a constant current, too, in an helium atmosphere. The phase diagram of the Y-Ho system is fairly simple, and indicates an unrestricted mutual solubility of the components. In alloys rich in yttrium, at temperatures close to melting, a phase transition from the hcp structure to the bcc is noted. The experiment showed that the temperature dependences of the properties studied are monotonous nondecreasing in nature. The transfer of heat is carried out mainly by an electronic mechanism. Collectivated electrons have a multiband energy structure. Within the measurement error, there are no anomalous changes in the properties near the temperatures of the structural transitions. The lattice component of the thermal conductivity is estimated. Concentration dependencies on the whole have the character established in [1], however, additional features were found. In particular, a noticeable difference in properties is recorded only for regions in which the holmium concentration is less than 30%. As a consequence, the Nordheim rule for these alloys is not satisfied. The magnetic contribution to the scattering of carriers is not described in the framework of the available models. This work was supported by the Russian Foundation for Basic Research (grants No. 11-08-00275 and No. 14-08-00228).

-
1. Ivliyev A. D., Kurichenko A. A., Vekshin I. M. //HighTemperature, 2016. V. 54, No. 2, P. 206.
 2. Ivliyev A. D. //HighTemperature, 2009. V. 47, No. 5, P. 737.

THERMODYNAMIC PROPERTIES OF DIATOMIC ARGON COMPOUNDS***Maltsev M.A.,*^{1,2} Morozov I.V.,¹ Osina E.L.¹***¹*JIHT RAS, Moscow, Russia, ²MIPT, Dolgoprudny, Russia***maksim.malcev@phystech.edu*

The diatomic argon compounds are of importance for different plasma sources that contain argon as a basic gas. One of these applications is the mass spectrometry with inductively coupled plasma (ICP-MS). In such experiments the signals from the argon compounds can disturb measured spectra significantly. Therefore for accurate processing of the ICP-MS results it is necessary to obtain the thermodynamic functions of the compounds of argon with other gases (H, O, etc.) and metal ions. It allows to estimate concentrations of the these compounds in the ICP-MS plasma.

In this work we report on thermodynamic properties of the following substances: ArV⁺, ArCo⁺, ArAr, ArAr⁺, ArH and ArH⁺. As a starting point we use DFT and quantum-chemistry data to find an appropriate model for the interatomic interaction potential. Then the rovibronic spectra is obtained via numerical solution of the Schrödinger equation [1] for each electronic state that contribute to the total internal partition function. The thermodynamic properties are calculated from the partition function within the ideal gas approximation using developed program that described in [2]. This method differs from the typical approach based on the use of molecular constants. Thermodynamic functions are prepared for importing into IVTANTHERMO database [3].

-
1. Le Roy R.J. A Computer program for solving the radial Shroedinger equation for bound and quasibound levels // J. Quant. Spectrosc. Radiat. Transfer. 2016. V. 186. P. 167.
 2. Maltsev M.A., Kulikov A.N., Morozov I.V. Thermodynamic properties of vanadium and cobalt argide ions, VAR⁺ and CoAr⁺ // Journal Conference Series. 2016. V. 774. P. 012023
 3. Belov G.V., Dyachkov S.A., Levashov P.R. et al. The IVTANTHERMO-Online database for thermodynamic properties of individual substances with web interface // J. Phys. Conf. Ser. 2018. V. 946 P. 012120.

HEAT OF FUSION OF REFRACTORY HCP METALS FROM FIRST-PRINCIPLE SIMULATIONS AND TROUTON'S RULE***Minakov D. V.,* Levashov P.R.****JIHT RAS, Moscow, Russia***minakovd@ihed.ras.ru*

There is a well-known empirical systematic relation for the enthalpy of vaporization and boiling temperature proposed by F.T. Trouton and known as Trouton's rule. A similar relation is often used for the estimation of enthalpy of fusion of refractory metals in case of lack of accurate consistent experimental data. The closely packed metals with hcp and fcc lattice are generally considered to have a similar entropy of fusion [1, 2]. According to this suggestion an analysis of entropy of fusion of such refractory fcc metals as rhodium, platinum and iridium leads to estimations of enthalpy of fusion for refractory HCP metals rhenium and osmium of around 60.4 and 57.9 kJ/mol correspondingly. These thermal properties are currently provided by some handbooks, including the well-known CRC Handbook of Chemistry and Physics [3]. However, some experiments for rhenium based on the rapid pulse heating technique do not confirm the existing estimation and provide significantly lower values of heat of fusion of about 30 kJ/mol [4]. In this work we present direct calculations of heat of fusion of refractory hcp metals using first-principle method of quantum molecular dynamics. Our calculations do not confirm

high values of heat of fusion of hcp refractory metals, predicted by the linear extrapolation of thermal data for refractory fcc metals, however are in good agreement with measurements by the pulse-heating method.

-
1. H. Sawamura, Trans. Jpn. Inst. Met. 13, 225 (1972).
 2. V.Ya. Chekhovskoi, and S.A. Kats, High Temp.-High Pressures, 13, 611 (1981).
 3. CRC Handbook of Chemistry and Physics, 84th ed., edited by D. R. Lide (CRC Press, Boca Raton, Florida, 2003).
 4. J.W. Arblaster, Calphad, 20, 343 (1996).

INVESTIGATIONS OF LIQUID CARBON AT PRESSURES ABOVE 200 BAR

Bgasheva T. V., Vervikishko P.S., Sheindlin M.A., Valiano G.E.*

JIHT RAS, Moscow, Russia

**miptbusiness@gmail.com*

The properties of liquid carbon, such as density and electrical conductivity at pressures near the triple point, are poorly investigated. Analyzing the literature data [1], [2], it can be concluded that carbon in the liquid phase has dielectric properties, but at high pressures it conduct the current. Investigations of this transition are not presented in the literature. Thus, it is not difficult to come to the conclusion that the study of the liquid carbon properties at pressures from a triple point to several kilobars can be carried out only with the use of laser heating. In this work we use the method of laser heating of graphite in a chamber with a high pressure of He such in [3]. The results of experiments on the melting of carbon using laser heating technice in an at pressures up to 6000 bar are presents in this work. The sample is isotropic graphite of the EC-02 mark. The drops and cross sections of crystallized liquid carbon were analyzed by scanning electron microscopy. Part of the cross sections of the samples with the melt zone was obtained by the ion-cutting method. The fraction of pores in the cross sections through the melt zone was studied, which, assuming rapid solidification of the liquid at a cooling rate of 1 MK / s, gives an estimate for the density of liquid carbon. The dependence of the density of liquid carbon on pressure up to 6 kbar was obtained using this data.

-
1. F. P. Bundy Melting of Graphite at Very High Pressure The Journal of Chemical Physics 38, 618 (1963);
 2. G. R. Gathers, J. W. Shaner, D. A. Young. High temperature carbon equation of state UCBI-51644 September 4, 1974
 3. M.Musella, C.Ronchi, M.Brykin and M.Sheindlin. The molten state of graphite: An experimental study. //J. of Applied Physics, 84, No.5 (1998), p.2530-2537.

MASS-SPECTROMETRIC ANALYSIS OF LASER-INDUCED EVAPORATION OF PYROGRAPHITE UP TO 4400 K

Frolov A.M., Sheindlin M.A.*

JIHT RAS, Moscow, Russia

**matotz@gmail.com*

The investigation of a carbon sublimation at extremely high temperatures is possible only in a quasi-Langmuir evaporation regime. Formerly the vapor composition during the sublimation was investigated in [1] up to 4100 K only for a basal plane of a pyrographite. Taking into account the anisotropic structure of a graphite crystal it was very important to do a comparison study

of evaporation from different planes of graphite. In the present work the results on evaporation both from c and ab- planes of graphite taken as a model of an ideal crystal are presented. For analysis of a vapor composition the time-of-flight mass-spectrometry with laser heating with millisecond pulses was used. The comparison of the evaporation of different molecular components was made using the data on evaporation coefficients [2], measured at temperatures up to 2500 K. It was confirmed that usage of relative evaporation coefficients given in [2] gives adequate results on a vapor composition during graphite evaporation up to 4400 K.

-
1. Pflieger. R., Sheindlin M., Colle J.-Y. Advances in the mass spectrometric study of the laser vaporization of graphite. J. Appl. Phys. 2008. V. 104, P. 054902.
 2. Burns R.P., Jason A.J., Inghram M.G. Evaporation Coefficient of Graphite. J. Chem. Phys. 1964 V. 40. P. 1161

A TECHNIQUE FOR DETERMINING THE ACTIVE COMPONENT OF THE VOLTAGE DROP ACROSS A SAMPLE IN PULSED JOULE HEATING EXPERIMENTS

Kondratyev A.M., Rakhel A.D.*

JIHT RAS, Moscow, Russia

**cpl593h@mail.ru*

Pulsed Joule heating is widely used to study the properties of metals, graphite and some other conductive materials at high temperatures and pressures. The experimental technique that made it possible to obtain unique data on the thermophysical properties of expanded liquid metals and graphite cite Kondr1: 2016 is that a sample in the form of a thin strip is placed between two plates of sapphire (or quartz glass) and heated by an electric current pulse of 10-100 amplitude and rise time on the order of a microsecond. During heating the time dependences of the current flowing through the sample and the voltage drop across it are measured. This allows us to determine the time dependences for the heat dissipated in the sample and its resistance cite Kondr2: 2016. However, an alternating current flowing through the sample induces a significant electromotive force in the high-voltage divider circuit, which is used to measure the voltage drop across the sample. To determine the active component of the voltage drop, that is used to calculate dissipated heat and resistance, it is necessary to subtract this inductive contribution from the total (measured) voltage. In this paper, a method is presented that makes it possible to determine the active component of the voltage with reasonable accuracy. The method is that the voltage across the sample is measured simultaneously with the help of a voltage divider and a calibrated current shunt. The results of such measurements are discussed.

-
1. Kondratyev A. M., Korobenko V. N., and Rakhel A. D. // J. Phys.: Condens. Matter. 2016. V. 28. P. 265501.
 2. Kondratyev A. M., Korobenko V. N., and Rakhel A. D. // Carbon. 2016. V. 100. P. 537.

**HIGH-TEMPERATURE(UP TO 4000 K) INVESTIGATION OF VAPOR
COMPOSITION OF NONSTOICHIOMETRIC ZRC_x AND TAC_x IN THE
VICINITY OF THE HOMOGENEITY DOMAIN**

Petukhov S. V., Frolov A.M., Sheindlin M.A., Falyakhov T.M.*

JIHT RAS, Moscow, Russia

**petuhov.sergey@bk.ru*

Tantalum and zirconium carbides are promising materials for a range of high-temperature applications. However, the present data on evaporation of the materials is related to 60-70th [1, 2]. It was obtained using stationary heating techniques and thus limited at the temperature of 3000 K.

Nowadays there is a capability to analyze the vapor composition above melting point over the surface with a changing composition [3] using laser heating with millisecond pulses combined with time-of-flight mass-spectrometry. Using the method we investigated the vapor composition of zirconium and tantalum carbides with initial composition lying within the homogeneity domain. To measure the emissivity of substances in solid and liquid states the method of polychromatic pyrometry was used. The data on relative vapor pressures of different molecular species in vapor over the surface of liquid tantalum and zirconium carbides was obtained for the first time. It was shown that zirconium carbide vapor at temperatures above 3500 K consists mainly of zirconium and carbon atoms with small quantity of ZrC₂ and Zr₂C. Vapor over specimen with initial ratio of C/Zr>0.8 also contains C₂ and C₃ molecules which may appear due to evaporation of small inclusions of free carbon in carbide. It turned out that at the temperature above 4000 K the ration C/Zr in vapor over the surface tends to the value of about 0.2 irrespective of the initial composition.

The reported study was funded by RFBR according to the research project 18-38-00837.

-
1. Jackson H. F., Lee W. E. Properties and characteristics of ZrC. in Comprehensive nuclear materials. ed. R. J. M. Konings. 2012. Oxford. Elsevier. pp. 339-372.
 2. Deadmore D. L. Vaporization of Tantalum Carbide-Hafnium Carbide solid Solutions Journal of the American Ceramic Society. 1965. p. 357
 3. Pflieger R., Colle J.Y, Iosilevskiy I., Sheindlin M. Urania vapor composition at very high temperatures. J. Appl. Phys. 2011. 109, p. 03351

**THERMODYNAMICS OF THE SUBLIMATION OF LANTHANOID
TRIIODIDES**

Kudin L.S., Motalov V.B., Dunaev A.M.*

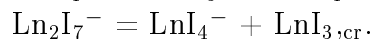
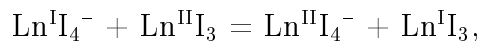
ISUCT, Ivanovo, Russia

**lkudin@yandex.ru*

The sublimation of the lanthanide triiodides LnI₃ (Ln = La, Ce, Pr, Gd, Tb, Tm, Lu) has been studied by high temperature mass spectrometry. The of LnI₃ samples were loaded into the molybdenum effusion cells with the evaporation to effusion area ratio ≥ 400 . A single-focusing magnetic sector mass spectrometer MI1201 was used in this investigation.

The ions LnI_n⁺ (n = 0-3), Ln₂I_n⁺ (n = 3-5), Ln₃I₈⁺ and the doubly charged ions LnI_n⁺⁺ (n = 0-2) were registered in electron ionization mass spectra of saturated vapor over all lanthanide triiodides in the temperature range of 800–1000 K and the energy of ionizing electrons of 40 eV. In thermionic emission mass spectra the I(LnI₃)_n⁻ negative ions with n = 0–4 were observed in the same temperature range. The mass spectra were found to be time-independent thereby indicating the thermal stability of the triiodides in the temperature range studied. Analysis

of the ionization energy curves and the temperature dependences of ion currents allowed us to conclude that the ions with one atom of lanthanide are formed by ionization of monomer molecules and the ions Ln_2I_n^+ and Ln_3I_8^+ are the products of dissociative ionization of dimer and trimer molecules, respectively. The partial vapor pressures of the molecular constituents were determined by the standard mass spectrometric procedure. For individual compounds and systems based on them, the equilibrium constants of the homogeneous and heterogeneous ion-molecular reactions



were measured. Here Ln^{I} and Ln^{II} are two different lanthanides. In the framework of techniques of the second and third laws of thermodynamics, the sublimation enthalpies in the form of monomer and polymer molecules and the enthalpies of ion-molecular reactions were determined. On the basis of the obtained results and the available literature data the formation enthalpies of the observed molecules and ions were calculated.

This work was supported by the Ministry of Education and Science of the Russian Federation (project 4.3232.2017/4.6).

INFLUENCE OF THE RARE EARTH METALS ON THE THERMOPHYSICAL PROPERTIES OF THE THERMOBARRIER COATINGS

Nagmutdinova A.I., Zaycev N.G., Mazilin I.V.*

OOO TSPC, Scherbinka, Russia

**a.nagmutdinova@tspc.ru*

The last few decades have witnessed a fast technical development. In this case metal materials of the cosmo-, avia- and energy apparatus and constructions at the present days have to operate in tough working conditions (hostile environments, high temperatures). Plasma spraying methods for deposition protective, thermobarrier coatings of different nature and properties are used to increase the lifetime of the details and sets. The thermal conductivity coefficient of the rare earth metals (Nd, Gd, La, Sm) zirconate coatings, done by plasma methods, were studied. Also, influence of the coatings thickness and porosity on coefficient of the thermal conductivity has been shown [1–3]. Investigations of the thermophysical properties of the coatings were estimated by use of impulse methods with LFA 457 analyzer. It is shown that specimen with $\text{Gd}_2\text{Zr}_2\text{O}_7$ coating demonstrate the lowest coefficient of the thermal conductivity at the temperature of 900C (0,86 W/m*K). And the specimen with lanthanum zirconia revealed the highest coefficient of the thermal conductivity. Also, it need to be noticed that correlation of the thermal conductivity coefficient depending on thickness and porosity is typical for coatings. The differences of this thermophysical parameter for Nd, Gd, La, Sm zirconate has been established. The influence of the coatings porosity and thickness on changes of thermal conductivity coefficient has been shown.

-
1. *MH Habibi* Hot corrosion behaviour of new candidates for thermal barrier coatings application in turbine simulated environments, 2014.
 2. *T.P. Chernyaeva and others* Metallophysics studies of the promising zirconia alloys. Questions of the atomic science and techniques (in Russian), 2000.
 3. *V.G. Zavodinsky* Investigation of the phase stability mechanism of the dioxide zirconium doped with magnesium and calcium. Perspective materials, I. 2, 2005.

OBSERVATION OF GRAPHITE MELTING DURING LASER HEATING IN VACUUM

Vasin A.A., Frolov A.M., Sheindlin M.A.*

JIHT RAS, Moscow, Russia

**av65536@gmail.com*

Experimental results on graphite melting are still very discrepant. For example, the heating using direct current transmission to study graphite melting near the triple point turned out to be impossible due to the low electroconductivity of liquid carbon. Laser melting [1] of the graphite at high pressure allowed to define the parameters of the carbon triple point: pressure of about 110 bar, temperature - 4800 K. In the present work it is reported that the formation of liquid carbon was observed for the first time on the surface of pyrographite heated in vacuum with a laser beam with the power up to 10^6 W/cm². Heating of the sample surface was performed applying the laser pulses of millisecond duration with increasing speed of power ascending, and that made it possible to reach the melting conditions, despite vacuum maintained in the chamber. The surface temperature was measured using a brightness pyrometer at the wavelength of 900 nm. The beginning of melting was registered through abrupt increasing of laser irradiation reflection from the samples surface. The measured melting temperature was about 4650 ± 50 K.

-
1. Musella M., Ronchi C., Brykin M., Sheindlin M. The molten state of graphite: an experimental study. *J. Appl. Phys.* 1998. 84. p. 2530

MELTING OF ANISOTROPIC GRAPHITE WITH VOLUME LIMITATION

*Konyukhov S.A.,*¹ Onufriev S.V.,² Savvatimskiy A.I.²*

¹MEPhI, Moscow, Russia, ²JIHT RAS, Moscow, Russia

**arcticdeer@yandex.ru*

At the moment, graphite is considered to be the most refractory material. But there are certain limitations on the study of its thermophysical properties near the melting point. In particular, graphite melts at a pressure above 120 atmospheres [1], so it is not possible to observe the liquid phase when graphite is heated under atmospheric conditions. To study the phase diagram at high temperatures, unsteady methods are used, such as pulsed laser or electric current heating. Pulsed heating by current makes it possible to create an overpressure during the experiment itself due to the limitation of the volume around the samples [2].

For the samples, a high-density graphite grade UPV-1T (analog HOPG) was used. Based on the results of the experiments, the values of the input energy of the beginning and the end of melting were recorded: the beginning of melting ($E = 11.5$ kJ/g), the end ($E = 21$ kJ/g). The electrical resistivity of liquid carbon is close to a constant value when its expansion is limited.

In the solid phase, before melting, the heat capacity (under conditions close to C_p) is 2 J/gK and steeply increases (by a factor of 2 J/gK) even before the melting begins. In the liquid phase (above the melting point), the specific heat decreases to 2 J/gK. The sharp increase in the heat capacity to the melting point and the sharp decrease after melting can be explained by the appearance of Frenkel's nonequilibrium pair defects in the solid phase-to ensure loss of long-range order and melting. In the liquid phase, these defects annihilate at almost the same rate (the characteristic time is 1 microsecond).

-
1. N.A. Gokcen, E.T. Chang, T.M. Poston, D.I. Spencer, Determination of graphite-liquid-vapour triple point by laser heating, *High Temp. Sci.* 8 (1976) 81

2. Savvatimskiy A I 2013 and 2014 (second edition) Graphite melting and liquid carbon properties Publishing house Fizmatkniga Moscow (in Russian)

PROPERTIES OF CARBIDES IN SOLID AND LIQUID CONDITION (2000 TO 6000 K)

*Seredkin N.N.,^{*1} Onufriev S. V.,² Savvatimskiy A.I.,² Muboyadzhyan S.A.,³ Evdokimov S.A.³*

¹MEPhI, Moscow, Russia, ²JIHT RAS, Moscow, Russia, ³VIAM, Moscow, Russia

*nikser12@yandex.ru

The purpose of this work is to experimentally study the properties of refractory carbides in the melting range and liquid phase. First of all, this refers to the electrical resistivity, as well as to the thermal properties (enthalpy, heat capacity, introduced energy). The most refractory materials needed for aviation and space technology are carbon compounds with metals. However, graphite melts only at pressures above 120 atmospheres [1], and it does not have high impact strength, like refractory metals.

The results of the study of the properties of refractory carbides over the widest temperature range are also important for nuclear power engineering, since nuclear fuel in the form of spherical micro-fuel elements is covered with protective layers of carbides and graphite.

By the method of pulsed current heating (3-5 us), samples of zirconium carbide (with a high content of carbon) were investigated [2]. The temperature was measured on samples in the form of a wedge-shaped model of a black body. The heat capacity, electrical resistivity (referred to the original dimensions) and Joule heating energy were obtained depending on the measured temperature. The onset of the phase transition (solidus) for ZrC + C was fixed at 3150 K, the termination of the phase transition (liquidus) at 3640 K. The properties obtained supplement the picture of the behavior of the substances shown in the phase diagrams.

-
1. N.A. Gokcen, E.T. Chang, T.M.Poston, D.I. Spencer, Determination of graphite-liquid-vapour triple point by laser heating, High Temp. Sci. 8, 1976, 81
 2. A.Kondratyev, S.Muboyajan, S.Onufriev, A.Savvatimskiy, Journal of Alloys and Compounds 631, 2015, 52-59

STRUCTURE AND PROPERTIES OF YBCO BEFORE AND AFTER SHORT-TERM EXPOSURE TO THE PLASMA FLOW

*Rabadanova A.E.,^{*1} Gadzhimagomedov S.Kh.,¹ Palchaev D.K.,¹ Ragimkhanov G.B.,¹ Isakaev E.Kh.,² Gadzhiev M.Kh.,² Demirov N.A.²*

¹DSU, Makhachkala, Russia, ²JIHT RAS, Moscow, Russia

*rabadanova.aida@mail.ru

The structure and properties of a ceramic high-temperature superconductor based on a complex YBa₂Cu₃O₇ oxide before and after a short-term exposure to a highly enthalpy flow of argon plasma are studied. These studies are aimed at optimizing the parameters ensuring the surface hardening of products made of highly porous nanostructured ceramics. They are part of research aimed at solving the problem of obtaining high-temperature superconductors with a gradient structure and properties. In the future, the possibility of forming a textured layer with high critical current values will be solved.

Samples of nanostructured ceramics based on YBa₂Cu₃O₇ were prepared by sintering at 1193 K for 1 hour of a nanopowder obtained by chemical technology. This technology provides

a high proportion of the superconducting phase with an oxygen index of 6.9 in one sintering step. However, despite the possibility of obtaining superconducting samples with densities from 2.5 g/cm³ to 6 g/cm³ by this method, they are characterized by low strength, since the contacts between the grains, which are agglomerates of nanoparticles, prove to be fragile. Approbation of hardening of the surface by a plasma flow led to positive results without significant changes in the initial structure and properties of this ceramics associated with oxygen stoichiometry and the recrystallization of nanoparticles. The established optimal processing parameters under the action of a high-enthalpy oxygen plasma flow allow to preserve oxygen stoichiometry, but just as after the action of the argon plasma flow, the ordered distribution of oxygen at the positions that provide the metallic conductivity path is violated.

The work was supported by the RFBR grant No. 18-08-00092a and the state assignments No. 3.5982.2017/8.9.

INFLUENCE OF QUENCHING ON ULTRASOUND SPEED IN STEELS

Roshchupkin V.V., Lyakhovitskii M.M., Pokrasin M.A., Minina N.A.,
Kudryavtsev E.M.*

IMET RAS, Moscow, Russia

**pokrasin@gmail.com*

The results of an experimental study of the ultrasound speed and the relative temperature expansion of 09G2S, 30HGSA, U8 and 45 steel in quenched and annealed states over a wide temperature range are presented. The chemical composition, application and conditions for heat treatment of steels are given in the database of steels. A characteristic feature of these steels is the presence of alpha-gamma transformation at high temperatures. An experimental study of the ultrasonic velocity was carried out according to the method developed by the GSSSD ME 216-2014. The obtained experimental data on the relative temperature expansion made it possible not only to increase the accuracy of the experimental data on the ultrasound velocity, the calculation formulas of which include the length of the sample, but also to calculate the temperature dependence of the density of steels. Wherein, the density at room temperature was determined with high accuracy by the hydrostatic weighing method. In addition, data on the ultrasound velocity and density make it possible to calculate the values of Young's modulus. Experimental data showed that the ultrasonic velocity in the quenched sample is much less than in the annealed sample. However, in the region of the phase transition, their values practically coincide, which indicates the annealing of the sample. Experimental and calculated values of the properties of steels in the temperature range from room temperature to the start of the phase transformation were processed by the least squares method, which allowed obtaining approximating equations in the indicated temperature range.

THE EFFECT OF THE MECHANICAL ACTIVATION ON THERMOPHYSICAL PROPERTIES OF POWDERED METALS

Popov D.A., Lebedev A.V., Ryazantseva A.A., Malkin A.I.*

IPCE RAS, Moscow, Russia

**alex.lebedev@rambler.ru*

We performed parallel measurements of specific heat and microstructure of a number of powdered metals after the mechanical activation in a high intensity planetary mill. X-ray diffraction and differential scanning calorimetry allowed us to establish that the microstructure and physicochemical properties of brittle and ductile metals change differently. The brittle

metals, exhibiting a size reduction of particles during the mechanical activation, in particular tungsten, demonstrate changes in the microstructure leading to a reduction of the crystal lattice parameters and emergence of additional internal compression strains. The specific heat of such metals increases during the entire period of the mechanical activation process. Temperature dependence of the specific heat changes at the same time. In the ductile metals, exhibiting an aggregation of particles during the mechanical activation, the change in the microstructure leads to an increase in the lattice parameters and emergence of internal tensile strains. The specific heat in this case decreases after the mechanical activation during 5 to 21 minutes.

EFFECT OF TEMPERATURE ON THE THERMAL DIFFUSIVITY AND HEAT CAPACITY OF SANDSTONE

*Abdulagatova Z.Z.,^{*1,2} Abdulagatov I.M.,^{1,2} Kallaev S.N.,² Omarov Z.M.,² Bakmaev A.G.²*

¹DGU, Makhachkala, Russia, ²IP DSC RAS, Makhachkala, Russia

**abdulagatova@yandex.ru*

The well-known contact-free, laser Flash method was used for measurement of the thermal diffusivity (a) of natural sandstone samples. The experimental procedure was conducted using the micro Flash apparatus (*LFA457*). The measurements have been made over the temperature range from (302.9 to 774.3)K. The isobaric heat capacities (CP) of the same sample were measured over the temperature range from (308 to 763)K using *DSC 204 F1*. Uncertainties of the thermal diffusivity and heat capacity measurements are 3% and 1%, respectively. Measured values of a and CP together with density data were used to calculate the thermal conductivity of sandstone. Theoretically based correlations for the thermal diffusivity (damped harmonic oscillator, DHO) and heat capacity (Debye and Einstein) theories were adopted to accurately represent the measured data. Correlation equations for the thermal diffusivity and heat capacity have been developed using the well-known theoretical asymptotic behavior of a and $CP(T)$ for various temperature ranges (low- and high-temperature limits). The microscopic nature of the effect of temperature on $a(T)$ and $\lambda(T)$ behavior of sandstone is discussed. Detailed interpretation and testing of the measured property data for sandstone using various existing theoretical and empirical models, in order to check their accuracy, predictive capability, and applicability, were provided.

EXPERIMENTAL DETERMINATION OF DESTRUCTION OF THERMALLY UNSTABLE SUBSTANCES

Dzhapparov T.A-G., Bazaev A.R.*

IGR DSC RAS, Makhachkala, Russia

**timur507@mail.ru*

In this work the technique of experimental determination of decomposition point of thermally unstable substances is offered. The available data on the thermal stability of aliphatic alcohols and their aqueous mixtures is contradictory [1–4]. By identification of increase of vapor pressure of the system in the constant volume piezometer during long-term time (about 48 hours) the decomposition points of the pure alcohols (methanol, ethanol, 1-propanol and 1-butanol) and of the alcohols dissolved in water are determined [5]. The dependence of decomposition point of the molecules of pure alcohols on the number of carbon atoms and of dissolved in water alcohols on their structure and concentration is determined. The rate of thermal decomposition of alcohol molecules depending on the temperature, carbon atoms, and

concentration is estimated. The effect of thermal destruction of alcohol molecules on changes of thermal coefficients (isothermal compressibility factor K_T , coefficient of volumetric expansion α thermal coefficient of pressure β), and main thermodynamic properties (C_v , C_p , H , S , U , F , G) of water+alcohol mixtures is examined.

1. Barnard J. A. and Hughes H. W. D. Trans. Faraday Soc. 1960. N56. P. 55-63.
2. Straty G.C. and others. J. Int. Journal of Thermophysics. 1986. N5. P.1077-1089.
3. Bazaev. E.A., Bazaev A.R., Abdurashidova A.A. High Pressure. 2007. V 47. N2. P. 215-227.
4. Kalafati D.D., Rasskazov D.S., Petrov E.K. Teploenergetika. 1967. V.14. P. 77-81.
5. Dzhapparov T.A., Bazaev A.R. Teplofizika i aeromekhanika. 2012. V.19. N6. P. 793-798.

DENSITY AND SURFACE TENSION OF ALLOY URANIUM–CHROMIUM IN LIQUID PHASE

Kachalov V. V.

JIHT RAS, Moscow, Russia

ongk@mail.ru

Method of maximum pressure in gas bubble in two-capillary modification are measured density and surface tension of liquid alloy 94.2% mas. uranium–5,8% mas. chromium in the interval of temperatures $T_{\text{melt.}}-1900$ K. As method of research method of maximum pressure in gas bubble is chosen. To advantages of method well developed theory, constant updating of the surface of formed bubble during experiment relates, from given one experiment density and surface tension of under study corium receive. However at traditional execution of this method with one capillary tube a series of methodical difficulties arises. First, accuracy of measurement of surface tension is limited of accuracy of registration of the capillary tube immersing depth to corium. Secondly, it is necessary to correct for curvature of the meniscus in the crucible which is defined by boundary angle of coating with the crucible material corium and surface tension of under study substance which can change during experiment In given work two-capillary outline of method of maximum pressure in gas bubble for the first time offered in [1] is realised. Application of two capillary tubes of various diameters immersed to corium, eliminates necessity of the account of curvature of the meniscus in the crucible, and immersing depth enters amendment, size of which is small as compared with measured sizes.

At research of density of high-temperature and chemically active substances because of complexity of filling pyknometer and difficulties connected with the control of the level of corium in dilatometer, method of maximum pressure in gas bubble becomes to competitive that two the most common methods of density research.

Experimental installation and the technique of execution of measurements are described. Confidential error of received data is appreciated. Experimental data of density and surface tension of alloy uranium–chromium are received for the first time. In investigated temperatures interval properties of corium decrease linear with growth of temperature:

$$\rho \cdot 10^3 = 19.11 - 2.2215T,$$

$$\sigma = 2548.8 - 0.5960T,$$

where ρ –density in kg/m^3 , σ –surface tension in mN/m , T –temperature in K.

Confidential error measuring ρ and σ are appreciated equal $\pm 28 \text{ kg/m}^3$ and $\pm 52 \text{ mN/m}$.

Reliability of experimental data received on given technique on this experimental installation, is recognised in modern reviews and reference books by results of research of density and surface tension of uranium up to temperatures 2100 K [2, 3].

It is shown that within the limits of accuracy of experimental data of density of uranium and chromium molar volume of alloy uranium-chromium is described by the equation of the type additivity

$$\nu_{\text{alloy}} = \nu_1\chi + \nu_2(1 - \chi),$$

ν_{alloy} , ν_1 , ν_2 – molar volumes of alloy and his components, χ – molar concentration of the component.

1. Sudgen, S. J. J. Chem. Soc. 1922. V. 121. P. 858
2. Fokin, L.R., Liquid Uranium, Density Isobar of 1406-4500 K, Sbornik dokladov mezhvedomstvennogo seminara TF-2007 (Collection of Papers to TF-2007 Inter-departmental Seminar), Obninsk: State Scientific Center of the Russian Federation-Leipunskii Institute of Energy Physics, 2008, p. 400.
3. Thermal properties of materials of nuclear equipment / under red. P.L. Kirillov, M.: 2007.

DENSITY AND MAGNETIC SUSCEPTIBILITY OF CoFeSiBNb ALLOY

Rusanov B.A., Sidorov V.E., Mikhailov V.A., Popel P.S.*

USPU, Ekaterinburg, Russia

**rusfive@mail.ru*

Present paper has results of the density and magnetic susceptibility of the $Co_{48}Fe_{25}B_{19}Si_4Nb_4$ alloy. Compared with other compounds, this alloy shows a high ability to form bulk metallic glasses.

Alloy $Co_{48}Fe_{25}B_{19}Si_4Nb_4$ is melted from initial components in the Leybold-Heraeus IS01/III induction furnace. Rods with a diameter of 2 mm were obtained by suction casting into a copper water-cooled ingot.

The kinetics of crystallization of the alloy was studied using a differential scanning calorimeter NETZSCH at heating rates of 5, 10, 20 and 40°C/min. Density was measured by the absolute method of penetrating gamma radiation in the temperature range from 20 to 1550°C. The magnetic susceptibility was investigated by the relative version of the Faraday method in the temperature range from 800 to 1500°C. The experiments were carried out in an atmosphere of pure helium at a heating rate of 3°C/min. Used crucibles of beryllium oxide.

The temperature dependence of density of composition in the liquid state is close to linear. With a decrease in its temperature from the maximum, its precrystallization supercooling by almost 100°C was noted. The cooling curve in the solid state down to room temperature lies substantially above the heating curve.

There are two transformation points on the temperature dependences of the magnetic susceptibility. The first of these is not observed on the temperature dependences of the density and in calorimetric experiments and corresponds, apparently, to the polymorphic transformation, the second corresponds to the melting of the sample. In the liquid state, the temperature dependences of the magnetic susceptibility can be approximated by the generalized Curie-Weiss law. Based on the results obtained, the effective magnetic moment, the density of states at the Fermi level, and the paramagnetic Curie temperature are calculated.

The reported study was funded by RFBR according to the research project 18-03-00433.

**THERMAL DIFFUSIVITY OF THE NI-V SYSTEM WITH VANADIUM
CONTENT UP TO 22 at.% AT HIGH TEMPERATURES**

Akhtyamov E.R.,¹ ***Polev V.F.***,² ***Korshunov I.G.***,² ***Kurichenko A.A.***,²
Gorbatov V.I.*^{2,3}

¹*UralNIIstrom, Chelyabinsk, Russia,* ²*URSMU, Ekaterinburg, Russia,* ³*ITP UB RAS,
Ekaterinburg, Russia*

**gorbatov@ursmu.ru*

This study is a continuation of the work [1], in which it was noted that when dissolving from 8 to 17 at.% vanadium in pure nickel, the thermal diffusivity polytherms undergo a small jump, blurred in the temperature range 1050–1170 K. In the phase diagram, this range of temperatures and concentrations corresponds to the region of the solid solution that on the right borders the region of the two-phase state (Ni)+Ni₃V, and below 680 K — with the ordering region Ni₈V. The studies performed in [2] on samples with a content of 16–19 at.% V showed that when quenched from high temperatures, a modulated structure is formed in them, which upon subsequent annealing below 1080 K leads to the formation of two-phase state (Ni)+Ni₃V.

In this paper we report the results of measurements of the temperature dependences of the thermal diffusivity, the resistivity, and the thermoelectric power of Ni-V alloys with a vanadium content of 7 to 22 at.% at high temperatures in the thermal cycling regime with an average heating-cooling rate of 0.06 K/c.

It is established that in the temperature range from 1050 to 1170 K the phonon component of thermal conductivity (in contrast to the electronic component) undergoes a jump, the magnitude of which increases with increasing vanadium concentration in alloys. In this case, the polytherms of the resistivity undergo a break near ~900 K, and the angle of the kink decreases with increasing vanadium concentration. Proceeding from this, it is assumed that the observed anomalies of the polytherm of thermal diffusivity of Ni-V alloys with a vanadium concentration lower than 16 at.% are associated with the formation of modulated structures of the dissolved component in these alloys.

-
1. Polev V.F., Startseva M.I., Gorbatov V.I., Glagoleva Yu.V., Korshunov I.G. // *The Physics of Metals and Metallography*. 2012. V. 113. No. 1. P. 39.
 2. Moreen H.A., Taggart R., Polonis D.H. // *Metallurgical Transactions*. 1974. V. 5. P. 79

ON PHASE TRANSITIONS IN DIFFERENT METALS

Rososhek A.,^{*1} Efimov S.,¹ Tewari S.,¹ Yanuka D.,² Krasik Ya.E.¹

¹*Technion, Haifa, Israel, ²Imperial College, London, United Kingdom (Great Britain)*

**sasharos@campus.technion.ac.il*

Results of underwater electrical explosion of single wires made from Cu, Al, T, Mo and Ta are presented and analyzed. Experimental research was carried out using microsecond timescale generators having 33/180 kA, 33/45 kV and 1200 ns of current amplitude, resistive voltage and rise-time respectively. The discharge current was measured by a current viewing resistor or Rogowski coil and the resistive voltage was calculated from the measured voltage by a voltage divider accounting for inductive voltage. These data coupled with data from Optronis Optoscope SC-10 streak camera and 1D MHD simulation was used to study the phase transitions in different metals at extreme conditions, i.e. the moment when a transition occurs, life-time of a phase and energy density in the wire at the moment of transition.

ABLATION OF TITANIUM BY FEMTOSECOND LASER PULSES

Struleva E. V.,* Komarov P.S.

JIHT RAS, Moscow, Russia

**struleva.evgenia@yandex.ru*

Rapid heating of metals by femtosecond laser pulses (FLI) and subsequent nonequilibrium bulk melting of the surface layer at picosecond times is accompanied by the development of cavitation processes, the growth of bubbles in the vapor phase in the melt in the rarefaction wave, and the ablation of its part in the form of a thin spall layer in the condensed state [1].

In the present work, an experimental study was made of laser ablation of titanium by heating with powerful FLI with an intensity $10^{12} \div 10^{13}$ W/cm².

Using the "pump-probe" microscopy, the threshold of thermomechanical ablation of titanium by the absorbed energy was measured. For this, the value of the reflection coefficient near the ablation threshold was determined. Using the interference microscopy method, the crater depth was estimated for various excess energy densities above the threshold value. Studies were made of the shape of ablation craters and the relief of the nanostructured surface of titanium samples in the region of laser action by atomic force microscopy. The dependence of the depth of the crater on the energy density of the heating pulse was obtained.

1. Anisimov S.I., Luk'yanchuk B.S. // Phys.-Usp. 2002. V. 45. No. 3. P. 293.

MICROWAVE DOPPLER DIAGNOSTICS OF SHOCK-COMPRESSED ARGON PLASMA

Bogdanov E.N., Zhernokletov M.V., Kozlov G.A., Medvedev A.B., Rodionov A.V.*

FSUE RFNC - VNIIEF, Sarov, Russia

**postmaster@ifv.vniief.ru*

Using the method of microwave diagnostics [1] based on radiointerferometers with wavelengths of 3.2 and 2.1 mm, the kinematic and electrophysical characteristics of plasma of shock-compressed argon initially located at atmospheric pressure were studied. The study was carried out in the pressure range from 12 MPa to 62 MPa and shock wave velocities from 3.1 km/s to 6.6 km/s. The obtained data on the kinematic parameters agree with the known data and the calculation from the modified Van der Waals model [2]. An array of reflection coefficients of electromagnetic radiation was obtained at the wavelengths of 3.2 and 2.1 mm from a shock wave front on whose basis the electron conduction and the electron density in the shock wave front were estimated. The experimental data are consistent with the calculation of the modified Van der Waals model in the velocity range $D=3.1-3.6$ km/s. With the further enhancement of velocity a phenomenon of constancy of a reflection coefficient was observed.

1. Microwave diagnostics. Chapter 5 in the book Nonperturbative diagnostic techniques of fast processes/Edited by Doctor of Technical Sciences A. L. Mikhaylov.-Sarov: FSUE RFNC-VNIIEF, 2015.-p.322.
2. Medvedev A.V. Equation of state and coefficients of argon transfer on the basis of the modified Van der Waals model up to pressures of 100 GPa // FGV, 2010, v. 46, 4, p. 116-126.

THERMOPHYSICAL PROPERTIES OF THE LOW-TEMPERATURE PLASMA OF METALS

Apfelbaum E.M.

JIHT RAS, Moscow, Russia

apfel_e@mail.ru

Various thermophysical properties of substances are studied for more than a century. Here we will consider the equations of state and the electronic transport coefficients - electrical conductivity, thermal conductivity and thermal power. However, their investigations for different metals at high temperatures ($T \geq T_0$, $T_0 \approx 5$ kK) have evident hinders. At first, these high-temperature states are difficult to obtain in measurements. At second, the reliable theories exist whether at very low densities (almost ideal gas or ideal plasma at T increase), or at the liquid metal near the melting curves. In the other area the theories and calculations exist as well, but they are not so reliable and give rise to ambiguous results. However, during recent two dozen years new measurements have appeared for the plasma of metals [1, 2]. In this experiments the properties under study were obtained in wide range of parameters. These data allows one to check and to make more precise the existing techniques of calculations.

Previously we have developed a model for calculations of the considered properties in the region of low-temperature plasma of metals (see [3] and references therein). It is applicable to the region of the temperatures $T=10-100$ kK and the densities lower than the critical one. It is based on the chemical approach, which considers a substance as a mixture of electrons, positive ions, atoms etc. Within this approach it is possible to find not only the thermodynamical functions but the concentrations of the components as well, i. e. the chemical composition. Further the composition is used to calculate the electronic transport coefficients within the relaxation time approximation. Presently we present the results of calculations by means of the

above model for a number of metals, for instance, Ni, Fe and Mo. Our results were compared with the data of calculations and measurements of other researchers. The comparison have shown good agreement.

-
1. DaSilva A.W., Vunni G.B. // *Phys. Rev.* 2011. V. 83. No. 3. 037402.
 2. Clerouin J. et. al. // *Phys. Plasmas* 2012. V. 19. No. 8. 082702.
 3. Apfelbaum E. M. // *High Temp.* 2017. V. 55. No. 1. P. 1.

THERMOPHYSICAL PROPERTIES OF DENSE LEAD PLASMA

Korobenko V.N.,* Rakhel A.D.

JIHT RAS, Moscow, Russia

**vkorobenko@gmail.com*

Study of thermophysical properties of non-ideal plasmas is a rather complex experimental task. For such plasma the ionization degree should be of the order of unity and the potential energy of interactions between the ions is comparable with the kinetic energy of their thermal motion. To create such plasma, it is possible to compress a gas by means of a strong shock wave. On the other hand, the plasma can be created by heating of a metal sample by an electric current pulse so that it expands homogeneously to the plasma state [1]. Due to the remoteness of the plasma state from the initial state of the sample on the phase diagram, the problem of maintaining the homogeneity of the sample becomes particularly complex. In the present work the experimental technique [1] is used to study the thermophysical properties of dense plasma of lead. A lead sample in the form of a foil strip with the thickness of 10 - 30 micrometers was sandwiched between two sapphire plates (or silica glass plates). Thermodynamic functions and electrical resistivity of lead plasma have been measured in the density range from 0.36 to 0.04 of the normal solid density. For this plasma we have determined the dependencies of electrical resistivity, the Gruneisen coefficient, and the speed of sound on density and specific enthalpy. Thermal expansion of the sample was measured by the Michelson interferometer. This interferometer allowed us to reduce the multi-beam interference and thus to improve the accuracy of the measurements of density compared to the results obtained by means of the interferometer [2].

-
1. Kondratyev A. M., Korobenko V. N., and Rakhel A. D. // *J. Phys.: Condens. Matter.* 2016. V. 28. P. 265501.
 2. Kondratyev A. M., Korobenko V. N., and Rakhel A. D. // *Carbon.* 2016. V. 100. P. 537.

THERMOPHYSICAL PROPERTIES OF DENSE MOLECULAR GASES IN QUASICHEMICAL REPRESENTATION

Gryaznov V.K.,*¹ Iosilevskiy I.L.^{2,3}

¹IPCP RAS, Chernogolovka, Russia, ²JIHT RAS, Moscow, Russia, ³MIPT, Dolgoprudny, Russia

**grvk@fcp.ac.ru*

The interest in the study of the thermodynamic properties of molecular gases at high pressures and temperatures is associated both with their wide distribution in nature and with wide use in various high-energy devices. At pressures of the megabar range, where a high density of matter is accompanied by a strong Coulomb interaction (strongly coupled

plasma), the thermophysical properties of gases were theoretically described both in frames of a quasi-chemical approach (free energy model) and by first principles methods using direct numerical simulation of a system of nuclei and electrons. Despite the progress achieved in both experimental and theoretical investigations, further study of the properties of dense gases in these range of parameters is of great importance. The currently available experimental data on the caloric and thermal equation of state overlap the pressure range from kilobars to tens of megabars and high densities. Recently, theoretical results have been obtained, both in frames of the quasi-chemical approach (the chemical model of plasma), and using first-principle methods in a wide range of parameters. This work presents the results of the calculation of hydrogen isochores in a wide range of temperatures, the shock adiabat of deuterium and nitrogen, and deuterium isentropes up to megabar pressures. The results were obtained using codes that implement advanced models of the SAHA family. Calculations have shown that in the considered range of dynamic pressures, compressed molecular gases represent a strongly coupled partially degenerate plasma with densities close to the density of condensed matter. The results of the calculations are presented in comparison with experimental data and the data obtained by the first principle modeling. It is shown that the presented approach allows to obtain an adequate description of the thermophysical properties of molecular gases in a wide range of temperatures and pressures, providing satisfactory agreement with both experiment and other theoretical approaches.

ELECTRICAL CONDUCTIVITY OF POLYTETRAFLUOROETHYLENE IN THE MEGABAR RANGE OF QUASI-ISENTROPIC COMPRESSION

Golyshev A.A.,^{*1} *Sobolev D.V.*,² *Molodets A.M.*¹

¹*ICP RAS, Chernogolovka, Russia,* ²*MSU, Moscow, Russia*

**golyshev@icp.ac.ru*

Polytetrafluoroethylene (PTFE, DuPont Teflon) is one of the widely used as insulator due to its unique properties such as chemical resistance and robustness against decomposition, high dielectric strength, and others (see [1, 2] and references herein). Therefore, PTFE is used as an insulator not only under ordinary conditions, but also when measuring the electrical resistivity of materials under dynamic loading conditions. As is known, the electrical resistance of most materials under extreme conditions of high pressures of shock compression can decrease. PTFE in this case is not an exception, its electrical resistance decreases with pressure. Accordingly, measurements of the electrical conductivity of PTFE under shock compression were carried out (see [1–3]).

In practice, measuring the electrical resistivity of shock-compressed materials often require measurements in the phase diagram range with reduced temperatures (see, for example, [4]). In this connection measurements of the electrical resistivity of PTFE in the region of the high (megabar) pressure-low temperature (due to a decrease to cryogenic initial temperatures) were carried out and presented in the report.

In the experiments carried out to measure the electrical conductivity of PTFE under the above conditions the high-conductivity state of PTFE was registered. It is shown that the least electrical resistivity of PTFE is recorded at a pressure of ~ 80 -100 GPa. The effect of an abrupt decrease in the electrical resistivity of a shocked PTFE is reversible: in release wave at a pressure of 80 GPa, the electrical resistance of PTFE returns to practically the initial value.

-
1. Tarzhanov V.I., Zhugin Yu.N., Krupnikov K.K. // JAMT. 1997. V.38. No.6. pp.826-832.
 2. Bordzilovskii S.A., Karakhanov C.M. // CESW. 2002. V.38. No.6. pp.722-727.
 3. Golyshev A.A., Molodets A.M., // CESW. 2013. V.49. No.2. pp.219-224.

4. Ananin A.V., Dremin A.N., Kanel G.I. // CESW. 1981. V.17. No.3. pp.320-326.

DYNAMICAL CONDUCTIVITY OF THE NONIDEAL PLASMA ON THE BASIS OF THE EFFECTIVE POTENTIAL

*Shalenov E.O.,*¹ Dzhumagulova K.N.,¹ Ramazanov T.S.,¹ Röpke G.,² Reinholz H.²*

¹*IETP, al-Farabi KazNU, Almaty, Kazakhstan,* ²*University of Rostock, Rostock, Germany*

**shalenov.erik@mail.ru*

During the last few years many papers about the transport properties of dense plasmas have been published. The electrical conductivity in fully ionized hydrogen plasma is well investigated [1–3]. The dynamical conductivity and dynamical collision frequency of dense semiclassical hydrogen plasmas on the basis of the effective interaction potential [4] (taking into account screening and diffraction effects) are presented. Semiclassical method has been used for the calculation of the collision frequency. Using generalized Drude formula, the dynamical conductivity has been investigated. The influence of electron-electron interactions was taken into account at the level of collision frequency via renormalization factor. The results of the dynamical conductivity show good agreement with the data of other authors, notably with the molecular-dynamics (MD) simulation, which also includes electron-electron interactions.

-
1. Nurekenov Kh. T., Baimbetov F. B., Redmer R., Röpke G. // Contrib. Plasma Phys. 1997. V.37. P. 473.
 2. Reinholz H., Röpke G., Rosmej S., and Redmer R. // Phys. Rev. E 2015. V.91. P.043105.
 3. Arkhipov Yu. V., Baimbetov F. B., Davletov A. E., Starikov. K. V. // J. Plasma Physics 2002. V.68. P. 81.
 4. Shalenov E. O., Rosmej S., Reinholz H., Röpke G., Dzhumagulova K. N., Ramazanov T. S. // Contrib. Plasma Phys. 2017. V. 57. P. 486.

EXPERIMENTAL OBSERVATION OF DECREASE IN PROBABILITY OF ATOMIC HIGHLY EXCITED STATE REALIZATION IN HELIUM ARC PLASMA AT ATMOSPHERIC PRESSURE

*Kavyrshin D.I.,*² Kutuzov D.S.,¹ Chinnov V.F.²*

¹*RRC KI, Moscow, Russia,* ²*JIHT RAS, Moscow, Russia*

**dimakav@rambler.ru*

This work is dedicated to experimental study of distributions of helium atom excited states with energies close to ionization threshold. By utilizing a spectrometer with absolute intensity calibration we were able to obtain concentrations of radiating particles from the intensities of observed HeI spectral lines, and we found that helium arc plasma at atmospheric pressure was substantially deviated from the ionization equilibrium state. The distribution of excited state populations with the principal quantum number $n > 4$ decreases at a rate increasing as their energy reaches ionization threshold. Thus, spectral lines corresponding to transitions from $n \geq 7$ were not observed in the spectra. Thus, in turn, we were able to experimentally confirm the phenomenon theoretically predicted by a large number of works of highly excited state realization probability decrease in helium arc plasma at atmospheric pressure [1] and presence of ionization-type nonequilibrium distributions of excited states [2]. Although the obtained distribution cannot be described by Boltzmann law with electron temperature, we have been able to determine electron temperature and concentration in plasma. Electron concentration was found by analyzing widening of spectral lines contours due to Stark effect, its value being

$n_e = 9 \cdot 10^{16} \text{ cm}^{-3}$, which is about 20% lower than its value for equilibrium state. The presence of HeII lines in the observed spectra allowed us to determine electron temperature T_e using our knowledge of electron concentration n_e and the relation between atomic and ion spectral line intensities. Its value was found to be $T_e = 3 \text{ eV}$, the difference between values found from relations between different line pairs was less than 10%. The reported study was funded by RFBR according to the research project No. 18-32-00292.

-
1. G.K. Kobzev, Yu.K. Kurilenkov, G.E. Norman // TVT. Vol.15. Issue 1. pp. 193-196. 1977
 2. Jonkers J., Vos H.P.C., van der Mullen J.A.M., Timmermans E.A.H.// Spectrochimica Acta B. 1996. V. 51 No. 5. P. 457.

TRANSPORT PROPERTIES OF HOT DENSE PLASMA

*Kodanova S.K, Ramazanov T.S., Issanova M.K.**

KazNU, Almaty, Kazakhstan

**issanova@physics.kz*

Investigation of transport properties in dense plasmas is one of the key issues in the physics of inertial confinement fusion (ICF), warm dense matter driven by heavy ion beams [1]. Calculation of parameters of inertial fusion drivers of heavy ion beams requires adequate quantitative description of the interaction of heavy ion beams with dense plasma in a wide range of parameters. Consequently, knowledge of transport properties in the plasma will enable us to calculate the design of thermonuclear target more accurately. These properties of plasma have to be calculated accurately taking into account both quantum and collective effects in plasmas. One of the important values that describing the transport coefficients of deuterium-tritium plasma is the Coulomb logarithm [2]. The Coulomb logarithm was obtained on the basis of effective potentials. These interaction potentials take into consideration long-range many particle screening effects as well as short-range quantum-mechanical effects [3]. For inertial confinement fusion applications, we have calculated of the viscosity, diffusion, thermal conductivity, and electrical conductivity of dense plasma in a wide range of densities and temperatures. The results obtained for viscosity, diffusion, thermal conductivity, and electrical conductivity are compared with the available experimental data [4] and the results of quantum molecular-dynamics simulation [5].

-
1. Fortov V.E. // Extreme states of matter on Earth and in the Cosmos, Springer, 2009.
 2. Ramazanov T. S., Kodanova S. K., Moldabekov Zh. A., Issanova M. K. // Phys. Plasmas 2013. V. 20. P. 112702.
 3. Kodanova S.K., Ramazanov T. S., Issanova M. K., Moldabekov Zh. A., Nigmatova G. // Contrib. Plasma Phys. 2015. V.55. No.2-3. P.271.
 4. Adams J.R., Shilkin N.S., Fortov V.E., Gryaznov V.K., Mintsev V.B., Redmer R., Reinholz H., and Ropke G. // Phys. Plasmas 2007. V. 14. P. 062303.
 5. Hu .X., Collins L. A., Boehly T. R., Kress J. D., Goncharov V. N. and Skupsky S. // Phys. Rev. E. 2014. V. 89. P.043105 .

**DEVELOPMENT OF ONLINE RESOURCES TO ASSESS THE
EFFECTIVENESS OF SOME GAS TURBINE PLANTS**

Ochkov V.F.,¹ *Ustyuzhanin E.E.*,*¹ *Znamensky B.E.*,¹ *Rykov S. V.*,² *Rykov V.A.*²

¹*MPEI (TU), Moscow, Russia*, ²*SPbSU ITMO, Saint-Petersburg, Russia*

*evgust@gmail.com

An analysis of Internet resources is fulfilled in the report. The resources contain such information as: (a) data on the thermal properties, $R = (\rho, h, s \dots)$, of substances, (b) numerical data on the energy criteria Z of gas turbine plants (GTP). It is shown that currently typical Internet resources have the form of text files. These resources are developed in a number of organizations (JIHT RAS, NIST etc.). For example, such a file contains tabulated R properties and does not use the software to calculate these properties. The resources allow the client to implement a number of options. The latter include: (a) "introduction" of boundary conditions, $Y = (p, T \dots)$, (b) "calculation" of the value of R using the software (SW) in the form of "exe-file", here p, T are the pressure and the temperature those are the arguments in the exe-file to calculate $R(p, T)$. In this case, the exe-file is closed to the user: there is no such option as "copying" the mathematical formula, $R(p, T)$, used for the calculation of the R property of the working substance. Some researchers have designed Internet resources to calculate the properties of R . These researchers include the authors of this report. This SW has the form of an open interactive Internet resource (OI). The computational part of the OI-resource is connected: (1) with the formula, $R(p, T)$, or with the equation of state (EOS), which calculates R property, 2) with Mathcad code named Code_1(R, Y). The code let us determine R property. The interactive part of the OI-resource is based on the computer science and Internet technologies.

We have considered the methodological techniques and tools, which can be used: (a) to create an OI-resource, (b) to place the OS-resource on a remote server, (c) to implement a number of new options for clients. These options include, for example, "copying" the mathematical formula/EOS or the code as a whole. In the report, OI-resources are focused on the joint use of some tools: (1) the code used for the design of a power plants, (2) OI-resource that allows us to calculate R properties at specified points of GTP cycle. We have got some results obtained on the basis of these resources. These results are discussed, including data on the internal efficiency, $Z_1(R, Y)$, of some GTP, here: $Y = (Y_1$ is the temperature at the entrance to the turbine unit, Y_2 is the degree of the pressure increase in the compressor unit, etc.). The optimization of the objective function, $Z_1(R, Y)$, of GTP is performed.

**ON IMPORTANCE OF THE MULTI-LEVEL CHEMICAL OBJECTS
DESCRIPTION IN ONTOLOGIES FOR INFORMATION SYSTEMS
INTEGRATION IN INORGANIC MATERIALS SCIENCE**

Dudarev V.A.,* *Kiselyova N.N.*

IMET RAS, Moscow, Russia

*vic_dudarev@mail.ru

In past years ontologies (on OWL) usage becomes popular for problem domains description and creating basis for thematic information systems (IS) integration. For example, in inorganic materials science several ontologies are known to consolidate information [1] [2]. One of their significant drawbacks is an unjustified description simplification for substance (or material).

The importance of multilevel chemical object description is shown by the example of IS developed in IMET RAS. «Diagram» IS (<http://diag.imet-db.ru>) describes phase diagrams of double and triple chemical systems. In another «Crystal» IS properties are described at other detail levels of chemical objects: the melting temperature is described at the substance (or compound) level, and the hardness — at its crystal structure information level [3].

Thus, developing the ontology for IS information integration on inorganic substances properties, it is necessary to implement means for properties definition at different levels of chemical objects description and to ensure an automatic matching for the upper-level hierarchy properties with the current chemical object.

The work was carried out with the partial financial support of the Russian Foundation for Basic Research, projects 17-07-01362, 18-07-00080. The work was carried out according to the government task No. 007-00129-18-00.

-
1. Ashino T. Materials ontology: an infrastructure for exchange materials information and knowledge // Data Science Journal. Volume 9. 8 July 2010. pp. 54-61.
 2. Erkimbaev A.O., Zitserman V.Yu., Kobzev G.A., Serebryakov V.A., Shiolashvili L.N. Ontology-based problem domain modelling for data on substances and materials properties integration // Proc of XV All-Russian Joint Conference «Internet and modern society» (IMS-2012). Saint Petersburg, 2012. pp. 38-47.
 3. Dudarev V.A. Information systems integration in inorganic chemistry and materials science. Moscow: URSS, 2016. 314 p.

ONTOLOGY-BASED METHODS OF THERMOPHYSICAL DATA INTEGRATION

Kosinov A. V., Erkimbaev A. O., Zitserman V. Yu., Kobzev G. A.*

JIHT RAS, Moscow, Russia

**adilbek@mail.ru*

The work analyzes the approaches to the problem of thermophysical data integration using modern information technologies (IT). To implement this task, the authors proposed a combined use of methods of Semantic Web and Big Data, which ensures that the variability of the data structure and the coverage of large numerical arrays typical of thermophysical data are taken into account [1]. Application of ontologies for description of metadata of the integrated distributed sources and JSON-format files for thermophysical data storage are offered. In order to organize the data management of such a two-layer system, the Apache Spark [2] toolkit was used from the Big Data technology stack.

A number of existing data integration platforms based on similar methods have been studied [3–5]. At the same time, a number of proposed components and IT solutions are worthy of attention and in the future can be used for the thermophysical data integration.

The test results of the developed integration tools for working with the THERMAL database are presented. The stages of data preparation and conversion into a new format are demonstrated.

-
1. Erkimbaev A.O., Zitserman V.Yu., Kobzev G.A., Kosinov A.V. Standardization of Storage and Retrieval of Semi-structured Thermophysical Data in JSON-documents Associated with the Ontology. Proceedings of the XIX International Conference Data Analytics and Management in Data Intensive Domains (DAMDID/RCDL'2017), Moscow, Russia, October 10-13, 2017, URL: <http://ceur-ws.org/Vol-2022/paper36.pdf> (available at 22.04.2018)
 2. Apache Spark, <http://spark.apache.org/docs/> (available at 22.04.2018)
 3. Open Semantic Framework (OSF), <http://opensemanticframework.org/> (available at 22.04.2018)

4. MOMIS DataRIVER, <http://www.datariver.it/data-integration/momis/> (available at 22.04.2018)
5. Karma: A Data Integration Tool, <http://usc-isi-i2.github.io/karma/#pub> (available at 22.04.2018)

INFORMATION SYSTEMS FOR INORGANIC MATERIALS SCIENCE

Kiselyova N.N., Dudarev V.A., Stolyarenko A.V.*

IMET RAS, Moscow, Russia

**kis-japan@mail.ru*

In recent years in the developed countries the initiatives aimed to the infrastructure organization for access to data about materials were announced and supported by the governments. In 2011 the USA started a project, called Materials Genome Initiative (MGI) [1]. In 2014 National Data Service announced a project of creation of repository for experimental and calculated data [2]. In 2015 EU supported a program Novel Materials Discovery Laboratory [3]. The analogous programs were announced in Japan [4], China [5] and India [6]. In spite of the fact that hundreds of millions of dollars are spent for these programs implementation, their results is economically profitable since they allow considerable cost reduction for new materials development.

IMET RAS experience in development and integration of Internet databases (DBs) on inorganic substances and materials properties together with computer-assisted design for new substances based on data mining technologies [7] is a premise for successful accomplishment of materials infrastructure project in Russia. The special Information-Analytical System (IAS) was developed in IMET RAS. It includes the virtually integrated DBs system on inorganic substances and materials properties [8], the subsystems for regularities search in data and new substances prediction and their properties estimation, the knowledge base and other subsystems.

Work was supported in a part by the RFBR, projects nos. 17-07-01362 and 18-07-00080 and State task N. 007-00129-18-00.

-
1. Materials Genome Initiative. <https://www.mgi.gov> — (visited on 23.03.2018).
 2. The Materials Data Facility. <https://materialsdatafacility.org> — (visited on 23.03.2018).
 3. The Novel Materials Discovery Laboratory. <http://nomad-lab.eu> — (visited on 23.03.2018).
 4. Center for Materials Research by Information Integration. <http://www.nims.go.jp/eng/research/MII-I/index.html> — (visited on 23.03.2018).
 5. Lu X.-G. // Sci. Bull. 2015. V. 60. N. 22. P.1966.
 6. First National Conference on Mapping the Materials Genome. Ed. V. Kumar, G. Roy, V.K. Jayaraman, S. Sukumar and N. Sukumar. New Delhi: Group Excel India, 2013.
 7. Kiselyova N.N., Dudarev V.A., Stolyarenko A.V. High Temperature. 2016. V. 54. N. 2. P. 215.
 8. DBs of IMET RAS. <http://www.imet-db.ru> — (visited on: 23.03.2018).

EVAPORATION THERMODYNAMICS OF YTTRIUM TRIFLUORIDE IN THE FORM OF MOLECULES YF₃ AND Y₂F₆**Gorokhov L.N.,¹ Osina E.L.,*¹ Kovtun D.M.²**¹JIHT RAS, Moscow, Russia, ²MSU, Moscow, Russia

*j-osina@yandex.ru

Due to the ongoing work on obtaining reliable thermodynamic data of yttrium halides, new calculations of functions for YF₃ and Y₂F₆ in gas phase were performed using quantum-chemical calculations by MP2 and CCSD(T) methods. Enthalpy of sublimation of yttrium trifluoride in the form of monomer was updated whereas enthalpy of YF₃(g) formation was calculated on the basis of existing data on vapor pressure of yttrium trifluoride using new thermodynamic functions of YF₃ molecules. Ab initio calculations of dissociation energy of dimer molecules Y₂F₆ on monomer two YF₃ was carried out. Using this data sublimation enthalpy of yttrium trifluoride in dimer form was found and formation enthalpy of Y₂F₆(g) was calculated. The composition of yttrium trifluoride vapor was calculated as follows: the ratio of Y₂F₆ pressure to that of YF₃ in the range between 1400 and 3000 K increased from 10⁻⁴ to 10⁻². The thermodynamic and thermochemical values obtained were introduced into IVTANTERMO database.

THERMODYNAMIC FUNCTIONS AND ENERGY STABILITY OF YTTRIUM TRICHLORIDE AND ITS DIMER**Gorokhov L.N.,¹ Osina E.L.,*¹ Osin S.B.²**¹JIHT RAS, Moscow, Russia, ²MSU, Moscow, Russia

*j-osina@yandex.ru

Experimental and theoretical data on the structure and vibrational frequencies of yttrium trichloride and its dimer was critically analyzed. The analysis enabled to choose the values of molecular constants and to perform thermodynamic functions calculations. Enthalpy of sublimation of yttrium trichloride in the form of monomer was updated whereas enthalpy of YCl₃(g) formation was calculated on the basis of existing data on vapor pressure of yttrium trichloride using new thermodynamic functions of YCl₃ molecules. Enthalpy of sublimation of yttrium trichloride in the form of a dimer was found and the enthalpy of Y₂Cl₆(g) formation was calculated using literature data on the composition of vapor at the temperature of 1312 K. The composition of yttrium trichloride vapor in the temperature range between 1317 and 1646 K was calculated: the ratio of Y₂Cl₆ pressure to that of YCl₃ increased from 0.15 to 0.21. The obtained values are added to IVTANTERMO software.

**THERMOPHYSICAL PROPERTIES OF NANOFLUIDS. EXPECTATIONS
AND REALITY**

Rudyak V. Ya.

¹*NSUACE, Novosibirsk, Russia,* ²*SFU, Krasnoyarsk, Russia*
valery.rudyak@mail.ru

Interest in nanofluids, borned a quarter of a century ago, continues to grow steadily. It is connected, on the one hand, with the existing applications of nanofluids (in perfumery and cosmetic industry, in bio- and medical technologies, at creating new materials, etc.) [1]. On the other hand, the boom of nanofluid researches was initiated by the expectations of various thermophysical applications (as coolants, refrigerants, etc.). All these expectations stimulated the active studying the thermophysical properties of nanofluids. Unexpectedly, the results obtained were extremely contradictory and gave rise to a lot of speculation. Only today certain clarity has been achieved regarding the features of the thermophysical characteristics of nanofluids.

In the present paper these properties are systematically discussed. Both experimental data and molecular dynamics data obtained directly by the author and his group are presented and analyzed. It was shown that the thermophysical properties of the nanofluids are not described by the classical theories. The reasons of such behavior are explained. The structure of nanofluid has been studied. The mechanisms determining the viscosity and thermal conductivity of nanofluids are formulated.

This work was supported by Russian Foundation of Basic Research (grants No. 17-01-00040 and No. 17-58-45023) and Russian Science Foundation (Project No. 17-79-20218).

-
1. Rudyak V.Ya., Minakov A.V. Modern problems of micro- and nanofluidics. Novosibirsk: Nauka, 2016.

**SURFACE TENSION OF LIQUID MERCURY IN VACUUM, IN THE
MEDIUM OF OXYGEN. EXPERIMENT**

*Fokin L.R.,*¹ Alchagirov B.B.,² Kokov Z.A.,² Korotkov P.K.,² Elimkhanov D.Z.³*

¹*JIHT RAS, Moscow, Russia,* ²*KBSU, Nalchik, Russia,* ³*ChSU, Grozny, Russia*

**Ifokin@mail.ru*

The operation of various devices and technical devices with mercury is carried out in a variety of conditions, so the study of the influence of the gaseous medium and vapors on the thermal properties of Hg remains an urgent task. But in the literature there are not enough reliable data that allow one to unequivocally judge the degree of influence of oxygen on the surface tension (ST) of mercury [1]. In this connection, in the present paper, the problem of the experimental study of the effect of air and oxygen on the surface tension of high-purity mercury at room temperatures is posed and is being solved. The experiments used mercury grade P-0 with a content of 99.9997% Hg. Before the measurements of the ST, the mercury was subjected to high-vacuum distillation and "distilled" it into glass ampoules, which were then soldered to the measuring cell, by the known method of a large drop. To prevent the mercury from sputtering and contacting it with atmospheric air inside the ampoule, mercury was blocked by a thin hemispherical glass partition, and a metal "firing pin" was placed in a glass "shirt" for subsequent opening of the ampoule with Hg in a vacuum inside the measuring

cell itself. Similarly, glass ampoules of about 0.2 liter capacity were prepared, which, after preliminary heat treatment in high vacuum, were filled with certified atmospheric air or oxygen and also were soldered to a measuring cell. The results of measuring the effect of oxygen on the mercury surface tension at 293 K, obtained in a continuous mode in a vacuum (1180 min) and an oxygen atmosphere (1460 min) on the same surface of the Hg drop, indicate that under vacuum conditions the surface tension of mercury is 475 ± 4 mN/m and remains fairly stable during the entire measurement period (1180 min). After the oxygen is introduced into the measuring cell and the beginning of exposure of the surface of mercury in oxygen, Hg is very rapidly reduced to 360 mN/m and then remains practically constant and equal to about 330 mN/m.

The paper gives possible explanations for the results obtained, as well as their discussion and comparison with the literature data.

1. Kozin L.F and Hansen S.C. Mercury Handbook: Chemistry, Applications and Environmental Impact // Published by the Royal Society of Chemistry. 2013. S. 324

EFFECT OF INSTABILITY ON THE CRITICAL BEHAVIOR OF HEAT CAPACITY FOR ETHANOL + DIAMOND NANOFUID

*Abdulagatov I.M.,*¹ Polikhronidi N.G.,² Batyrova R.G.²*

¹DSU, Makhachkala, Russia, ²IP DSC RAS, Makhachkala, Russia

*ilmutdina@gmail.com

A deeper understanding of the thermodynamic properties of nanofluids can lead to marked improvements in their industrial applications (environmental, mechanical, chemical, biological, and geothermal industries). However, using nanofluids in high-temperatures and high-pressures and other severe environmental conditions (high pH-condition, salinity, for example) are related with some problems. For example, nanoparticle dispersions are often difficult to stabilize in harsh downhole environments [1] when nanoparticle dispersions applied to enhanced oil recovery. Also, the interaction between the base fluid and solid nanoparticles (for example, wetting properties, hydrophilic or hydrophobic properties, structure of the transition zone between the bulk liquid and solid surface) plays an important role in observed properties of nanofluids. Since most nanoparticles employed a dispersant (or stabilizer) or surfactants for stabilizing of the nanofluids, their effect on measuring properties is still unclear, for example, surfactants thermal decomposition is considerable affecting on the nanofluid properties, therefore, on their practical applications. Thermal decomposition of the surfactants leads to destabilization of nanofluids, i.e., agglomeration or precipitation of nanoparticles and subsequent damage to the technological process. Thus, instability renders the nanofluid ineffective and often leads to unexpected results. Due to surfactant thermal decomposition the dispersion can quickly become unstable and agglomerate when the base fluid is subjected to change in pH, or encounters increased salinity and temperature. Among different factors, the effect of temperature on destabilization of nanofluid is extremely important [1]. However, the effect of temperature on the stability and the measuring properties of nanofluids is very poorly understood. In the present work we have studied the effect of thermal instability on nanofluid ethanol+diamond (3 to 10 nm size) critical behavior. We experimentally found that at temperatures above 500 K thermal destabilization of the nanofluid completely changes the temperature behavior of heat capacity. For example, the phase transition temperature of the nanofluid considerably shifts to high temperature in comparison with pure ethanol. Also, heat capacity discontinuity for pure ethanol near the critical point is smoothed for nanofluid.

This work was supported by Russian Foundation of Basic Research (RFBR) grants 16 08 00536 and 18 08 00500

1. McElfresh P., Wood M., Ector D. // SPE 154758, SPE Int. Oilfield Nanotechnology Conference, Noordwijk, The Netherlands. 12-14 June. 2012.

SURFACE TENSION OF LITHIUM ALLOYS: STATE OF RESEARCH (REVIEW)

Alchagirov B.B., Kyasova O.Kh., Uzdenova A.N.*

KBSU, Nalchik, Russia

**boris@alchagirov.ru*

Great interest in the study of lithium alloys is caused by the possibility of their use as electrodes in batteries with high energy density and thermoelectric converters, as well as promising materials for the development and application of coolant in nuclear power plants on fast neutrons and other areas of new technology. In this regard, there is a need to obtain reliable information about the thermophysical properties of metallic system alloys involving lithium. In this paper, the task is to give a brief overview of the state of surface tension research (ST) - one of the most important energy characteristics of surface substance for this class of materials.

An analysis of the study results of the concentration dependences of the lithium-ion alloys in the literature shows that the surface tension (ST) has been studied for only a dozen binary systems, including Al-Li, Bi-Li, Ga-Li, In-Li, Sn-Li, Pb-Li, Zn -Li, etc. Studies of the ST triple alloys involving lithium only unfolds [1, 2]. In our opinion, this state of research is explained by the fact that the study of the physicochemical properties of lithium alloys is a very difficult experimental task, starting with the problems of synthesizing and homogenization of samples of the considered class of objects, as well as the measurements themselves.

Thus, from the analysis of literary and own results of researches of ST of lithium alloys, it follows that:

- 1) most concentration dependences of surface tension of lithium alloys are studied in narrow intervals of compositions, mainly in the form of small additives of lithium to metals;
- 2) a significant fraction of the concentration dependences a ST of lithium alloys available in the literature are based only on several experimental points;
- 3) in the binary alloys considered, lithium additions to low-melting p-metals reduce the ST of the solvent-metal, i.e. exhibit a sufficiently high surface activity, which all the more the surface tension of the solvent metal in comparison with the ST of lithium.

-
1. Trybula M.E., Gancarz T., Gasior W.// Fluid Phase Equilibria. V.421. P. 39–48. 2016.
 2. Alchagirov B.B., Dyshekova F.F.// High Temp. V.54. No.6. P. 815–819. 2016.

CHANGE IN THE PHASE DIAGRAM OF A SIMPLE MATTER WITH A DECREASE IN THE SIZE OF THE NANOSYSTEM

Magomedov M. N.

IPG DSC RAS, Makhachkala, Russia

mahmag4@mail.ru

The statistical three-phase model of a simple matter developed earlier in [1] is generalized to the case of a nano-system. Analytic expressions for the Helmholtz free energy and the state equation, which are valid for arbitrary values of the density, temperature, and number of atoms

in the system are obtained on the basis of the Mie-Lennard-Jones paired potential of the interatomic interaction.

Calculations of the argon state equation showed that, when the number of atoms in the system decreases, the S-loop on the isotherm of the state equation for the phase transition (PT) of crystal-liquid (C-L) decreases, and at a certain number of atoms (N_0), the PTC-L S-loop disappears. It is shown that the value of N_0 increases when the shape of the nano-system deviates from the most energetically optimal shape. The value of N_0 increases with increasing temperature on the isotherm. In a cluster of $N < N_0$ atoms the PTCL already no.

As the number of atoms decreases, the liquid-gas phase transition (PTL-G) S-loop also decreases. The critical point parameters for PTL-G at decreasing number of atoms vary: the critical temperature and pressure decrease, and the critical specific volume increases.

Earlier, both in experiments and in computer modeling, it was noted that with a decrease in the nano-system size, both a convergence of the size dependences of the melting and crystallization temperatures is observed, as well as a decrease in the latent heat and in the specific volume jump at melting. Proceeding from these facts, and studying the extrapolation of size dependencies to the small dimensions, in [2] pointed out the possible disappearance of the PTC-L with a decrease in the number of atoms in the nano-system. In this work, it is shown that this disappearance of the S-loop of the PTC-L is due to an increase in the fraction of delocalized atoms at a decrease in the size of the nano-system.

This work has been supported by the Russian Foundation for Basic Research (grant No. 16-03-00041_a) and the program of the Presidium of the Russian Academy of Sciences (project No. I.13).

-
1. M.N. Magomedov. Vestnik Moskovskogo Tekhnicheskogo Universiteta im. N.E. Baumana, Ser.: Estestvennye Nauki, 2013, 2, 28-42.
 2. M.N. Magomedov. Technical Physics, 2014, 59, 5, 675-681.

EQUATION OF ISOTHERM OF SURFACE TENSION OF BINARY METAL SYSTEMS

Kalazhokov K.K., Kalazhokov Z.K., Kalazhokov Z.K.*

KBSU, Nalchik, Russia

**khh49@mail.ru*

In [1] from the analysis of experimental data on the dependence of the surface tension (ST, $\sigma(x)$) on the composition of the melt of binary metal systems, the equation of the isotherm ST is proposed

$$\sigma(x) = \beta \frac{(F-1)(1-x)x}{1+(F-1)x} + \sigma_A(1-x) - \sigma_B x, \quad (1)$$

where β and F are parameters of the equation (1) that do not depend on the composition, σ_A and σ_B - ST of the pure components of the $A - B$ system, and x is the thermodynamic concentration of the second component of the system.

To prove the validity of (1) for binary systems with monotonic change of ST depending on the composition, we rewrite it as a linear function

$$y(x) = \frac{(1-x)x}{\Delta\sigma(x)} = \frac{1}{\beta(F-1)} + \frac{1}{\beta}x, \quad (2)$$

where

$$\Delta\sigma(x) = \sigma(x) - \sigma_A(1-x) - \sigma_B x, \quad (3)$$

where $\sigma(x)$ is the PN of the melt of x , measured in the experiment.

The straight line (2) is constructed using experimental data $\sigma(x)$ for binary systems: 1 - alkali metals; 2 - p-metals; 3 - p-metal+alkali metal; 4 - refractory metal+p-metal . For all these systems, the expression (2) is satisfactory and it is shown that it describes all kinds of experimental isotherms of PN binary systems with a monotonous change of PN with high accuracy - the permissible relative deviations from the experiment are about 1%.

The high accuracy of the description of experimental isotherms by the equation (1) allows to construct methods of forecasting of surface properties of binary and triple systems with a minimum number of reference measurements.

-
1. Kalazhokov Zamir Kh., Zikhova K.V., Kalazhokov Z.Kh., Kalazhokov Kh.Kh., Taova T.M. Calculation of isotherms for surface tension of melts for multicomponent metal systems. // High Temperature. - 2012. - V.50 N3. - P.469-472.

NANODIAMON DGRAPHITIZATION AT HEATING AND IRRADIATION

Zakatilova E.I., Efremov V.P.*

JIHT RAS, Moscow, Russia

**ei.zakatilova@mail.ru*

Nanodiamonds are an interesting physical object and attractive material for many industrial applications. At industrial conditions nanodiamonds are obtained as detonation product. The sizes of detonation nanodiamonds depend on conditions of explosion. At explosion in inert atmosphere the products consist of nanodiamonds. At explosion in water environment the products are microdiamonds.

In this work the graphitization and thermal stability of detonation nano and microdiamonds were studied. Received data showed that the temperature of graphitization of nanodiamond particles lies in wide range and the temperature of graphitization beginning depend on the particle size. It is shown the high thermal stability of microdiamonds. It is established the influence of heating rate on the size of nanodiamond conglomerates.

The analysis of literature shows that the graphitization processes take place at irradiation. Depending on the type and irradiation dose the point defects, amorphous and graphite phases can form in the diamond structure. Annealing of irradiation samples showed the defect structure restore to ideal lattice and the release of stored energy.

With the appearance of powerful laboratory radiation sources (femtosecond laser), the possibility to receive nanodiamonds by irradiation of carbon media was appearance. Today this possibility determines the high interest to thermophysical properties of nanodiamond.

SIZE DEPENDENCE OF MOLYBDENUM MELTING AND CRYSTALLIZATION TEMPERATURES

Akhmedov E.N.

IGR DSC RAS, Makhachkala, Russia

aen-code@yandex.ru

Based on the RP-model, presented in [1], the state equation (P) of molybdenum has been calculated. Interatomic interaction was described by the Mi-Lennard-Jones pair potential. The potential parameters were determined by fitting to the state equation, the bulk modulus, and the coefficient of thermal expansion of molybdenum [2].

Proceeding from the Lindemann criterion under isobaric conditions ($P = 0$), the melting temperature (T_m) has been calculated for nanocrystals with different size and surface shape. It was found that the value T_m decreases with the decrease of the atoms number (N) in the nanocrystal, and it is more noticeable when the shape deviates from the most energetically optimal (a cube for the RP-model).

The surface pressure compress the nanocrystal and to keep isobaric conditions $P = 0$ the interatomic distance must be increased that facilitates melting process.

For the RP-model curves $T_m(N, P = 0)$ end at N_{cr} – minimum possible size of a nanocrystal. For a cube $N_{cr} = 10$, and N_{cr} increases with the nanocrystal shape deformation. If we assume that the value of N_{cr} is the size of the crystalline nucleus with the particular surface shape at $P(N_{cr}) = 0$, then we can get the size dependence of the crystallization start temperature T_{cr} . Extrapolation of the isobaric dependence $T_{cr}^*(N_{cr}^{-\frac{1}{3}}) = T_{cr}(N_{cr}^{-\frac{1}{3}})/T_m(\infty)$ to a macrocrystal ($N_{cr}^{-\frac{1}{3}} = 0$) showed that the value $T_{cr}^*(N_{cr}^{-\frac{1}{3}} = 0)$ is 0.713 for rod-like and 0.857 for plate-like shapes of the nanocrystal. This agrees with the Turnbull rule, which allows us to state that obtained dependence $T_{cr}^*(N_{cr}^{-\frac{1}{3}})$ describes the dimensional dependence of the molybdenum crystallization start temperature at $P = 0$.

This paper has been supported by Russian Foundation for Basic Research (Grant No. 16-03-00041_a) and the Program of the Presidium of the Russian Academy of Sciences (project No. I.13).

-
1. M.N. Magomedov. Crystallography Reports, 2017, 62, 3, 480-496.
 2. E.N. EAhmedov. Journal of Physics and Chemistry of Solids, 2018, 121, 62-66.

A GENERALIZED MODEL OF THE KAPITZA RESISTANCE

Khvesyuk V.I.

BMSTU, Moscow, Russia

khvesyuk@bmstu.ru

At present, the problem of the development of the theory of Kapitza resistance between solids is particularly relevant due to growth of nanotechnology, where these resistances play an important and sometimes main role in the heat transport. The theory of acoustic mismatch (AMM) for this phenomenon previously presented in [1, 2]. However, this model contains a number of limitations that do not take into account the important properties of acoustic wave propagation in solids. 1) Only longitudinal waves are taken into account. 2) It is not considered that refraction and reflection of acoustic waves cause simultaneously both longitudinal and transverse waves [3, 4]. 3) It does not take into account the phenomenon of total internal reflection, which makes a significant contribution to the Kapitza resistance. These facts significantly change the formulation of the problem, especially, the boundary conditions on the contact surface (interface).

This work presents a new model that takes into consideration all specified properties of acoustic waves. A number of estimations were carried out which show a good agreement with the experimental data, better than in previous works.

Work was supported by Russian Ministry of Science and Education, project 16.8107.2017/6.7.

-
1. Khalatnikov I.M. // JETP Lett. 1975. Vol. 22(11).P. 581
 2. Little W.A. // Can. J. Phys. 1959. Vol. 37. P. 334
 3. Landau L.D. , Lifshitz E.M. Theory of Elasticity. (3rd ed.). Butterworth-Heinemann. 1986.

4. Krasilnikov V.A., Krylov V.V. Introduction to Physical Acoustics. Moscow: Nauka (in Russian). 1984.

NANO-SCALE INHOMOGENEITY IN NiO

*Shulyatev D.A.,^{*1} Ponomareva A.V.,¹ Mukhamedov B.,¹ Abrikosov I.A.,¹
Bozhko S.I.,² Ionov A.M.,² Mazilkin A.A.,² Smirnova I.A.,² Walls B.,³ Shvets I.V.³*

¹NUST MISIS, Moscow, Russia, ²ISSP RAS, Chernogolovka, Russia, ³CRANN, Dublin,
Ireland

**shulyatev@mail.ru*

The aim of this work was to study the inhomogeneity of NiO (and Ni_{1-x}Li_xO) single crystals grown by floating zone melting. Different types of inhomogeneities varied from mm-scale to nano-scale were observed by X-ray diffraction, electron microscopy, LEED, AFM and STM/STS. In particular, AFM/STM images reveal the unusual granular structures onto NiO(100) surface with a typical granula size of a few nanometers. The nano-granular structure was also studied by low-energy electron diffraction (LEED) and transmission electron microscopy (TEM). The estimation of coherent area size from width of LEED spots and TEM images is in good agreement with STM - AFM data. The first principles calculations shown that the possible reason of the nanogranular structure formation is the lattice distortions induced by Ni vacancy. According to the DFT calculations the diameter of the area of the atomic displacements around the Ni vacancy is 1.2 nm. That is very close to the size of the granules observed by STM.

EMPIRICAL ESTIMATIONS OF SURFACE TENSION OF GRAIN BOUNDARIES IN PURE SUBSTANCES

Prokofjev S.I.

ISSP RAS, Chernogolovka, Russia

prokof@issp.ac.ru

In the framework of the model that treats grain boundaries as a homogeneous liquid-like layer in a solid matrix, empirical equations are obtained describing the temperature dependences of the average surface tension of high-angle grain boundaries in pure substances. The proposed expressions relate the surface tension of grain boundaries with the melting point, enthalpy of melting and the molar volume of pure elements in the solid state at the melting point. On their basis empirical expressions connecting the surface tension of the grain boundaries with the surface tension of the elements in the solid and liquid states at the melting point are also obtained. The proposed empirical relationships can be useful for quantifying of the average surface tension of high-angle grain boundaries in elementary solids at a not too low homologous temperature. Parameters of temperature dependences of the average surface tension of high-angle grain boundaries in 57 elements are given. The estimated error in determining of the values of the surface tension of the grain boundaries is comparable with the errors of their experimental determination.

HEAT CAPACITY AND THERMAL CONDUCTIVITY OF SEMICONDUCTOR NANOFILMS AND NANOWIRES

Barinov A.A., Liu B.*

BMSTU, Moscow, Russia

**barinovE6@bmstu.ru*

Semiconductor nanofilms and nanowires are a classic example of structures in which mean free path of heat carriers (phonons) is comparable to the characteristic size of the sample. This condition leads to the so-called size effect – dependence of properties on the characteristic size and geometry of the sample [1, 2]. The method based on the solution of the Boltzmann transport equation in the relaxation time approximation is widely used to estimate the size influence on thermodynamic properties [3]. In this case, specific quantitative calculations required, firstly, the dispersion law (the dependence of phonon frequency on polarization and wave vector), and secondly, the relaxation times of phonons between consistent interactions.

In this paper, the dispersion relations are obtained from the solution of elasticity equation for continuous media for film and cylinder [4, 5] with free boundaries.

Relaxation time was determined according to the Matthiessen rule as a combination of 1) time between consistent phonon interactions (three-phonon processes), 2) time of scattering on inhomogeneities (impurities) of the crystal lattice and 3) time between successive interactions with the sample boundaries [3].

Dependences of heat capacity and thermal conductivity on temperature and characteristic size of the structure for semiconductor nanofilms and nanowires were obtained. Results of the research can be used for the estimations of heat-transfer processes in advanced semiconductor devices.

Work was supported by Russian Ministry of Science and Education, project 16.8107.2017/6.7.

-
1. Khvesyuk V.I. // Engineering Journal: Science and Innovation, 2013. Vol. 5(17). <http://engjournal.ru/catalog/machin/crigen/721.html>
 2. Khvesyuk V.I., Skryabin A.S. // High Temp. 2017. Vol. 55(3). P. 434.
 3. Khvesyuk V.I., Barinov A.A. // J. Phys.: Conf. Ser. 2017. Vol. 891. P. 012352.
 4. Victorov I.A. Fizicheskie osnovy primeneniya ultrazvukovykh voln Releya i Lemba v tehnike. (rus) M.: Nauka, 1966
 5. Physical Acoustics: Principles and Methods: Vol. 1, Part A / Edited by U. Mezon. Academic Press, 1964.

STUDY OF THE ABSORBING SPECTRA OF NANOSTRUCTURED MATERIALS BASED ON THIN FILMS OF METAL OXIDES IN THE MIDDLE IR RANGE

Skryabin A.S., Vesnin V.R., Tsygankov P.A., Chirkov A.Yu.*

BMSTU, Moscow, Russia

**terra107@yandex.ru*

At present, an increase in the absorption coefficient A_λ of materials in the middle IR range is very important for the development of promising bolometric sensors and intensification of radiation heat transfer. For example, thin-film (with typical thicknesses $h = 10 \dots 100$ nm) coatings on various substrates can be IR absorbers [1]. In this case, films of metals, semiconductors, as well as their oxides, nitrides, etc. are used [2].

Using the Drude theory [3] the optical properties of some metals (Ti, Cr, etc.) have been calculated. As a result, the spectral refractive indices n_λ , the extinction coefficients k_λ , and the

absorption coefficients A_λ were determined at $\lambda = 2.5 \dots 15 \mu\text{m}$ and $T = 300 \dots 1000 \text{ K}$.

The creation of samples of thin-film absorbers based on titanium oxides was carried out by ion-beam sputtering of a Ti target in a mixture of argon and oxygen at a gas mixture pressure of about 3 mPa, followed by deposition of atoms on a silicate glass substrate. The resulting coatings were subjected to a complex study in order to establish the features of their structure and to obtain data on their absorbing rate.

It was shown that the characteristic thickness of the films is about 600 nm. The absorption spectra of the original substrate as well as the coated substrates were studied for two cases: i) a radiation incident on the coating side and ii) on the filmless side. For all the systems studied, the dependences are essentially nonmonotonic in nature with the presence of several extrema in the investigated range of λ .

Summarizing the results of the studies, one can say that thin-film coatings based on Ti oxides with a thickness of $\approx 600 \text{ nm}$ can be recommended to increase the absorption of middle IR radiation. The use of such coatings makes it possible to achieve a mean integral absorption $\bar{A}_\lambda \approx 0.37 \dots 0.39$ in the range $\lambda = 2.5 \dots 15 \mu\text{m}$, which is 3...4 times higher than that of silicate glass substrates.

-
1. Lodenquai J.P. // Solar Energy, Vol. 53. No 2. pp. 209-210.
 2. Jiang B. et al. // ECS Transactions, Vol. 64. No 8. pp. 179-183.
 3. Arnold G.S. // Applied Optics, Vol. 23. No9. pp. 1434-1436.

STUDY OF NOVEL EPOXY COMPOSITIONS WITH SILVER NANOPARTICLES BY DIFFERENTIAL SCANNING CALORIMETRY AND REFRACTOMETRY¹

Khasanova R.R.,^{*1} Zhavoronok E.S.,¹ Shabatin A.V.,² Senchikhin I.N.²

¹MTU (MITHT), Moscow, Russia, ²IPCE RAS, Moscow, Russia

**khasanova_r@mail.ru*

Metal-polymer nanocomposites (and specifically containing silver nanoparticles) have unique optical, thermophysical and bactericidal properties, that is why their development and study are of current interest. One of the interesting types of such materials is nanocomposites formed by curing epoxy resins (ER) containing nanoparticles precursor (salt). An important condition of such nanocomposite formation is the salt dissolving in the oligomeric matrix. Therefore, the goal of the research is to study silver reduction from its precursor (nitrate) in epoxy matrices.

The main objects of the study were epoxy resin Epikote 828 with $M_n=375$ (Hexion, USA) and polyglycidyl ether of oligoxypropylene triol Laproxide 703 with $M_n=732$ and $f_{EP}=2.43$ (Macromer, Russia). The metal precursor was silver nitrate (Merck, Germany). The studies were carried out by differential scanning calorimeter DSC Q-100 (TA Instruments, USA) in the range 188-473K in an argon atmosphere at the heating rate of 10 K/min. Refractive index was detected by URL-1 instrument at 22 °C by standard techniques.

Experimental results indicate that the rate of silver ions reduction is influenced by the salt dissolution rate and the silver nitrate solvation possibility in the epoxy resin. Influence of ER chemical nature on Ag⁺ reduction in the epoxy matrix is demonstrated. Our results allow to optimize the synthesis of silver nanoparticles in ER stable dispersions. On the basis of the dispersions it is planned to develop epoxyamine nanocomposites with improved optical and other properties.

¹The work was partially supported by the Russian Foundation for Basic Research (Project No. 17-08-00630).

EXPERIMENTAL INVESTIGATION OF VISCOSITY COEFFICIENT OF NANOFLUIDS

*Pryazhnikov M. I.,^{*1,2} Minakov A. V.,^{1,2} Rudyak V. Ya.^{1,3}*

¹*SFU, Krasnoyarsk, Russia,* ²*ITP SB RAS, Novosibirsk-90, Russia,* ³*NSUACE (Sibstrin), Novosibirsk, Russia*

**arrivent@yandex.ru*

There is an increasing interest in nanofluids in the last two decades. This is due to existing and possible future applications. Since nanofluid flows usually occur in applications, the their viscosity plays a decisive role. Discussions are still ongoing, despite the considerable experimental data (see, for example, the reviews [1–4]). The contradiction associated with question depends on whether the viscosity of nanofluids on particles size and, if so, how [4].

The paper presents the results of experimental study of viscosity coefficient of nanofluids. The several tens of nanofluids based on water, ethylene glycol and engine oil with particles SiO_2 , Al_2O_3 , TiO_2 , ZrO_2 , CuO , Fe_2O_3 , Fe_3O_4 , as well as diamond were studied. The volume concentrations of particles ranged from 0.1 to 8%. The their size was changed from 5 to 150 nm. Nanopowders were purchased from JSC “Plasmoterm” (Moscow) and LLC “Advanced powder technology” (Tomsk, Fe_3O_4 , and CuO nanopowders). All nanofluids used in the described experiments were prepared by the so-called two-step method [5].

Measurement of viscosity coefficient of the nanofluid was carried out with the help of “Brookfield DV2T” rotational viscometer with interchangeable spindles. We used also a rotational viscometer OFITE-900. All measurements are performed at 25°C.

The study has been conducted at partial financial support of the Russian Science Foundation (project 17-79-20218).

1. Hosseini S.Sh., Shahrjerdi A., Vazifeshenas Y. // Aust. J. Basic Appl. Sci. 2011. V. 5. No. 10. P. 417.
2. Mahbulul I.M., Saidur R., Amalina M.A. // Int. J. Heat Mass Transfer. 2012. V. 55. P. 874.
3. Murshed S.M.S., Estelle P. // Renew. Sust. Energy Rev. 2017. V. 76. P. 1134.
4. Koca D.H., Doganay S., Turgut A., Tavman I.H., Saidur R., Mahbulul I.M. // Renew. Sust. Energy Rev. 2018. V. 82. P. 1664.
5. Rudyak V.Ya., Minakov A.V., Smetanina M.S., Pryazhnikov M.I. // Dokl. Phys. 2016. V. 61. No. 3. P. 152.

NANOPOROUS CARBON MATERIALS FOR SUPERCAPACITORS

Vervikishko D.E., Kochanova S.A., Dolzhenko A.V., Shkolnikov E.I.*

JIHT RAS, Moscow, Russia

**vitkina-darya@yandex.ru*

Carbon materials are widely used as electrode structures for supercapacitors. The reason for this is a number of unique properties of carbon, such as high corrosion resistance, sufficient electronic conductivity, high temperature stability, the ability to adjust specific surface values and other parameters of the porous structure during synthesis. In addition, the variety of forms of carbon materials also allows more flexible approach to the choice of supercapacitor electrode materials. The properties of the carbon electrode are influenced by the properties of the carbon electrode such as: the type of feedstock, its dispersion and elemental composition, pre-pyrolysis and activation regimes, modification after activation, etc. Various materials can be used as activation raw materials: polymers, petroleum pitch, fossil coal, plant biomass (peat, wood and its components, nutshells), etc. An important condition from the technical and economic standpoint is the low cost, availability and uniformity of raw materials. To effectively form a

double electrical layer in supercapacitors, it is necessary to provide a highly developed surface of electrode materials. That is why one of the most common electrode materials is activated carbon with a large specific surface area. An important role is played by the state of the surface of the carbon material (for example, the presence of surface C-O groups, the contact angle, and other physicochemical characteristics).

This work is devoted to the development and investigation of highly efficient activated carbons from wood. Extensive work has been done to determine the optimum modes of synthesis of these carbon materials to achieve high specific electrochemical characteristics of supercapacitors with aqueous and organic electrolytes. It is shown that the developed materials have high resource stability. More than 1 200 000 charge-discharge cycles of a supercapacitor with an electrolyte of 1M tetraethylammonium tetrafluoroborate have been achieved. The nanoporous structure of activated coals has been studied, hypotheses about the influence of the parameters of the porous structure on the specific electrochemical characteristics have been made.

Work is performed at the expense of a grant of the Russian scientific fund (project number No. 14-50-00124).

BIOCIDAL ACTIVITY OF HYDROPHOBICATED OLIGOHEXAMETHYLENUGANIDINES IN EPOXY SYSTEMS

***Kosakovich E.O.*¹, *Zhavoronok E.S.*¹, *Safonov A.V.*², *Senchikhin I.N.*^{*2}**

¹MTU (MIFCT), Moscow, Russia, ²IPCE RAS, Moscow, Russia

**isenchikhin.ras@gmail.com*

Long-term usage of antibacterial and antifungal agents may cause resistance occurrence of many bacteria and parasitic fungi to active substances. That is why new antimicrobial derivatives development is up-to-date problem. Among modern microbial-resistant materials the group of oligohexamethyleneguanidines (OGMG) is of special interest, because it is promising additive for various polymer materials. The purpose of the study was to modify the epoxy-amine systems by OCMG derivatives, and to investigate general thermophysical properties and biocidal activity of the cured materials as well.

The main objects of the study were epoxy epoxy resin (ER) Epikote 828 with $M_n = 375$ (Hexion, USA) and polyglycidyl ether of oligooxypropylene triol Laproxide 703 with $M_n = 732$ and $f_{EP} = 2.43$ (Macromer, Russia); OGMG palmitate and stearate synthesized from OGMG hydrochloride ($M_n = 951$, branching coefficient equals 0.47 equivalents per mole. OGMR salts — ER adducts were synthesized in autoclave at manometric pressure of 4 atm for 2 hours. The synthesis products were introduced into epoxy-amine mixture, after that curing process was carried out till fully cross-linked polymer was obtained. Further experiments samples (films) were prepared by coating technique. Glass transition temperature evolution of curing systems with variable OGMG content was analysed; the polymer products thermal stability and some mechanical characteristics were evaluated. Fully cured films antibacterial activity was verified by MTT assay. Samples were held for a week in inoculated by *P. putida* K12 strain nutrient medium (based on the yeast extract, tryptone and dextrose) and biocidal response was detected. The study results had demonstrated the perspectiveness of hydrophobized OCMG modified epoxy-amine polymers employing as antibacterial materials.

The work was partially supported by the Russian Foundation for Basic Research, Project No. 18-08-01252A.

INFLUENCE OF GAS TEMPERATURE ON NUCLEATION AND GROWTH OF DUST NANOPARTICLES IN HIGH-FREQUENCY PLASMA

*Orazbayev S.A.,^{*1,2} Zhumadylov R.E.,² Zhunisbekov A.T.,¹ Ramazanov T.S.,¹ Gabdullin M.T.,² Dosbolayev M.K.,^{1,2} Batryshev D.G.²*

¹*IETP, Almaty, Kazakhstan, ²NNLOT, Almaty, Kazakhstan*

**sagi.orazbayev@gmail.com*

The trend of development of nanomaterials already allows us to clearly see that one of the most promising areas in nanotechnology is the synthesis of carbon nanomaterials. In turn, nanoparticles are isolated solid-phase objects, the sizes of which in all three dimensions are from 1 to 100 nm. To date, many interesting discoveries related to the physicochemical characteristics of a carbon nanomaterial (CNM) are being studied. This reveals great potential for the application of UNM in various fields not only of science, but also in construction, energy, electronics, and so on. In this paper, the method of chemical deposition from gas phase with plasma enhancement (PECVD) was used to obtain carbon nanomaterials. The production of carbon nanoparticles is carried out in a high-frequency discharge plasma of 13.56 MHz, a matching device of type L. This installation consists of a vacuum chamber in which a system of cylindrical tubes with electrodes is integrated. The electrodes are made in the form of plane-parallel disks located at a distance of 20 mm. The temperature in the vacuum chamber is regulated by a cooling and heating system using liquid nitrogen and a heater. Thus, the temperature of the plasma-forming medium can be varied in the range from -20 to 1000C. On the active electrodes in the capacitive discharge, a constant current is induced, the self-bias voltage of which directly affects the concentration of the electron flow in the plasma. To study plasmochemical synthesis and the formation of nanoparticles, a method based on measuring the self-bias voltage VDC is used. The resulting nanoparticles are analyzed using an electronic scanning microscope Quanta 3D, micrographs are taken. In this research paper, carbon nanoparticles were synthesized by the PECVD method and it was found that various parameters, such as the temperature in the working chamber, the self-bias voltage, the gas pressure, etc., directly affect their formation. For example, it became known that in the case of increasing the temperature from room to 1000 C, the time of formation of carbon nanoparticles increases by 4 times.

References

J. Lin, S. Orazbayev, M. Hénault, Th. Lecas, K. Takahashi and L. Boufendi. Effects of gas temperature, pressure, and discharge power on nucleation time of nanoparticles in low pressure C2H2/Ar RF plasmas // *Journal of Applied Physics* 122, 163302 (2017)

=====

**THERMOPHYSICAL MEASUREMENT
TECHNIQUES**

=====

**MEASURING OF HEAT FLUX IN THE RANGE FROM 5 UP TO 2500
KILOWATT PER METER SQUARED**

Osadchii S.M., Potapov B.G., Sokolov N.A.*

VNIIFTRI, Mendeleevo, Russia

**osm@vniiftri.ru*

Measuring of density of high intensity radiation heat flux is great importance for experimental studies, technological processes and materials testing [1-3]. A significant problem for the development of standards that ensure the unity of measurements of high-intensity fluxes is the creation of a source of high-power heat flux in the laboratory. The source must ensure the stability of the radiation in time and uniformity of the heat flux density on the area, which one exceeds the size of the receiving area of the sensors. A xenon high-pressure gas-discharge lamp with a power of 7 kW and an elliptical reflector with a diameter of 380 mm focusing the heat rays from the arc of the gas-discharge lamp and forming a heat flux of high intensity were chosen as a source of heat flux. To obtain a uniform heat flux in the apparatus, a quartz lightguide is used. The geometry of lightguide was calculated to redistribute the flux density uniformly across the section. The achieved uniformity of the heat flux density is 2 % on area 100 mm². Radiometer-calorimeter is used for absolute measuring of the heat flux on the exit of the lightguide. Radiometer-calorimeter measures the heat flux density by substitution the electric power. On the base of this apparatus "The state standard of unit of radiation heat flux density in the range from 5 up to 2500 kW/m²" was developed and certified in VNIIFTRI. Systematic error is less, than 2.9 % , RMS error is less, than 0.3 % [3].

1. Enaleev R.S., Krasina I. V., Gasilov V.S., O.A. Tuchkova O.A., Khairullina L. I. The measurement of high-intensity heat flows, VESTNIK KTU, vol. 16, No. 15, 2013, p. 298-302.

2. Murphy A.V., Tsai B.K., Saunders R.D. Comparative Calibration of Heat Flux Sensor in Two Black body Facilities// Journal of Research of the National Institute of Standards and Technology, V. 104, 1999,.p. 487.

3. Osadchii S.M., Potapov B.G. State standard of the unit of radiation heat flux density in the range from 5 up to 2500 kW/m², Almanac of Modern Metrology 12, 2017, p. 65-72.

**SIGNAL PROCESSING ALGORITHMS FOR MEASURING
THERMOPHYSICAL PROPERTIES USING TEMPERATURE WAVES
METHOD**

Chernoskutov M. Yu., Ivliev A.D., Meshkov V. V.*

RSVPU, Yekaterinburg, Russia

**mikhail.chernoskutov@gmail.com*

In the temperature waves method [1] information about thermophysical characteristics of the studied substance is contained in the parameters of the first harmonic of the temperature wave passed through the sample. Specifically, the main information parameters of the corresponding problem are the initial phase and amplitude of the temperature wave. In addition to these parameters, the calculation requires knowledge of the sample thickness and wave frequency. These parameters are usually determined by standard methods with the necessary accuracy.

Analog-to-digital signal conversion allows you to get a file that contains information about

temperature fluctuations over several periods of the temperature wave. Further processing of such a signal should provide a sufficiently accurate estimate of the parameter values, subject to the presence of noise. Optimal processing of weak signals contains the Fourier transform operation [2].

We use several techniques to speed up the analysis. First, with a priori known frequency of thermal waves [3], we set polling frequency of sensors such that a data file contains the same number of samples per period each time. This allows further use of reference tables of sine and cosine signal, without performing their calculation each time and save time during multiple processing. Secondly, we use a personal computer with a multi-core processor, which allows us to split the analysis into several parts and process them in parallel. Then the complex amplitude of the temperature wave is determined and the thermophysical characteristics are calculated.

The work was supported by RFBR (grants No. 11-08-00275 and No. 14-08-00228).

1. Ivliyev, A.D. High Temp (2009) 47: 737. <https://doi.org/10.1134/S0018151X09050162>
2. Van Trees H. Detection, Estimation and Modulation Theory. V. 1. // N-Y. John Wiley and Sons, Inc., 1968
3. Chernskutov, M.Y., Ivliyev, A.D. I& Meshkov, V.V. High Temp (2017) 55: 618. <https://doi.org/10.1134/S0018151X17030075>

DEFINITION OF THE TEMPERATURE CONDUCTIVITY OF A CARBON FILM BASED ON THE DATA OF PHOTOMETRIC ANALYSIS OF THE SPECTRA OF BRIGHTNESS OF THE REFLECTION FROM ITS SURFACE.

Ermishkin V.A., Minina N.A., Kudryavtsev E.M., Pokrasin M.A.*

IMET RAS, Moscow, Russia

**minina1951@rambler.ru*

Based on the method of photometric analysis of structural images (PHASI), which was previously developed in the IMET RAS, a procedure was proposed for determining the coefficient of thermal diffusivity on samples from the foil of the materials under study. Using this technique, the process of heat propagation was analyzed and estimates of the thermal diffusivity of copper, aluminum and carbon in the present work, were obtained in which an inhomogeneous temperature field was excited by means of a single laser pulse emitted from a continuously operating laser on carbon dioxide directed to one of the foci of an elliptical target (sample). The target surface during the experiment was continuously recorded on a video camera. Single-frame processing of video recording with the selected periodicity by the PHASI method allowed, to analyze the propagation features over the target surface and to obtain quantitative characteristics of this process. According to these data, temporal and spatial local characteristics of their changes were obtained; first and second partial derivatives with respect to time and coordinates included in the heat equation, from which the thermal diffusivity of the target material was determined. The developed technique made it possible to directly determine the values of thermal diffusivity coefficients, in contrast to the standard method based on the separate determination of thermal conductivity, heat capacity, and density. A comparison of the values obtained for the thermal diffusivity coefficients for carbon with its values calculated from the reference data of thermophysical characteristics showed fairly good agreement between them. The work was carried out according to the state assignment No 007-00129-18-00 and with the financial support of the Russian Foundation for Basic Research (grant No. 17–08–00098a).

DIGITAL SYSTEM FOR THE COLLECTION AND PROCESSING OF INFORMATION AND MANAGEMENT OF THE THERMOPHYSICAL HIGH TEMPERATURE INSTALLATION

*Kurichenko A. A.,¹ Gorbatov V. I.,¹ Ivliyev A. D.*²*

¹USMU, Ekaterinburg, Russia, ²RSVPU, Ekaterinburg, Russia

*ad_i48@mail.ru

The installation implementing the well-known method of temperature waves [1], the main functional devices of which operate under the control of a computer and microcontrollers, is described. The unit consists of an optical quantum generator (laser), an amplitude modulator, a vacuum chamber for the test sample, equipped with electrothermal equipment and a gas supply system, as well as measuring sensors and a digital signal processing system. The modulator transforms the radiation of continuous-wave laser into a stream of thermal pulses acting on the surface of a flat sample. A temperature wave is excited in the sample. The operation of the amplitude modulator is rigidly connected with the operation of the reference voltage generator, which generates a signal that allows to judge the phase of oscillations of the heat flow. The modulation frequency is set at the command of the computer in the range from 1 to 100 Hz and stabilized [2]. The temperature wave passes through the sample. Fluctuations in the temperature of the second flat surface of the sample with the help of a thermocouple and a photo sensor are converted into electrical signals, which, after passing through the analog normalizing circuits, enter the analog-to-digital Converter (ADC), and then into a computer. The operation of the normalizing circuits is controlled by the computer [3], so that the ADC aperture is used effectively. The computer performs Fourier transform signal and reference voltage, which allows you to determine the phase shift of the signal and its amplitude. According to these parameters, the computer calculates the thermal diffusivity and relative heat capacity of the sample. The heating rate of the sample is controlled by a computer, so the entire measurement process takes place automatically.

-
1. Ivliyev A. D. //HighTemperature, 2009. V. 47, No. 5, P. 737.
 2. Vekshina O. A., Vekshin I. M., Kurichenko A. A., Ivliyev A. D. // Measurement Techniques, 2010, V. 53, No. 6. P. 668.
 3. Vekshin I. M., Vekshina O. A., Kurichenko A. A., Ivliyev A. D. // Measurement Techniques, 2012, V. 55, No. 11. P. 1263.

INFRARED SYSTEM FOR THERMAL RESISTANCE MEASUREMENT OF MICROOBJECTS

Senchenko V.N., Konovalov P.A., Ilichev M.V., Kapustin D.I.*

JIHT RAS, Moscow, Russia

*pyrolab@mail333.com

The original measuring system and method of temperature fields measuring of integrated circuits chips for controlling of thermal resistance between a chip and its case under production conditions is presented. The developed system based on infrared microbolometric matrix and allows integrated circuits chips temperature fields controlling with the high spatial resolution up to 15 microns. The infrared system allows temperature measuring over the range (40 – 200) C, and also allows to spot small gains of IC chips temperature around (1 – 2) C at various operating modes. The instrumental error of temperature measuring does not exceed ± 0.5 C for a blackbody model. For determination of thermal resistance in the system included special bulk copper heat load that provides IC case temperature stabilization in range (40 – 170) C at

drift less than ± 0.1 C.

The system consists of the opto-electronic block with a microbolometric matrix, the infra-red objective with fluid-flow temperature stabilization of the case at level (18 ± 0.01) C, the heat load with adjustable temperature, a precision fluid-flow thermostat with the solid-state cooling medium.

Approach of the method novelty consists in application of self-correction of the measured temperature on effective emissivity of the object that allows without special black coating of IC chips controls thermal resistance between an IC chip and its case under manufacturing conditions.

This work is supported by RFBR (grant No. 18-08-00923).

INVESTIGATION OF PHASE TRANSITIONS OF N-ALKANES NANOEMULSIONS BY MEANS OF DYNAMIC AND STATIC LIGHT SCATTERING

Kuryakov V.N.,¹ *Ivanova D.D.**²

¹*OGRI RAS, Moscow, Russia*, ²*MUCTR, Moscow, Russia*

**ivanovad.97@mail.ru*

In this work we present the results of studies of phase transitions (melting, crystallization, rotational phases of paraffins) by dynamic and static light scattering in aqueous emulsions of individual paraffins C₁₉H₄₀, C₂₀H₄₂, C₂₁H₄₄, C₂₃H₄₈, C₂₄H₅₀, C₂₅H₅₂, C₂₆H₅₄, and C₂₈H₅₈ and some binary mixtures of these paraffins. Emulsions were prepared by ultrasonic dispersion without the use of surfactants and remained stable throughout the year; the characteristic emulsion size is about 100 nm. Paraffin emulsions are promising material for Phase Change Materials (PCM) applications (heat transfer, heat storage, conditioning).

Using the dynamic and static light scattering methods, these emulsions were studied in a wide temperature range. Authors proposed a new method for determining the temperatures of phase transitions of paraffins based on an analysis of the temperature dependences of the intensity of scattered light [1,2]. The phase transition temperatures of individual paraffins determined in this paper agree well with the available published data.

-
1. V.N. Kuryakov et al 2018 IOP Conf. Ser.: Mater. Sci. Eng. 347 012034. <https://doi.org/10.1088/1757-899X/347/1/012034>.
 2. Ivanova D. D., Kienskaya K. I., Kuryakov V.N. Uspekhi v khimii i khimicheskoy tekhnologii: sb. nauch. tr. [The successes of chemistry and chemical technology, a collection of scientific papers], 2017, V. XXXI, 4 (185), 88-90.

EXPERIMENTAL STUDY OF THERMAL CONDUCTIVITY OF THERMALLY CONDUCTIVE STRIPS FOR ELECTRONIC EQUIPMENT

Sukhikh A.A.,* *Kuznetsov K.I.*, *Skorodumov S.V.*

MPEI (TU), Moscow, Russia

**SukhikhAA@mpei.ru*

The object of research - CONDUCTIVITY OF THERMALLY CONDUCTIVE STRIPS - domestic analogues of the materials of the series SilPad, GapPad and Bond-Play of foreign production, widely represented in the market of electronic equipment. To perform this task, a unit for measuring the thermal conductivity by the method of a flat layer with a stationary heat flux was developed and manufactured. The range of work from the level of nitrogen temperature

to +150 ° C, in addition, the installation is designed in such a way that it can be measuring during loading of the specimen pressurized to 1200 kPa. In order to eliminate heat leaks from the sample due to natural convection, it is provided that the measuring cell is vacuumed, which also ensures that there is no condensation and freezing of water vapor from the ambient air inside the cell when working in the low-temperature range. The geometric configuration of the samples: discs with a diameter of 15 mm and a thickness of 0.5 to 5 mm. Certification experiments were carried out on a sample of optical colorless glass brand TF1 (GOST 13659-96) with a certified characteristic of the dependence of thermal conductivity on temperature in the range of 50-500 K.

1. Tsvetkov F. F., Grigoriev B. A. Heat And Mass Transfer. Textbook for high schools. 2nd edition revised and enlarged // M. publishing house of MPEI, 2005. 550 C. 2. Mereusta E. V., Butov A. R. Investigation of the thermal conductivity for workers fluorocarbon composition method of a plane layer// Potential of modern science. 2016. No. 3. C. 23-31.

METHODS AND MEANS OF THERMOPHYSICAL CHARACTERISTICS MEASUREMENT FOR VEGETABLES AND FRUITS TISSUES

Divin A.G., Ponomarev S.V., Lyubimova D.A.*

TSTU, Tambov, Russia

**agdv@yandex.ru*

The thermophysical characteristics of vegetables and fruits plant tissues depend on their type and variety, structure, water content, as well as the presence of mechanical damages or phyto-diseases. The last circumstance makes it possible to apply thermal methods of non-destructive and noncontact control with using the technical vision systems in the infrared range of the spectrum (8000-14000 nm) when sorting out agricultural products. To determine the regime parameters of the thermal effect, it is necessary to know the real control object thermophysical characteristics in the surface and subsurface plant tissues, which is possible with the use of both contactless and contact measurement methods.

To implement non-contact measurements, the absolute method was used [1], in which the object surface heating was organized by using a laser with a power of 0.5 W and a wavelength of 405 nm through a surface area in the form of a circle during several minutes. To obtain the initial information about the surface temperature of the body, a thermal imager A35 model by FLIR Company was used. The software developed in the LabVIEW 2016 environment serves for image processing, temperature measurement and calculation of thermal conductivity and thermal diffusivity of the tissue.

To determine the thermophysical characteristics of the subsurface plant tissues, a contact regular mode method of the third kind and a pulsed flat-layer method were used.

Conducted calibration measurements on standard samples allowed to reach a maximum thermal conductivity error not more than 7 %.

This work supported by of the Ministry of Education and Science of the Russian Federation in the framework of the Agreement N 14.577.21.0214 (RFMEFI57716X0214)

-
1. Ponomarev S.V., Mishchenko S.V., Divin A.G., Vertogradsky V.A., Churikov A.A. Theoretical and practical basis of thermophysical measurements. M.: FIZMATLIT, 2008.
 2. Lyubimova D.A., Ponomarev S.V., Divin A.G.// Measurement Techniques. 2015. Vol. 57. Num. 12. P. 1423-1429.

**INVESTIGATION OF THE DIFFUSION OF ALLOYING ELEMENTS IN
MULTI COMPONENT ALLOYS OF THE CR-NI SYSTEM USING THE
PHOTOMETRIC ANALYSIS OF THE RADIATION BRIGHTNESS SPECTRA**

Ermishkin V.A., Mikhaylov D.L., Minina N.A., Belousov O.K., Palyi N.A.*

IMET RAS, Moscow, Russia

**minina1951@rambler.ru*

In this paper we consider the results of studying the diffusion of chromium and boron in an alloy G 35 (USA), in the chemical composition of which there were 12 elements. It should be noted that boron on the alloy passport was not specified, but its presence and concentration were established during the current study by the method of photometric analysis of structural images (PHASI), developed in IMET RAS. The method of PHASI is based on comparison according to the differential scheme of the spectra of the brightness of the reflection of visible light from the fragments of the surface of the object under study and their images before, during and after heating. The study was performed in situ in a high temperature metallographic microscope. The digital camera allowed in a periodic mode to register the image of the investigated fragment of the sample surface. Analysis of the data obtained by the PHASI method made it possible to establish the time and radial dependences of the partial derivatives of the concentrations of the first and second order alloying elements that appear in the diffusion equation. A complete analysis of the obtained experimental data made it possible to obtain temperature dependences of the diffusion coefficients of chromium and boron. The obtained values of activation energies of diffusion for these elements are close in magnitude to their estimates known from the literature data. The work was carried out according to the state assignment No 007–00129–18–00 and with the financial support of the Russian Foundation for Basic Research (grant No. 17–08–00098a).

**HIGH-TEMPERATURE TEST BENCH FOR THERMAL SHOCK
RESISTANCE CONTROL CERAMIC COATINGS**

Artamonov A.V., Mazilin I.V., Zaitsev N.G.*

TSPC, Moscow, Russia

**art-bass@mail.ru*

One of the most important thermophysical characteristics (thermal shock resistance) of the ceramic coatings, in particular thermal barrier coatings (TBC), formed on component used at high temperatures. The surface temperature of the components with the TBC during operation can be cyclically changed over a wide interval in a fairly short period of time, which can lead to the TBC damage due to the occurrence of high mechanical stresses, which usually are caused by the differences in the thermal expansion coefficients of coating materials and the base [1]. For this reason, particular interest is the possibility of controlling the thermal shock resistance of the TBC under conditions close to operational ones. The paper presents the results of the TBC thermal shock resistance control. Coatings were formed by use of atmospheric plasma spraying method. One-sided gas heating by a propane-oxygen burner were used to simulate the operating conditions of the components of the hot paths of the gas turbine engine. Differences in the damage mechanisms of TBCs which were formed with use of stabilized material ($ZrO_2-7.5Y_2O_3$) and ($ZrO_2-7.5Y_2O_3$) stabilized and further modified, during powder preparation process, with carbon nanotubes (0.1 wt. %). The influence of the additionally introduced modifier on the TBC thermal shock resistance is discussed.

1. Irene Spitsberg, Jim Steibel Thermal and environmental barrier coatings for SiC/SiC CMCs in aircraft engine applications. Int. J. Appl. Ceram. Technol., 1 [4] 291-301, 2004.

FEATURES OF OHMIC HEATING OF THE SILICONIZED SILICON CARBIDE AT MEASUREMENT OF THERMAL PROPERTIES IN THE FIELD OF HIGH TEMPERATURES

Kostanovskiy A. V., Pronkin A. A., Zeodinov M. G., Kostanovskaya M. E.*

JIHT RAS, Moscow, Russia

**pronkin.a.a@gmail.com*

The silicified silicium carbide SiC+Si is high-temperature material. However, heaters from the silicified silicium carbide usually are used at a temperature below 1600 K.

Basic circuit of the equipment on which features of ohmic heating of the siliconized silicon carbide are realized and investigated at temperatures over 1600 K are presented. It is shown that use of the personal computer original program with two-parameter (current and temperature) a feed-back for regulation of tension brought to an exemplar, and an express inventory allowed to realize the steady steady thermal conditions necessary for determination of resistance. Specific electrical resistance of the siliconized silicon carbide is measured in temperature range 1200–2200 K.

THERMOPHYSICAL PROPERTIES OF THIN FILM COATINGS BASED ON THE HOLLOW MICROSPHERES

Prorokova M. V., Bukhmirov V. V., Gaskov A. K., Suleymanov M. G.*

ISPU, Ivanovo, Russia

**prorokova_mv@list.ru*

The attention of researchers and engineers is currently attracted to energy-saving paints, which are used to reduce heat losses during transport and consumption of thermal energy. Paints based on hollow microspheres have a number of advantages in comparison with traditional types of thermal insulation: low thermal conductivity, low moisture absorption, low corrosion activity and sufficient mechanical strength. Thin-film energy-saving coatings have the properties of paints, which greatly simplifies the process of applying the composition to an insulated surface.

Despite the listed advantages, the thermophysical properties of energy-saving paints have not been adequately studied. The data on the values of the thermophysical coefficients presented in the scientific and technical literature differ by at least an order of magnitude. Therefore, the study of the thermophysical properties of energy-saving paints is currently an urgent task, the solution of which will increase the accuracy of thermal engineering calculations.

The report presents the results of an experimental study of the thermophysical properties of energy-saving paints, in particular, an experimental stand for estimating the coefficient of thermal conductivity and a stand for estimating the coefficient of thermal diffusivity of paints based on hollow glass microspheres and the base in the form of styrene acrylic dispersion «Akrilan 101».

According to the results of a series of experiments, the average value of the thermal conductivity in the temperature range 293 — 373 K was 0,019 — 0,028 W/mK. A range of values for the thermal diffusivity was also obtained.

New experimental data on thermophysical properties of thin-film coatings (energy-saving paints) increase the accuracy of thermal engineering calculations in determining heat losses in multi-layered enclosing structures.

INCREASING CHEMICAL PURITY FUSED BY HIGH TEMPERATURE ANNEALING IN VACUUM

Grigorenko A. V., Belyaev G. E., Vlaskin M. S., Lipatova I. A., Zhuk A. Z.*

JIHT RAS, Moscow, Russia

**belyaev_g@yahoo.com*

The aim of this work was to investigation of the white fused alumina refining process under high temperature in a vacuum. The annealing temperature was 2023 K (1750° C), the pressure in the vacuum chamber was not worse than 3×10^{-3} Pa (2×10^{-5} Torr.)

Three types of industrial samples white fused alumina were investigated. Samples were extracted from the upper part of the 6-ton ingot – the so-called crust, as well as from its middle and bottom parts.

Before and after annealing, granulometric measurements were carried out for each sample by laser diffraction. Average size of samples granules before/after vacuum heat treatment [μm]: ingot crust – 16 / 25, middle part of ingot – 32 / 32, bottom part of ingot – 64 / 65 The chemical composition of the samples (60 elements) was studied by ICP M–S. As a result of heat treatment of samples in vacuum, the total amount of impurities in electro-corundum decreased by approximately an order of magnitude. After processing, the samples of electro-corundum were practically completely purified from impurities such as Na, Mg, K, Mn and Zn. The iron content in the samples was reduced by a factor of 8–10.

The purification process, vacuum refining of corundum consists of three main stages: i) impurity diffusion in the volume of particles to the surface; ii) evaporation of the impurity from the surface of the particle; iii) impurity diffusion along the pores of the particle.

It was shown the possibility of industrial white fused alumina powders purification by high temperature vacuum annealing. The presented results can be used to produce on industrial scale corundum abrasive and refractory materials of high purity.

INFLUENCE OF THE BACKGROUND RADIANCE ON THE MEASURED TOTAL DIRECT POWER OF PT–10%RH ALLOY SPECIMEN

Mendeleyev V. Ya., Kachalov V. V.*

JIHT RAS, Moscow, Russia

**v_mendeleyev@ihed.ras.ru*

When measuring the total direct thermal power radiated by materials in gas environments, it is necessary to either exclude or, if not possible, take into consideration the emission of heated background [1]. An experimental setup was used to determine the contribution of the background to the measured total direct radiance power for Pt–10%Rh alloy specimen.

The experimental setup consisted of an electric heater, a sensor to measure the radiance of a specimen, and a two-part copper housing with water cooled walls. The measuring sensor resembled a water cooler diaphragm and a thermocouple detector [2] behind it. The two parts of the copper housing were installed in between the heater and the water cooler diaphragm, and in between the water cooled diaphragm and the detector. A screen painted by black absorber [3] was mounted on the water cooled diaphragm on the specimen's side. Measurements were taken in the range of temperatures between 72°C and 640°C.

The performed study showed that the main influence on the measured total direct power is caused by the background radiance of the heater unshielded by the specimen and reflected from inner walls of the copper housing. Application of the thermal radiation absorbing material [3] on the inner cavity of the housing allowed measuring the total direct power radiated by the Pt–10%Rh alloy specimen with uncertainty of 2.5% at the temperature of 640°C.

1. R. B. Pérez-Sáez, L. del Campo, M. J. Tello // Int. J. Thermophys. 2008. V. 29. P. 1141.
2. Thermal Power Sensor Head, <https://www.thorlabs.com/thorproduct.cfm?partnumber=S302C>
3. A. V. Grigorevskiy, L. V. Kiseleva, N. V. Strapolova // Astrophys. Space. Sci. Proc. 2013. V.32. P. 177.

PRECISION MEASUREMENTS OF THERMODYNAMIC PARAMETERS OF LOW-BOILING METALLIC LIQUIDS

Blagonravov L.A., Modenov A.A.*

MSU, Moscow, Russia

**blagonravovla@mail.ru*

The results of an investigation of the thermophysical properties of cesium in the region of the anomalous behavior of these properties are given in [1] Interpretation of anomalies is difficult, because of the small magnitude of the effects. In the area of forced growth of the adiabatic thermal pressure coefficient (a.t.c.p.), the magnitude of the effect was 5% with a random error of 2%. The proposed work attempts to increase the accuracy of measurements. It is studied thermodynamic derivatives, namely a.t.c.p.

$$\chi = \left(\frac{1}{T}\right)\left(\frac{\partial T}{\partial p}\right)_s = \frac{\alpha_p}{c_p\rho} \quad (1)$$

where α_p -thermal expansion coefficient and $c_p\rho$ -heat capacity of the volume unit. For the measurement a unit is used in which the pressure change is carried out in a cycle mode. The software allows simultaneous averaging the values of the pressure oscillation amplitude and the amplitude of the temperature oscillation response with subsequent determination of their relationship. It is used in the unit an improved pressure modulator, allowing to create pressure oscillations form close to a sine wave (the value of the second harmonic is not more than 10%). The response temperature variations of the sample were recorded with the help of a precision nano-voltmeter RS-810 with synchronous digital detector. A supercapacitor (ionistor) of large capacity was used to separate the constant and periodic temperature signals, so that it became possible to record simultaneously the amplitude of pressure oscillations, the amplitude of the temperature oscillations of the sample and its current temperature. The technique currently used guarantees the determination of a.t.c.p. with a random error estimated at 0.5 –1%, which allows for a more complete study of the nature of the anomalies of thermodynamic parameters. Several series of the a.t.c.p. measurements were performed with liquid cesium in the temperature range of 320 - 620 K.

-
1. L.A.Blagonravov, S.N.Skovorod'ko, A.S.Krylov, L.A.Orlov et al. Phase Transition in Liquid Cesium near 590 K // J.Non-Cryst Solids 277 (2000) 182-187.

**ON THE DETERMINATION OF THE TRUE TEMPERATURE OF
REFRACTORY METALS BY RADIATION IN THE
"GRAY" APPROXIMATION**

Rusin S.P.

JIHT RAS, Moscow, Russia

sprusin@yandex.ru

As known, radiation thermometers (pyrometers) do not require direct contact with the measured object and have a high speed. Therefore, they are widely used in thermophysical research. However, in this case, it is necessary to know the emissivity ϵ of the site of sight at a given wavelength in the direction of radiation. Moreover, the value of ϵ , as a rule, is unknown.

In this report, the simultaneous determination of the thermodynamic (true) temperature and the emissivity of opaque, free-radiating object from the registered thermal radiation spectrum in the "gray" approximation is considered. It is assumed that in a given spectral interval $\ln \epsilon = a_1 + a_2/\lambda$, where, a_1, a_2 are constant coefficients. It is shown that a measured object can radiate as a "gray" body, even in the case when its emissivity is changing several times over the spectrum. A relation is presented for estimating the accuracy of the "gray" approximation. For refractory metals, the spectral intensities distribution in the visible spectrum of radiation is compared. The use of a tungsten helix as a source of illumination is discussed. Approaches based on more realistic models for emissivity are discussed.

**INTERFERENCE DIAGNOSTICS THE DYNAMICS OF THE TARGET
SURFACE MOVEMENT DURING ABLATION USING A
FREQUENCY-MODULATED LASER PULSE**

Komarov P.S., Struleva E.V.*

JIHT RAS, Moscow, Russia

**komarov-p@yandex.ru*

A technique has been developed for femtosecond spectral interferometry using frequency-modulated diagnostic pulses for the continuous recording of the displacement of the metal film surface. The method of continuous registration on the basis that different spectral components of the diagnostic pulse probe the heated region of the target at different times. The technique allows to obtain images with high spatial and temporal resolution of samples in the picosecond time range.

For the diagnosis of deformation used Michelson interferometer with transfer image (Linnik configuration) of the surface of the sample onto the entrance slit of the spectrometer. The expansion into the spectrum of the frequency-modulated signal from the output of the interferometer was carried out using a diffraction spectrometer. The recording of optical signals at the output of the spectrometer was performed by a CCD camera.

The realized measurement scheme provides continuous registration of the displacement of the sample surface as a function of time with spatial resolution and different time resolution, determined by the dispersion of the spectrometer.

INVESTIGATION OF THERMAL PROPERTIES OF THE PLEXIGLASS ON THE APPARATUS TAU-5

Sviridenko V. I.

VNIIFTRI, Mendeleevo, Russia

visvirid@vniiftri.ru

Apparatus TAU-5 is designed to measure the thermal conductivity and temperature conductivity of solid samples (with an error of 2 % and 5-8 %, respectively) in the temperature range from 80 to 360 K by absolute non-stationary method of a heated circle [1-4]. The method is based on heating by a known heat flux from a thin circular sensor placed between two samples from the test material or between a sample from the test material and a sample from a material with known properties. By recording the dependence of the sensor temperature versus time when it is heated by direct current, information about the thermal properties of the material is obtained. Automatic mode of measurement and subsequent calculation of the recorded results are provided by computer-measuring system "AKSAMIT-6.13" and software. Apparatus TAU-5 was certified as the State working standard of the unit of thermal conductivity of the 2-nd category in the range of 0.02-15 W/m/K. Plexiglass in a symmetrical version was studied at TAU-5, as the most common and reliable material for the standard samples of 3-rd category. The investigation showed hysteresis in the measurement results of the thermal conductivity of the plexiglass. Above 200 K the plexiglass exhibit higher thermal conductivity when the sample is heated than when it is cooled. The discrepancy comes up to 2 %, which is comparable with the error of the standard samples of the 3-rd category 3 %.

1. Karlsru G., Eger D. thermal Conductivity of solids., "Science 1964 487c.
2. Beck J. V. International Journal Of Heat Mass Transfer, 1981. V. 24, p. 155-164.
3. Sviridenko V. I., Ushakov S. I. Method of determining thermal characteristics of materials. Inventor's certificate No 1602184, 22.06.1990.
4. Sviridenko V. I., Ushakov S. I. Investigation of thermophysical characteristics of quartz glass by non-stationary method. V All-Union scientific and technical conference "Metrological support of thermophysical measurements at low temperatures Khabarovsk. Abstracts, part I, 1988, pp. 36-37.

=====
**COMPUTER SIMULATIONS IN
THERMOPHYSICS**
=====

**NEW OPPORTUNITIES IN THE APPLICATION OF THE ClayFF FORCE
FIELD FOR ATOMISTIC COMPUTER MODELING OF NATURAL AND
SYNTHETIC NANOPOROUS MATERIALS AND THEIR HYDRATED
INTERFACES**

Kalinichev A. G.

¹*IMT Atlantique, Nantes, France,* ²*IL-SAMMA, Moscow, Russia*

kalinich@subatech.in2p3.fr

Molecular-level knowledge of the thermodynamic, structural, and transport properties of water and aqueous solutions confined in nanopores and at interfaces with clays, cement, and other natural and synthetic inorganic nanomaterials is crucial for quantitative understanding and prediction of many technological and environmental processes, including rock weathering, geological nuclear waste storage, water desalination, geological carbon sequestration, etc. Atomistic computational modeling is capable to significantly complement the experimental investigations of such systems by providing invaluable atomic-scale picture of the materials and processes involved, leading to a greatly improved understanding of the specific effects of the substrate structure and composition on the structure, dynamics and reactivity of the interfacial and nano-confined aqueous solutions. However, accurate and realistic molecular scale simulations of such materials as clays are often challenging, because of the great diversity of their chemical composition the significant degree of their structural and compositional disorder. ClayFF was originally developed in response to a strong need for a robust and flexible force field for classical atomistic simulations of such materials and interfaces, as well as their interactions with organic and bio- molecules in aqueous environment [1]. This lecture will provide a brief overview of the fundamental assumptions and limitations of the ClayFF approach to the atomistic modeling of these complex systems and demonstrate new opportunities offered by recent improvements of ClayFF, specifically addressing the simulation of a wide range of materials related primarily to clay and cement chemistry [2-4]. [1] R.T. Cygan, J.-J. Liang, A.G. Kalinichev (2004) *J. Phys. Chem. B*, 108, 1255-1266. [2] M.Szczerba, A.G.Kalinichev (2016) *Clays Clay Min.*, 64, 488-502. [3] I. Androniuk, C. Landesman, P. Henocq, A.G. Kalinichev (2017) *Physics and Chemistry of the Earth A/B/C*, 99, 194-203. [4] M.Pouvreau, J.A.Greathouse, R.T.Cygan, A.G.Kalinichev (2017) *J. Phys. Chem. C.*, 121, 14757-14771.

**VISCOSITY OF LIQUID HYDROCARBON MIXTURES: MOLECULAR
DYNAMICS SIMULATIONS AND MIXING RULES**

Pisarev V. V.

JIHT RAS, Moscow, Russia

pisarevvv@gmail.com

The work presents the results of molecular dynamics calculations of viscosity of liquid mixtures in the methane–n-butane–n-pentane system. The TraPPE-EH forcefield [1] is used for hydrocarbons. The viscosity calculations are made using a nonequilibrium molecular dynamics technique [2].

The viscosities of pure components and mixtures are found to agree with the Batchinski equation $\eta = C/(v - b)$, where η is the viscosity, v is the molar volume, C and b are constant characteristic to a liquid. To predict the viscosities of mixtures with arbitrary composition,

Batchinski mixing rule, Arrhenius mixing rule and cubic root mixing rule are tested. The states of pure substances with the same molecular volumes as in mixtures are suggested as the basis states for mixing rules. The Batchinski mixing rule shows the best correspondence between the viscosities predicted by the mixing rules and calculated from direct MD simulations.

The proposed technique allowed us to apply the mixing rules to stable and metastable liquids and liquids with dissolved gas, while typically the mixing rules are only applied to mixtures of liquids.

The work has been supported by the Russian Science Foundation grant no.17-79-20391.

-
1. Chen B. and Siepmann J.I. // J. Phys. Chem. B, 1998. V. 103. P. 5370-5379.
 2. Müller-Plathe F. // Phys. Rev. E. 1998. V. 415. No. 3. P. 604.

THE INFLUENCE OF INTERACTIONS BETWEEN PHONONS ON HEAT TRANSFER

Khvesyuk V.I., Barinov A.A., Qiao W.*

BMSTU, Moscow, Russia

**khvesyuk@bmstu.ru*

The processes of heat transfer in solids are determined by the kinetics of quasi-particles gas called phonons. This is the similarity to the kinetics of classical gases. However, the nature of phonon interactions is much more complex than the interactions of atoms and molecules. First of all, there are a large number of factors affecting phonon kinetics [1, 2]. Such as 1) triple interaction of phonons, accompanied by their merger or decay. 2) Existence of different types of phonons. 3) Availability of different types of interaction processes with phonons. 4) Mean free path of phonons have various dependences on the energy for different polarization types. 5) Another important subject is the phonon interactions with impurities and imperfections of the crystal structure. It is interesting to estimate the relative contributions of these factors to the intensity and nature of heat transfer depending on the temperature of the solid.

In this work, the analysis of listed factors is based on a specially developed code using the Monte Carlo method.

The obtained results are necessary to get more information about the complex processes of heat transfer in solids and to develop the tools that can solve relevant thermal transport problems using Monte Carlo method.

Work was supported by Russian Ministry of Science and Education, project 16.8107.2017/6.7.

-
1. Peierls R.E. Quantum Theory of Solids. Clarendon Press, Oxford. 1955.
 2. Klemens P.G. // Solid StatePhys. – Adv. Res. Appl. 1958. Vol. 7:1-98.

**NUMERICAL AND EXPERIMENTAL INVESTIGATION OF FORMATION
OF WEAKLY CONDUCTIVE LIQUID DIELECTRIC FLOWS CAUSED BY A
HIGH NONUNIFORM ELECTRICAL FIELD**

*Apfelbaum M.S., Gadzhiev M.Kh., Doludenko A.N.**

JIHT RAS, Moscow, Russia

**adoludenko@gmail.com*

A quasi-exponential formula for the current-voltage characteristics of low conductive dielectric fluids in the presence of high-voltage electric field was obtained analytically by solving the system of equations [1]. These equations are for the pre-breakdown charge formation in quasi-neutral media such as transformer oil. The high-voltage electric field is created by the "wire on plane" system of electrodes.

The formation of jets of a weakly conducting liquid formed under the action of an applied electric field of electrodes is studied. The McCormack method, the local mesh refinement and the account of influence of the space charge in fluid on the initial electric field were used for the numerical analysis of fluid flow characteristics. In addition, the results of experimental studies of fluid motion in this statement of the problem are presented. The characteristic velocities of fluid flow in the interelectrode region are given. Images of vortex structures and fluid flows are obtained. The results are presented for several values of the applied DC voltage.

This work was supported by the Russian Foundation for Basic Research (project no. 18-0800136).

-
1. Apfelbaum M.S. and Apfelbaum E.M. // Plasma Phys. Rep. 1998 V. 24 P. 850-856.

COMPOUND THERMODYNAMIC PROPERTIES EVALUATION MODEL

Shults O. V.

RFNC-VNIITF, Snezhinsk, Russia

o.v.shults@vniitf.ru

At present there are many databases and reference books on thermodynamic properties of individual substances, but still there remain a great number of chemical compounds, which thermodynamic properties are described poorly or not described at all.

The problem of missing data on chemical compound properties can be solved by generalizing the available data and taking it as a basis for modelling quantitative structure-property relationships. The paper presents such a model, based on fragmental descriptors approach, which summarizes data on heat capacity, enthalpy, and entropy of compounds. The model allows us to obtain thermodynamic function values for arbitrary compounds made up from fragments derived when analyzing the database of thermodynamic properties for individual substances.

The test calculations by the model are in good agreement with reference data. The relative enthalpy error is about 5%, the estimated entropy error is about 2%, and heat capacity error is 1%.

The reported study was funded by RFBR according to the research project 17-01-00873.

ON-LATTICE MODELS TO STUDY EVOLUTION OF HEA AT ATOMIC SCALE

Meshkov E.A., Novoselov I.I., Yanilkin A.V.*

VNIIA, Moscow, Russia

**novoselov@vniia.ru*

High-entropy alloys (HEA) is a new perspective class of metallic materials. These alloys contain at least four principle elements in approximately equal concentrations. HEAs with outstanding properties have already been discovered. For instance, some of the alloys have excellent mechanical properties at elevated temperatures; others demonstrate good corrosion resistance, and even enhanced radiation tolerance.

However, these effects remain unexplained, since simulation of HEAs at atomic scale is hindered by complex chemical composition of the material. In particular, quantum molecular dynamics (MD) could not reach required time- and space-scales, while classical MD does not provide sufficient accuracy. Therefore, a new approach is needed, which will be capable of accurate and yet computationally feasible description of HEAs at atomic scale.

Such approach is proposed in this work. We describe evolution of a HEA in the framework of kinetic Monte-Carlo, coupled to on-lattice interatomic potential [1]. The model reproduces the results of quantum-mechanical calculations with error less than 5 meV/atom. The proposed approach allows to reveal ordering of FeCoNiCr, and formation of Fe and Cr super-lattices.

The reported study was funded by RFBR according to the research project No. 18-32-00736.

-
1. Shapeev A. // Computational Materials Science. 2017. V. 139. P. 26

CONTINUAL FLUID FILTRATION MODEL

Zakharov S.A.,^{1,2} Pisarev V.V.,¹ Chudanov V.V.¹*

¹JIHT RAS, Moscow, Russia, ²MIPT, Dolgoprudny, Russia

**stepanzh@gmail.com*

This work is aimed to design a program using the model described in [1]. The model includes two continuity equations: for vapor (1) and liquid phases (2). Filtration velocity is defined by Darcy's law with relative permeability functions $f_i(s)$, phases' pressures are supposed to be equal:

$$\begin{aligned} \frac{\partial m\rho_1 s}{\partial t} &= -\frac{\partial \rho_1 u_1}{\partial x} + F_1, \\ \frac{\partial m\rho_2(1-s)}{\partial t} &= -\frac{\partial \rho_2 u_2}{\partial x} + F_2, \\ u_i &= -\frac{k f_i(s)}{\eta_i} \frac{\partial P}{\partial x}, i = 1, 2. \end{aligned}$$

The hydrodynamic equations are combined with equations of state:

$$\rho_i = \frac{\mu_i(P, T)}{z_i(P, T)} \frac{P}{RT}, i = 1, 2.$$

The calculation of supercompressibilities z_i is processed using cubic equation of state, designed by Brusilovsky [2].

This work describes different attitudes for solution of the hydrodynamic equations and their discrete analogues. The validation of the numerical models is provided. The numerical stability

and accuracy is analyzed. The main purpose of the work is describing flows that includes retrograde condensation.

The research is financially supported by Russian Science Foundation (project ID 17-79-20391).

-
1. Zaichenko, V.M., Maikov, I.L., Torchinskii, V.M. et al. High Temp (2009) 47: 669. <https://doi.org/10.1134/S0018151X09050083>
 2. Batalin, O.Yu., Brusilovskii, A.I., and Zakharov, M.Yu., Fazovye ravnovesiya v sistemakh prirodnykh uglevodorodov (Phase Equilibria in Natural Hydrocarbon Systems), Moscow: Nedra, 1992.

NUMERICAL ESTIMATION OF THERMAL CONDUCTIVITY OF EXFOLIATED VERMICULITE

*Skurikhin A. V.,*¹ Kostanovsky A. V.¹*

¹MPEI (TU), Moscow, Russia, ²

**SkurikhinAV@mpei.ru*

An effective method of reducing the volumetric weight and thermal conductivity of thermal insulation materials (TIM) can be using of natural porous fillers, such as exfoliated vermiculite, which is obtained by firing vermiculite concentrate. This material has a number of unique properties: low density, low thermal conductivity, relatively high melting point, chemically inert, durable, environmentally safe [1, 2]. Such properties provide the prospect of its use as a filler in the manufacture of TIM and other materials used in construction, agriculture, chemical industry and energy. Recently the most popular method of prediction of properties of novel composite materials by taking into account a structure, matrix and constituent characteristics is numerical simulation. In this paper we propose a model to describe a structure of exfoliated vermiculite, present the results of calculating the problem of determining heat flux, temperature field and temperature gradient inside its grain using [3, 4] techniques and computing a thermal conductivity and comparing it on the base of data from literature sources.

-
1. Kalyanov N.N. et al. Vermiculite and perlite are porous aggregates for heat insulation products and concretes. Edited by V.A. Kitaeva. State publishing house of literature of building, architecture and construction materials, Moscow: 1961 - 150 p.
 2. K.N. Dubenetsky, A.P. Pozhnin Vermiculite. Stroyizdat, Leningrad department, 1971 - 176 p.
 3. Kellet B.S. The steady flow of heat through hot glass, Journal of the Optical Society of America, Volume 42, Number 5, May 1952.
 4. Sergeev O.A., Men A.A. Thermophysical properties of semitransparent materials. M., Publishing house of standards, 1977, 288 p.

COMPUTATIONAL APPROACHES TO DETERMINING ISOTHERMAL COMPRESSIBILITY AND FLUCTUATION PARAMETER OF LIQUIDS

Nedyalkov Yu. V., Postnikov E. B.*

Kursk SU, Kursk, Russia

**ynedyalkov@gmail.com*

The Fluctuation Theory-based Tait-like Equation of State (FT-EoS) proposed in the work [1], $\rho = \rho_0 + k^{-1} \log [k\rho_0\kappa_T^0(P - P_0) + 1]$, which is shown as a tool for the high accurate prediction of the density under high pressures in liquid matter, varying from organic to ionic

liquids [2], require a knowledge not only the density ρ_0 at normal or saturated pressure P_0 but also the isothermal compressibility as its derivative included into the parameter k at the respective conditions.

Here we consider practical spreadsheet-based program implementations of procedures for their computations based either on the reference experimental data, such as the density, the isobaric heat capacity, and the speed of sound, or on the purely predictive methods utilizing the data on molecular structure and parameters and a group contribution approach. The latter set of methods allows also determining the speed of sound in hydrocarbon liquids referring to properties presented in standard databases such as DIPPR 801 (AIChE) [3] discussed in the context of molecular packing and the density fluctuations. In addition, the general algorithm of the usage of parsing SMILES chemical identifier aimed to be used in different group contribution methods for calculating thermodynamic properties will be presented supplied with routines, which do not require a coding on user's end.

The work is supported by RFBR, Research Project No. 16-08-01203.

1. Postnikov E.B., Goncharov, A.L., Melent'ev, V.V. // Intern. J. Thermophys. 2014. V. 35. P. 2115.
2. Chorążewski M., Postnikov E.B., Jasiok B., Nedyalkov Yu.V., Jacquemin J. // Scientific Reports. 2017. V. 7: 5563
3. Postnikov E., Nedyalkov Y, Polishuk, I. // Mendeley Data. 2018 <http://dx.doi.org/10.17632/zshnj5c7v7.1>

KOLMOGOROV FLOW AND ITS NUMERICAL SIMULATION IN A FLAT CHANNEL

Fortova S. V.

ICAD RAS, Moscow, Russia

sfortova@mail.ru

Based on numerical experiments we investigate 2D flow of a weakly conductive inviscid compressible medium under the influence of the periodic external force. Direct numerical simulation using Euler equations allows to simulate periodic vortex structures in the flow, which are similar to the mode of “parquet” in the Kolmogorov's flow. The result of this work is a direct numerical simulation of the formation of the vortex flow regime of the “vortex parquet” type in a layer of weakly compressible normal medium based on the Euler equations. It is shown that the formation of this flow is significantly influenced by the initial conditions. Namely, a small perturbation of the velocity components leads to the appearance of a “vortex parquet”. During the numerical experiment, the instability of the formed flow and the transition to chaos were found. The results of this study once again emphasize the fact that the development of the turbulent process can occur in the absence of the influence of viscosity and walls.

MODELING OF THE ALUMINA CLEANING BY MEANS OF HIGH TEMPERATURE EVAPORATION INTO VACUUM

Ivanov P.P., Vlaskin M.S., Zhuk A.Z.*

JIHT RAS, Moscow, Russia

**peter-p-ivanov@yandex.ru*

Considering a porous granule to be an ensemble of solid micro-particles the mathematical model is developed for the high temperature vacuum cleaning of alumina from ferrous impurity [1]. Three parts of the process are identified: the diffusion in solid, the evaporation into vacuum

and the filtration through pores into outer space. Diffusion as a limiting factor is overwhelming compared with evaporation, and this issue makes possible the use of analytical solutions for the treatment of experimental data. The equation describing the abatement of impurity in time is found to be like:

$$\frac{d \ln(\rho_{AV})}{dt} = -\frac{1}{\chi} \quad \chi = \frac{R}{4} \left(\frac{\rho^*}{J^*} + \frac{R}{4D} \right) \quad J^* = \frac{p_{Fe}}{v_T} \quad v_T = \sqrt{\frac{2\pi kT}{m}}$$

Here χ - characteristic time of the cleaning, when the concentration of impurity falls $\exp(1)$ times, R - radius of the micro-particle, D - diffusion coefficient for the iron atoms in the alumina, ρ^* - initial uniform density of the impurity, J^* - evaporation flux into vacuum according to the equation of Hertz-Knudsen [2], v_T - thermal velocity of vaporized iron atoms, p_{Fe} - saturated iron vapor pressure accounting the relative density in the solid, m - the mass of the iron atom. The filtration of impurity atoms through pores of the granule, composed of solid spherical micro-particles, is described by the Knudsen diffusion model.

Results of the modeling show that the efficiency of the cleaning (less the time and more the depth) depends on the dimensions of solid micro-particles constituting the granule and on the porosity of granule. Reasonable cleaning time (about several hours) is observed for the radius of micro-particles at the level of 1 micron and for the high porosity of granules (0.3).

The work was supported through a grant of the Russian Science Foundation (project No. 14-50-00124).

1. Zhuk A.Z., Vlaskin M.S., Grigorenko A.V., Kislenco S.A., Shkolnikov E.I. Synthesis of high-purity α -Al₂O₃ from boehmite by high temperature vacuum treatment // Journal of Ceramic Processing Research. 2016. V. 17. N9. P. 910-918.
2. Jafar Safarian and Thorvald A. Engh. Vacuum evaporation of pure metals // Metallurgical and materials transactions. 2013. V. 44a. P. 747.

APPLICATION OF TURBULENCE PROBLEM SOLVER (TPS) SOFTWARE COMPLEX FOR FOR THE NUMERICAL SIMULATION OF THE EFFECTS OF FEMTOSECOND LASERS ON METALLIC SUBSTRATES.

*Shepelev V. V.,^{*1} Fortova S. V.,¹ Inogamov N. A.²*

¹ICAD RAS, Moscow, Russia, ²ITP RAS, Chernogolovka, Russia

^{*}vadim.aries@gmail.com

The work is dedicated to the use of the software package Turbulence Problem Solver (TPS) for numerical simulation of a wide range of laser problems. The capabilities of the package are demonstrated by the example of numerical simulation of the interaction of femtosecond laser pulses with thin metal bonds. The software package TPS developed by the authors is intended for numerical solution of hyperbolic systems of differential equations on multiprocessor computing systems with distributed memory. The package is a modern and expandable software product. The architecture of the package gives the researcher the opportunity to model different physical processes in a uniform way, using different numerical methods and program blocks containing specific initial, boundary conditions and source terms for each problem.

ON THE DEVELOPMENT OF THERMODYNAMIC MODELING TOOLS FOR COMPLEX HIGH-TEMPERATURE SYSTEMS

Belov G. V., Aristova N.M.*

JIHT RAS, Moscow, Russia

**gbelov@yandex.ru*

The calculations of the parameters of the equilibrium state of multicomponent heterogeneous systems are widely used in the practice of investigation of high-temperature processes with chemical reactions. Probably the first universal method of calculating equilibrium was presented in 1951 in the work of NASA employees “General Method and Thermodynamic Tables for Computation of Equilibrium Composition and Temperature of Chemical Reactions”. In the USSR, a method for calculating the equilibrium composition and properties of the combustion products of rocket fuels was also developed, a computer program and a database on the thermodynamic properties of substances were created, and in 1971 a reference book was prepared “Thermodynamic and thermophysical properties of combustion products”. Later in Baumsn Moscow Higher Technical School a method and a universal algorithm of thermodynamic calculation of multicomponent heterogeneous systems were developed and the program ASTRA was created. The program was used to solve a wide class of problems, in particular, metallurgical and plasma chemical problems. Based on the ASTRA algorithm, a program REAL has been developed for calculating the equilibrium composition and properties of complex thermodynamic systems using the nonideal gas model. Unfortunately, in real processes, thermodynamic equilibrium is not always achieved. For example, when the combustion products in a rocket engine nozzle expand, they are cooled, as a result the chemical reaction rates decrease, the composition is partially “frozen”. To analyze these and similar processes, it is necessary to use methods combining the capabilities of thermodynamics and kinetics. Such an approach has been used, in particular, in the creation of software systems CHEMKIN and Chemical Workbench.

COMPUTER SIMULATION OF THE THERMOPHYSICAL PROPERTIES OF THE RADIOACTIVE GRAPHITE-CO₂ SYSTEM

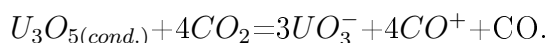
Barbin N.M.,^{1,2,3,4} Sidash I.A.,¹ Terentev D.I.,¹ Alekseev S.G.^{1,4}*

¹UISFS of EMERCOM of Russia, Yekaterinburg, Russia, ²UFU, Yekaterinburg, Russia,

³USAU, Yekaterinburg, Russia, ⁴SEC RLSUB RAS, SEC RLSUB RAS, Russia

**NMBarbin@mail.ru*

The thermophysical properties of the equilibrium system of radioactive graphite-carbon dioxide calculated by means of the program complex TERRA [1]. The main contribution to the thermophysical properties of the condensed system contributes carbon to the temperature of its combustion (973 K). At temperatures over 973 K the thermophysical properties of the system are determined by the vapor phase. On the basis of the obtained data highlighted 4 main temperature ranges in which happen changes of the thermophysical properties of the system. The change of thermophysical properties of the system in the temperature range from 373 to 673 K, presumably associated with the beginning of the reaction $U_3O_{5(cond.)} + 4CO_2 = 3UO_3^- + 4CO^+ + CO$. The change in the thermophysical properties of the system in the temperature range from 673 to 973 K is due to the course of the reaction $U_3O_{5(cond.)} + 4CO_2 = 3UO_3^- + 4CO^+ + CO$ and the disappearance of condensed C. The change in the thermophysical properties of the system in the temperature range from 973 to 2573 K is linear and is determined by the vapor-gas phase. The change in the thermophysical properties of the system in the temperature range from 2573 to 3273 K is due to the course of the reaction



1. Barbin N.M., Sidash I.A., Terentev D.I., Alekseev S.G. Computer modeling of thermal processes with calcium, strontium and cesium radionuclides when radioactive graphite is heated in the carbon dioxide atmosphere. *Izvestia Vysshikh Uchebnykh Zawedeniy. Yadernaya Energetika*, 2017. No. 1. P. 73-82.

THERMODYNAMIC MODELLING IN COMPUTING BACK-END MATERIAL BALANCE

Paukova A.E., Shults O.V., Peshkichev I.V., Pugachev V.Yu.*

RFNC-VNIITF, Snezhinsk, Russia

**paukovaee@mail.ru*

Within the framework of “Proryv” project [1] work is underway toward mathematical modelling of spent nuclear fuel (SNF) reprocessing and fuel fabrication technologies; the software complex (SC)VIZART [2] has been developed for validation and optimization of back-end process parameters.

In modelling back-up processes some uncertainties arise related both to SNF composition of candidate reactor facilities, and to newly developed processes. Full-scale experimental development is hampered by the absence of SNF samples, and the difficulty of processing actual highly-active compositions. One of the methods to evaluate technological parameters under such circumstances is thermodynamic modelling.

For this purpose RFNC-VNIITF is currently developing SC TeDy [3], which allows computing chemical-equilibrium compositions of systems of varying complexity. The computations use the data base containing information on substance properties typical of nuclear fuel cycle (NFC) technologies. SC TeDy is able to operate standalone as an application with user interface, and it is usable in balance computations.

The results of related computations by SC VIZART and SP TeDy are used by developers of SNF reprocessing and nuclear fuel fabrication technologies to analyze and evaluate different alternative technologies.

The reported study was funded by RFBR according to the research project No 17-01-00873.

1. Adamov E.O., Aleksakhin R.M., Bolshov L.A., Dedul A.V., Orlov V.V., Pershukov V.A., Rachkov V.I., Tolstoukhov D.A., Troyanov V.M. The project “PRORYV” is a technological base for large scale nuclear power engineering // *Izvestia RAN. Energetika*. 2015. No. 1. P. 5–12.
2. Schmidt O.V., Makeeva I.R., Liventsov S.N. Modelling of back-up technological limits as a tool to create and optimize industrial processes. // *Radiokhimiya*. 2016. V. 58. No. 4. P. 316–323.
3. Peshkichev I.V., Kuropatenko V.F., Makeeva I.R., et al. TeDy software complex to solve thermodynamic modelling problems. // *Vestnik UuUrGU. “Mathematical modelling and programming” series (Vestnik UuUrGUMMP)*. 2018. V. 11. No. 1. P. 84–94.

DEVELOPMENT OF THE DATABASE OF THERMODYNAMIC FUNCTIONS OF AIR IN A WIDE RANGE OF TEMPERATURES AND PRESSURES FOR SOFTWARE PACKAGES OF HYPERSONIC FLOW SIMULATION

Rozhdestvensky A. V.

MRDB, Miass, Russia

src@makeyev.ru

Increasing requirements for the accuracy and quality of aerodynamic calculations lead to an increase in the number of cells in the grid, which, despite the continuous growing performance of processors, forces researchers to look for ways to reduce the number of arithmetic operations per element of the grid. With reference to the problem of modeling the thermodynamic properties of air, the above arguments suggest the use of approximation of table-given thermodynamic and thermophysical data by bicubic splines $S(p, t) = \sum_{k=0}^3 \sum_{l=0}^3 a_{k,l} p^k t^l$. In this case, the total volume of the coefficients of the bi-cubic spline approximating the given table is equal to the size of the table multiplied by 16, which, in principle, allows to keep in the operating memory of the processor spline coefficients constructed from large tables. The above approach is applied to modeling the following thermodynamic and thermophysical values of air as functions of pressure and temperature: density, enthalpy, entropy, specific heat at constant pressure, sound velocity, dynamic viscosity and thermal conductivity. As a starting material for modeling these values at temperatures from 200 to 12000 degrees Kelvin and pressures from 0.001 to 300 atmospheres tables from the books [1] and [2] were chosen.

On the basis of the obtained realization of thermodynamic and thermophysical quantities, a "user-defined real gas model" was created in programming language "C" for the ANSYS FLUENT 18.2 package, which was then validated on the problems of flow around a blunt body with a hypersonic flow of air, taking into account the available experimental data.

-
1. Predvoditelev A.S. and others. *Tablitsy termodinamicheskikh funktsiy vozdukha* [Tables of thermodynamic functions of air]. Moscow, USSR Academy of Sciences Publ., 1957, 1962.
 2. Vargaftik N.B. *Spravochnik po teplofizicheskim svoistvam gazov i zhidkostey* [Handbook of thermophysical properties of gases and liquids]. Moscow, "Science" Publ, 1972

SYNERGETIC MECHANISM OF THERMAL DESTRUCTION OF TWO-PHASE CONTACT MATERIALS

*Kuanishev V.T.,*¹ Sachkov I.N.,² Sorogin I.G.,³ Sorogina T.I.²*

¹UISI, Ekaterinburg, Russia, ²UrFU, Ekaterinburg, Russia, ³USURT, Ekaterinburg, Russia

**kuan06@mail.ru*

One of the poorly studied factors of the electrical contacts degradation is the spatial inhomogeneity of the Joule heat release. The mechanism of the appearance of a kind of «thermal structure» when the topological defects of the structure and impurities contained in the metal become centers of intensive heat release is considered in work [1]. This paper reports on investigation of the possibility of synergetic mechanism of thermal cracks occurrence and growth in two-phase contact and resistive materials. To calculate the spatial distribution of Joule heat $q(x, y)$, a system containing weakly conducting circular inclusions and rectangular nonconductive cracks was considered [2].

The analysis of $q(x, y)$ and the values of effective conductivity σ_{ef} at varied values of crack length, conductivity σ_i and the concentration C_i of inclusions allow us to conclude that at a certain point on the surface of the inclusion under the considered conditions the peak of heat

release more than 5 times higher than the average value for the sample is formed, which leads to a concentration of thermal stresses.

1. Icryannikov V.I. // J. Eng. Physic. 1992. V. 62. N. 4. P. 617.
2. Kuanishev V.T., Sachkov I. N., Sorogin I. G., Sorogina T. I. // The concentration parameter thermal microstresses as the thermophysical characteristics of two-phase materials // Journal of Physics: Conf. Series. 2017. V. 891.

**THREE-DIMENSIONAL NUMERICAL MODELING OF DEVELOPMENT OF
THE INSTABILITY OF THE CONTACT SURFACE OF COLLIDING
METALLIC PLATES IN GAS DYNAMICS APPROACH**

*Fortova S. V., Utkin P.S.**

ICAD RAS, Moscow, Russia

**pavel_utk@mail.ru*

The work presents the results of the numerical modeling of the development of the instability of the contact surface of colliding metallic plates. Mathematical model is based on the Euler system of equations for the medium with two-terms equation of state. Parameters of the equation of state are calibrated using experimental and numerical data based on the real wide-range equations of state for the metals. Numerical algorithm is based on the Harten-Lax-van Leer scheme. Initial sinusoidal disturbance of the contact boundary between the plates after the rarefaction waves passing from the free boundaries of the plates obtained crater-shaped form. The fact qualitatively corresponds to the natural experiments.

**THERMOPHYSICAL PROPERTIES OF
MATERIALS FOR NUCLEAR POWER
ENGINEERING**

HEAT TRANSFER IN SUPERCRITICAL WATER

Rutin S.B., Skripov P.V.*

ITP UB RAS, Ekaterinburg, Russia

**ryutin.sergey@gmail.com*

The first experiments in the near supercritical region of parameters, carried out under unsteady conditions of heat transfer in various liquids, including water, revealed a conspicuous paradox. If in stationary conditions the peak of the isobaric heat capacity influences the results of the experiments, then under unsteady experiment the influence of this peak is completely absent. Moreover, the effect of a threshold decrease in the heat transfer intensity is detected, which is expressed the stronger the closer the pressure value to the critical value.

The observed effect is undoubtedly of fundamental importance, since the interpretation of the physical picture, expressed in the form of isobaric heat capacity peak, again becomes open.

The practical application of the effect is also examined. There are essential reasons to believe that the choice of operating pressure near the critical one, usually 25 MPa, is not optimal. In addition, according to the results of our experiments, a roadmap for further steps has been formulated, which makes it possible to approximate the development of nuclear reactors cooled by supercritical water.

This study was supported by the Russian Foundation for Basic Research (grant no. 16-08-00381-a) and by the Presidium of UB RAS Complex Program (grant no. 18-2-2-3).

**MODELS DESCRIBING EVOLUTION IN UO₂ FUEL PROPERTIES UNDER
IRRADIATION**

Likhanskii V. V.

SC "RC RF TRINITI", Moscow, Troitsk, Russia

likhansk@triniti.ru

The report reviews physical mechanisms and existing theoretical concepts on the evolution of the microstructure and thermo-mechanical properties of UO₂-based fuels irradiated in a nuclear reactor. The main parameters determining the rates of physico-chemical and thermomechanical processes are the temperature and specific fission rate of heavy-atom nuclei in the uranium dioxide fuel.

Modern fuel performance codes take into account the dependence of the thermal conductivity of nuclear fuel on temperature, burnup, porosity, stoichiometry, and the concentration of the dopants. The basic mechanisms of energy transfer in uranium dioxide are considered. Taking into account gas parameters in the fuel-pellet gap, as well as the spatial distribution of the plutonium isotopes build-up, is necessary for calculating temperature distribution. The report presents physical models for evolution of porosity and grain size in nuclear fuel under irradiation. Particular consideration is given to the effect of the formation and growth of a fine-grained rim-layer on the peripheral surface of the fuel pellets when certain burnup values are reached.

Since most of the physical processes in nuclear fuel are interdependent, it is necessary to develop fuel performance codes that are capable of correct modeling of the thermomechanics of fuel rods. The capabilities of the modern RTOP fuel performance code and its applications

for the tasks of fuel cycle assessment at NPPs with WWER reactors and justifying the safe operation of nuclear fuel are discussed. In many countries with highly developed nuclear power sector, research and development work is performed to increase safety and economic efficiency in the operation of nuclear fuel, and in subsequent stages of SNF storage and processing. To implement these tasks, modern computer technologies are used and new digital platforms are being developed.

The report presents several computational complexes for solving the problems of operating nuclear fuel, justifying the technology of dry storage of SNF produced in Russia, carrying out design works for justifying and introducing new fuels. These computational complexes are based on the series of RTOP codes, a thermal-hydraulics module and a StatVerSet module for performing probabilistic analysis and estimating the sensitivity of calculation results to the uncertainty of the parameter values.

PROCESSING OF HETEROGENEOUS DATA OF EXPERIMENTS AND CONSTRUCTION OF RECOMMENDED RELATIONS

*Chusov I.A.,^{*1} Didenko V.I.,¹ Obysov N.A.,² Novikov G.E.,² Pronyaev V.G.³*

¹*INPE MEPhI, Obninsk, Russia,* ²*Rosatom, Moscow, Russia,* ³*Atomstandart, Moscow, Russia*

**igrch@mail.ru*

The report describes the developed method of evaluation of heterogeneous thermodynamic and thermophysical experimental data, and its software implementation in the form of a complete software tool.

Under the term “heterogeneous ... data”, the authors understand the sets of experimental points obtained in different years (currently, the time range of accepted papers ranges from 1919 to 2014), by different authors or groups of authors, by different methods, with different degrees of purity of the materials and so on. The latter circumstance has become particularly relevant in the last two decades due to the significant improvement in the quality of measurements with the use of very precise measurement methods.

The main feature of thermophysical and thermodynamic data focused on atomic energy is relatively small sets of experimental values obtained by different authors. Usually their number does not exceed eight or ten points. And only recently, the works began to appear in which the number of experimental points is more than ten or fifteen. The reason for the “scarcity” of the experimental material is the extreme complexity and high cost of the experiment with parameters varying in a wide ranges.

The report describes the developed method of evaluation of experimental data taking into account the specifics of nuclear power and its program implementation.

The description of the developed database, its components and web-implementation is given.

**THEMOPHYSICAL PROPERTIES OF
MATERIALS FOR AVIATION, ROCKET AND
SPACE TECHNOLOGIES**

**ANALYSIS OF THE NITROGEN PLASMA JET DESTRUCTIVE EFFECT ON
THE HEAT-RESISTANT MATERIALS**

Khromov M.A., Chinnov V.F., Sargsyan M.A., Kavirshin D.I., Scherbakov V.M.,
Efimov A.V.*

JIHT RAS, Moscow, Russia

**volteg@mail.ru*

Processes of heat and mass transfer in the interaction zone of a high-temperature subsonic plasma stream with the surface of an ablating heat-resistant material determine the rate of its destruction [1–4]. Intensive work is being carried out to create and study new heat-shielding materials based on composites (SiC/C, HfB₂-SiC, etc.), and the mechanisms of their destruction under the influence of high-temperature and chemically active media are studied in detail [2–4]. The purpose of this study is to establish changes in the parameters and composition of the plasma in the destructive interaction zone of an incident high-enthalpy nitrogen plasma jet and samples from carbon-containing materials. The complex [4] created in the JIHT RAS provides the possibility for creating and studying the plasma of various gases (Ar, He, N₂, air) and their mixtures over a wide range of temperatures (T=10–30 kK), mass flows 0.2–5 g/s and velocities of 50–1000 m/s in the output section of the plasma torches. An experimental estimate of the mass loss rate of the sample material in real time is performed by the methods of two-position high-speed video imaging and the method of laser profilometry developed by the authors using a "laser knife" [5]. The studies used isotropic MPG-6 graphite with a cylindrical shape and density of $\rho \approx 1.70\text{--}1.8 \text{ g/cm}^3$, and anisotropic graphite UPV-1T with a density of $\rho \approx 2.1\text{--}2.2 \text{ g/cm}^3$ in the form of a parallelepiped with a characteristic thickness of 3–5 mm and a side of 15–25 mm.

At specific thermal loads of 1–2 kW/cm², experimental data revealed spatial-temporal changes in the samples materials decrease rate (3–20 mg/cm²s), their surface temperature (2000–3500 K), the electron temperature of the incident plasma stream (12000–6000 K), plasmochemical composition in the region of "injection" of the products of destruction.

A joint analysis of the spatial-temporal variations in the concentration of the main destruction byproducts, carbon atoms and the CN radical, and the rate of loss of the carbon-containing sample material, makes it possible to establish the relative role of the processes of heterogeneous ($C_{solid} + N \rightarrow CN$) and homogeneous ($C_{gas} + N + M \rightarrow CN + M$) carbon nitridation in the interaction zone.

The work is carried out with the partial support of the Russian Foundation for Basic Research on grants No 16-08-00323 and No 17-08-00816.

1. Mihatulina D.S., Polezhaev Yu.V., Reviznikov D.L. Teploobmen, termohimicheskoe i termoerozionnoe razrushenie teplovoy zashchity. Moscow, Yanus-K, 2011.
2. Helber B., Turchi A., Scoggins J.B., Hubin A., Magin T.E. // Int. J. Heat. Mass. Tran. 2016. V. 100. P. 810.
3. Lei L., Yiguang W., Liping L., Liyuang D., Guolin W., Yonghong L. // Carbon. 2016. V. 103. P. 73.
4. Chinnov V.F., Tyuftyaev A.S., Kavirshin D.I., Ageev A.G., Sargsyan M.A., Gadzhiev M.Kh. // High Temp. 2018. V. 56. No. 1. P. 25.
5. Ageev A.G., Kavirshin D.I., Sargsyan M.A., Gadzhiev M.Kh., Chinnov V.F. // Int. J. Heat. Mass. Tran. 2017. V. 107. P. 146.

THERMOPHYSICAL AND PHYSICOMECHANICAL PROPERTIES OF PRODUCTS OBTAINED BY SELECTIVE LASER MELTING

Kashapov N.F.,* Kashapov R.N., Kashapov L.N.

Engineering Institute of KFU, Kazan, Russia

**kashnail@gmail.com*

Additive Manufacturing is one of the fastest growing areas of engineering. They allow you to make any product layer-by-layer technology on the basis of a three dimensional model: a new product is “grown” from “nothing” (from a consumable material in the form of the powder or polymer “wire”). Depending on the technology, the object may receive various properties that differ from the properties of the primary consumable material.

The method of selective laser melting (SLM), one of the technologies of additive manufacturing, is increasingly used in the industry of the Republic of Tatarstan. Such large enterprises as KAPO OJSC, KMPO OJSC and Sokol Design Bureau are beginning to use this technology to create prototypes of metal powders, master models and molds for aviation equipment. To introduce this technology into production, it is necessary to investigate the properties of products obtained by selective laser melting.

The most widely used in the SLM production are powders of tool and stainless steels. One of such powders is stainless dispersion-hardening martensitic steel 17-4 PH (15-17.5 Cr, 3-5 Ni, 3-5 Cu, < 1 Mn, Si, 0.15-0.45 Nb, balance Fe). or a long time, steel 17-4 PH was the most popular among the dispersion-hardening grades, due to the flexible variation of its properties, and was actively used in the aerospace and chemical industries. But there are differences in thermophysical and physicomechanical characteristics between products created using SLM technology and products machined on lathes.

The aim of the work is to study the thermophysical and mechanical characteristics of metal products obtained using SLM technology from 17-4 PH steel powder.

To this end, the following tasks were solved: 1) forming samples from 17-4 PH steel powder using the SLM method; 2) carrying out heat treatment of samples; 3) conducting research on the thermophysical and mechanical characteristics of the samples before and after heat treatment; 4) determination of the optimal modes of SLM processes and heat treatment.

**CALORIMETRIC INVESTIGATION OF PHASE BEHAVIOR OF
HYDROCARBON MIXTURES WITH LOW CONTENT OF HIGH
MOLECULAR COMPONENTS (C4+)**

Buleiko V.M., Grigoriev B.A.*

Gazprom-VNIIGAZ, Moscow, Russia

**V_Buleiko@vniigaz.gazprom.ru*

The results of calorimetric investigations of phase behavior of binary mixture (methane-propane), ternary mixtures (methane-propane-heptane and methane-propane-decane) and seven-component mixtures (methane-ethane-propane-butane-pentane-heptane-decane and methane-ethane-propane-butane-isobutane-pentane-octane) are presented. The thermodynamic properties, phase behavior and kinetics of phase transitions of liquid and gaseous hydrocarbons have been studied in the temperature range from 100 to 370 K and in pressure range from 0.1 to 40 MPa. A method of precision adiabatic calorimetry makes possible to construct the phase diagrams of hydrocarbon mixtures, as well to determine with higher accuracy PVT data of condensate dew points. Phase transitions are determined by the discontinuity of directly measured specific heat and temperature derivative of pressure at constant volume. Our particular attention is paid to the hydrocarbon mixtures with low content of high molecular components (condensate-to-gas ratio), due to the fact that standard methods with the use of conventional PVT experiments not guarantee the efficiency and accuracy of phase diagram. Hydrocarbons with four and more carbon atoms are called C4+ components and the entity of all C4+ components is called C4+ fraction. A particular C4+ component will belong to the high molecular component. Our investigations show that if the content of C4+ fraction is less than 2.0 mol %, the phase behavior of hydrocarbon mixtures is qualitatively differed from traditional phase behavior. The region of phase state of hydrocarbon mixtures with low content of high molecular components includes the extensive domain of uncertainty and cannot be studied by conventional PVT experiments and cannot be prognosticate theoretically.

Data of our measurements show that phase diagrams of seven-component hydrocarbon mixture with low content of high molecular components are drastically transformed compared to traditional concepts. For example, hydrocarbon mixture (methane-ethane-propane-butane-pentane-heptane-decane) is separated into a macroscopic phase enriched by methane, ethane, propane and two microscopic phases enriched by isobutane-pentane, and heptane-decane. We define a macroscopic phase as the phase formed and enriched by components of high concentration in the original homogeneous state. A microscopic phase is the phase formed and enriched by components of low concentration in the original homogeneous state. It is found out that these phases are equilibrium phases. To prove that all phases are equilibrium phases the cooling regime of measurements is used. At cooling regime of measurements the same phase transitions as at heating regime occur. These phase transitions correspond to formation of two microscopic phases enriched by heptane-decane and isobutane-pentane and formation of macroscopic phases (liquid-vapor) enriched by methane-ethane-propane.

To reveal the impact of individual hydrocarbon components on seven-component phase diagram the binary and ternary mixtures, represented as that in a set of quasibinary mixtures, have been studied. The content of decane and heptane in ternary mixtures was less than 2.0 mol %. A ternary mixture methane-propane-decane is separated into a macroscopic phase enriched by methane-propane and a microscopic phase enriched by decane. A liquid phase of ternary mixture methane-propane-heptane is separated into layers (liquid-liquid).

This work was supported by the Russian Foundation for Fundamental Research under Grants No. 16-08-00032.

PHASE TRANSITIONS AND CRITICAL PROPERTIES OF 1-PROPANOL —N-HEXANE SYSTEM

*Bazaev A.R., Bazaev E.A.**

IGR DSC RAS, Makhachkala, Russia

**emilbazaev@mail.ru*

By the method of isochore fracture using experimental data on p, ρ, T -dependences of 1-propanol+n-hexane system (0.2, 0.5, 0.8 and 0.9 mol. fractions of n-hexane (x)) in two-phase, one-phase (gaseous and liquid) regions parameters of liquid–vapor phase transitions p_s, ρ_s, T_s [1, 2] are obtained. Using power function including scaling behavior parameters of critical points p_k, ρ_k, T_k are also obtained.

The dependence of pressure on density, temperature and composition of mixtures along the curve of phase coexistence is described by three parameters polynomial equation of state, represented by expansion of the compressibility factor $Z = p/RT\rho$ into a power series of reduced density $\omega = \rho/\rho_k$, and reduced temperature $\tau = T/T_k$ and composition x:

$$Z = \frac{p}{RT\rho_m} = 1 + \sum_{i=1}^m \sum_{j=0}^n \sum_{k=0}^s a_{ijk} \omega^i x^k / \tau^j,$$

and $p = RT\rho_m \left[1 + \sum_{i=1}^m \sum_{j=0}^n \sum_{k=0}^s a_{ijk} \omega^i x^k / \tau^j \right]$.

The average relative deviation of calculated values of pressure from experimental ones does not exceed 1%.

The dependence of density of mixtures along the curve of phase coexistence far from critical point in symmetrical part is described by equations:

$$\rho = \rho_k \left(1 \pm B_0 \tau^{\beta_0} + B_1 \tau^{\beta_1} \pm B_2 \tau^{\beta_2} + \dots \right),$$

$$(\rho_f - \rho_g) / 2\rho_k = B_0 \tau^{\beta_0} + B_2 \tau^{\beta_2} + B_4 \tau^{\beta_4} + \dots,$$

where $\tau = (T - T_k)/T_k$ and $\omega = (\rho - \rho_k)/\rho_k$.

The average relative error is 1.5%..

-
1. Bazaev E.A., Bazaev A.R., Dzhapparov T.A. Research of phase transitions and critical properties of ethanol+n-hydrocarbon binary mixtures // Vestnik Kazanskogo tekhnologicheskogo universiteta. 2010. N.2. pp. 242-249.
 2. Bazaev E.A., Bazaev A.R., Karabekova B.K. Phase transitions (liquid-vapor) and critical properties of n-propanol+n-pentane binary mixture. // Vestnik Kazanskogo tekhnologicheskogo universiteta. 2014. V.17. N.21. pp.89-92.

EFFECT OF MOISTURE ON HEAT TRANSFER IN LIQUID HYDROCARBONS UNDER IMPULSE HEATING OF A WIRE

Lukyanov K. V., Kotov A. N., Starostin A. A., Skripov P. V.*

ITP UB RAS, Ekaterinburg, Russia

**r.t.f@bk.ru*

Rapid local heating can be observed in friction units with oil lubrication, in cycles of cooking and burning of fuel in engines and reactive plants and other process units. As a rule, in real processes, liquid hydrocarbons may contain impurities of moisture. To study the effect of moisture in saturated hydrocarbons, the technique of powerful local heating of a wire probe was used. The main task was to elucidate the influence of the moisture impurity on the intensity of non-stationary heat transfer when the probe was heated above the normal boiling point of the components. Experiments were carried out on samples of hexane, decane, hexadecane with a moisture content of 5 to 35 ppm. Moisture additives were introduced from the vapor phase through the free surface of the liquid and controlled by the Karl Fischer method. It turned out that under conditions of pulsed heating, small impurities of moisture can exert a considerable influence not only on the boiling point of hydrocarbons, but also on the heat transfer intensity of these substances in a state of superheating, near the temperature of spontaneous boiling-up. The work was supported by the Russian Foundation for Basic Research, project No. 16-08-00381-a.

1. K.V. Lukyanov, A.A. Starostin and P.V. Skripov. Heat transfer under high-power heating of liquids. 4. The effect of water admixtures on the heat transfer in superheated hydrocarbons// Int. J. Heat and Mass Transfer. - 2017. - V. 106. P. 657-665.

2. Lukyanov KV, Kotov. AN, Starostin AA Pulse-thermal control of volatile impurities in dielectric process fluids. Sensors and systems. 2014. No10. - P.46-49.

INVESTIGATION OF HEAT FLUX IN HYDROCARBON FUELS AT THE FILM AND BUBBLE BOILING

*Zhukov S. A.,² Yanovskiy L. S.,^{1,2} Molokanov A. A.,^{1,2} Il'ina M. A.*¹*

¹CIAM, Moscow, Russia, ²IPCP RAS, Chernogolovka, Russia

**lapohka12@yandex.ru*

The issues of heat transfer during the boiling of fuels are of great interest to the developers of aviation units. Heat transfer during boiling of a liquid depends on the boiling regime. The heat flux is ten times greater than in the bubbling boiling mode versus the film mode at the same temperature of the surface. In the present work we have studied the process of heat transfer during boiling of fuels in the regime of ultra-intense bubble boiling, as well as other regimes under conditions of high-density heat flow [1].

The electrothermographic method using platinum filaments 100 μm in thickness was used as the main experimental method. Platinum filament has a strong dependence of electrical resistance from temperature. Its heating was carried out by means of a constant electric current. In this method, the heater, in addition to its direct function, is also used as a resistance thermometer. By removing its current-voltage characteristic, one can obtain information on the magnitude of the heat flux and surface temperature. Samples of aviation kerosene were taken as objects of research. Complete boiling curves were obtained for the temperatures of 18°C, 100°C, and 184°C It is found that under boiling conditions with underheating, the SPK-super-intense bubbly boiling regime is realized in the system. Under these conditions, the branch of bubbly boiling has an unusual "step-like" form. The transition (mixed) boiling is carried out in an autooscillatory mode. When the liquid reaches the boiling point, the above effects disappear.

1. Concerning the Magnitude of the Maximum Heat Flux and the Mechanisms of Superintensive Bubble Boiling. Zhukov S.A., Afanas'eva S.Yu., Ehmaev S.B. International Journal of Heat and Mass Transfer.

THERMOPHYSICAL PROPERTIES OF VOLATILE PRODUCTS OF BIOMASS LOW TEMPERATURE PYROLYSIS

*Director L.B., Sinelshchikov V.A.**

JIHT RAS, Moscow, Russia

**sinelshchikov@mail.ru*

In the low-temperature pyrolysis (torrefaction) of biomass as a result of thermal decomposition of the organic component there are formed volatile products consisting of non-condensable gases and vapors of high-molecular organic compounds. When developing torrefaction technologies and methods for utilization of volatile products, that are hazardous for the environment, data on thermophysical properties of pyrolysis gases and vapors are needed.

The aim of the paper was to calculate the heat capacity and the heating value of volatile products that are released during the biomass heating up to a temperature of 600 K. Data on the composition of volatile products formed at different temperatures and residence times were taken from [1]. As a parameter, determining the composition and thermophysical properties of volatile products, the weight losses in torrefaction process on dry ash free basis of the starting biomass was adopted. In calculations the values of heat capacity and enthalpy of formation of the organic compounds constituting the volatile products of torrefaction were taken from the NIST database [2]. In the absence of appropriate data, there was applied the method of group contributions [3], the essence of which is that the sought thermophysical quantity is calculated by summing the contributions of the individual structural and atomic groups forming the compound under consideration.

As a result the heating value and the temperature dependences of the heat capacity for volatile products formed during the torrefaction process at weight losses up to 17% were determined. The maximum difference in the values of heat capacity of volatile products corresponding to various weight losses does not exceed 6%.

-
1. Prins M.J., Ptasincki K.J., Janssen F.J.J.G. // J. Anal. Appl. Pyrolysis. 2006. V. 77. P. 35.
 2. NIST Chemistry WebBook, <http://webbook.nist.gov/chemistry/form-ser/>
 3. Joback K.G., Reid R.C. // Chem. Eng. Commun. 1987. V. 57. P. 233.

MANOMETRICAL INVESTIGATION OF THE SATURATED VAPOR PRESSURE AND CRITICAL TEMPERATURES OF HYDROCARBON COMPOUNDS

*Yanovsky L.S.,^{1,2} Varlamova N.I.,¹ Kazakov A.I.,² Molokanov A.A.,^{*1,2}
Plishkin N.A.,² Popov I.M.,¹ Il'ina1 M.A.,¹ Ezhov V.M.¹*

¹CIAM, Moscow, Russia, ²IPCP RAS, Chernogolovka, Russia

**molokanov@ciam.ru*

At present, there are no experimental data on the thermophysical properties of some hydrocarbon compounds of promising aviation fuels. The present work is devoted to the investigation of thermophysical properties and critical temperatures of hydrocarbon compounds by the manometric method, as well as to an assessment of the fulfillment of Raoult's law for

mixtures of hydrocarbon compounds. Promising components of aviation fuels: aliphatic cyclic hydrocarbons with high density, volumetric heat of combustion and high boiling temperature were studied in the research. The experimental manometric installation includes the thermostat, the pressure regulation system, the test chamber, and allows to determine the pressure of the test sample from 0 to 45 atm at temperatures from 15 textdegree C to 500 textdegree C [1]. Investigation of the saturated vapor pressure of the samples was carried out by measuring the equilibrium pressure during their isochoric heating. The vapor pressure of samples was not changed during the test chamber was held at a given temperature for 2 hours, i.e. the reaction of thermal decomposition with evolution of gases was not observed during vapor determination. It is established that the saturated vapor pressures of the samples studied in the interval 100-400 textdegree C are subject to Clapeyron-Clazius law. The dependence of the vapor pressure on temperature, enthalpy and evaporation entropy, boiling point and critical temperatures was determined for the hydrocarbon compounds.

-
1. V.V. Dubikhin, V.G. Matveev, G.M. Nasin. Thermal decomposition of 2,4,6-trinitrotoluene in melt and solutions // *Izvestiya Akademii Nauk*.

INTERACTION OF METHANE WITH THERMAL CARBON DIOXIDE PLASMA OBTAINED IN THE AC PLASMA TORCH

Subbotin D.I., Popov V.E., Safronov A.A., Popov S.D., Surov A.V., Kuchina J.A.,
Obraztsov N.B., Serba E.O., Nakonechny Gh.V., Spodobin V.A.*

IEE RAS, Saint-Petersburg, Russia

**subbotin1987@mail.ru*

Currently the problem of obtaining synthesis gas from natural gas (reforming) is topical. In this case main reagents are steam, carbon dioxide and oxygen. Carbon dioxide is a greenhouse gas, so its emissions into the atmosphere should be limited. However, the interaction of methane with carbon dioxide is a strong endothermic process. There are a number of scientific papers devoted to the interaction of CO₂-plasma with methane. For this, DBD, corona discharge, DC arc discharge and etc. are used. The report deals with the interaction of methane with carbon dioxide in a high-voltage three-phase AC plasma torch. The power source of the plasma torch consists of current-limiting reactors, the reactive power compensator and the high-voltage transformer (10 kV). The plasma torch consists of three arc channels with three rod copper electrodes. Carbon dioxide (3.7 g/s) and methane (1 g/s) are supplied to the near-electrode zone, and carbon dioxide (3.2 g/s) and methane (1.4 g/s) are supplied to the arc zone. The electric power of the plasma torch was 110 kW. The composition of the synthesis gas was determined by a mass spectrometer using calibration mixtures. The synthesis gas contained CO 50 percent vol. and H₂ 50 percent vol. without the formation of soot. This indicates a high efficiency of processing methane into synthesis gas.

THERMOPHYSICAL PROPERTIES OF COMPONENTS OF BIODIESEL FUEL AND RAW MATERIALS FOR ITS PRODUCTION

Nikitin E.D., Bogatishcheva N.S., Popov A.P., Faizullin M.Z.*

ITP UB RAS, Ekaterinburg, Russia

**e-nikitin@mail.ru*

Biodiesel is a renewable energy resource and has some advantages over petroleum fuels. Biodiesel is a blend of fatty acid methyl or ethyl esters and is produced through the esterification reaction from vegetable oils and animal fats which mainly consist of triglycerides. The paper presents the results of measuring the critical temperatures T_c , the critical pressures p_c , heat capacities C_p , and thermal diffusivities of some fatty acid methyl and ethyl esters and saturated triglycerides. These properties have been measured for the following compounds:

methyl esters of n-alkanoic acids $\text{CH}_3\text{O}_2\text{C}_n\text{H}_{2n-1}$ with the number of carbons $n = 6, 7, 8, 9, 10, 11, 12$, as well as oleic, linoleic, linolenic, and erucic acids;

ethyl esters of n-alkanoic acids $\text{C}_2\text{H}_5\text{O}_2\text{C}_n\text{H}_{2n-1}$ with the number of carbons $n = 10, 11, 12, 14, 16, 18$;

saturated triglycerides $\text{C}_3\text{H}_5[\text{O}_2\text{C}_n\text{H}_{2n-1}]_3$ with $n = 8, 10, 12, 14$.

The purities of the samples (Sigma-Aldrich, Alfa Aesar) were from 98.5 to 99.9 mol.%.

The compounds studied are thermally unstable at near-critical temperatures, so that the measurements of the critical properties have been made by the pulse-heating method developed by the authors (GSSSD 163-2010); the method provides ultra-low decomposition of compounds under study in the course of measuring the critical properties. The uncertainties of the measurement of the critical parameters are $\delta T_c = 0.01T_c$ and $\delta p_c = 0.03p_c$, where T_c is the absolute temperature. Equations for the calculation of the critical properties of n-alkanoic acid methyl (ethyl) esters have been obtained.

Heat capacity was measured with the help of a differential scanning calorimeter DSC 204 F1 Phoenix (Netzsch) with the uncertainty of 2%. The measurements of thermal diffusivity were taken by the laser flash technique using LFA 457 MicroFlash (Netzsch); the uncertainty is no more than 5%. Equations for the dependence of molar heat capacities and thermal diffusivities of the compounds studied on temperature have been obtained.

The study was supported by the Complex Program for Basic Research of the Ural Branch of the Russian Academy of Sciences N 18-2-2-13.

DETERMINING THE SPEED OF MULTICOMPONENT HYDROCARBON MIXTURE PHASE TRANSITIONS IN THE FREE VOLUME Al_2O_3 & MgO

*Bogdanov A. V.,¹ Grigoriev E. B.,¹ Sokotushenko V. N.*²*

¹LLC Gazprom VNIIGAZ, Razvilka, Russia, ²State University Dubna, Dubna, Russia

**sokotushenko@mail.ru*

To study the phase transition processes in the intensive pressure reduction in gas-condensate systems [1–3] a series of experiments on the sharp decrease and increase pressure in the PVT cell by different values relative to the initial pressure is carried out, corresponding to the equilibrium gas state. Basic controlled in the study parameters – pressure in the recombinator and temperature. Experiments to determine the relaxation time of phase transitions were performed by static method. In this case, the phase transition occurred in a stationary gas in a closed volume.

In the framework of mathematical formulation of the problem, one resolving equation with respect to the phase velocities is obtained from the system of fluid motion equations. The calculation of the thermodynamic properties (TDS) of a multicomponent hydrocarbon mixture

under volume change (adiabatic compression – expansion) is presented and sharp pressure fluctuations in the cell recombinator, as well as the relaxation time of phase transitions on the example of 4-component mixture: CH₄ – C₃H₈ – C₅H₁₂ – C₇H₁₆.

Comparison of the obtained pressure distribution by the developed mathematical model on the boundary sections of the recombinator cell with the obtained from the experiment data on the measurements of pressure at the corresponding points of the recombinator cell gives an error of less than 5%, that is a satisfactory result of the mathematical model approbation.

1. Grigoriev B.A., Gerasimov A.A., Grigoriev E.B. Fundamental equations of the state of hydrocarbons in the critical region. Interdisciplinary scientific and technical journal. Defense complex – scientific and technological progress of Russia. 2010. V. 3. P. 52-60.
2. Buleyko V.M., Vovchuk G.A., Grigoriev E.B., Fedoseev A.P. Experimental study of thermodynamic properties of gas hydrates in porous media under temperature and pressure conditions corresponding to the liquid state of the hydrocarbon hydrateforming components. News of gas science: Topical issues of studies of formation systems of hydrocarbon deposits. – Moscow: Gazprom VNIIGAZ. 2013. V. 1 (12).
3. Grigoriev B.A., Zaichenko V.M., Molchanov D.A., Sokotushenko V.N. Mathematical modeling of isothermal filtration of gas condensate mixture at different flow regimes. Lead gas science: Actual problems of studies of hydrocarbon deposits. – Moscow: Gazprom VNIIGAZ, 2016. – V. 4 (28). – P. 37-40.

STUDY OF SUPERHEAT AND CRITICAL PARAMETERS OF DIESEL FUEL WITH ADDING CASTOR OIL

Igolnikov A. A., Skripov P. V.*

ITP UB of RAS, Ekaterinburg, Russia

**alexander.igolnikov@bk.ru*

The extraction and use of non-renewable energy sources, such as oil and gas, are harmful to the environment. In this regard, alternative sources of energy are being developed, one of which is biofuel. It is a mixture of methyl or ethyl esters of fatty acids, and its production is based on the recycling of various vegetable oils. The use of biofuel as an additive to diesel fuel or its alternative in internal combustion engines can reduce carbon dioxide emissions, as well as nitrogen and sulfur oxides. In addition, such fuel is completely degraded in the environment by the action of bacteria, so it does not harm plants and animals.

The report will present the results of measurements of attainable superheat and critical parameters of castor oil solutions in diesel fuel at various concentrations of castor oil. The test samples are thermally unstable compounds. In this connection, the measurements were carried out by the method of pulse heating of a substance with a characteristic heating time of 1 millisecond.

This study was supported by the Russian Foundation for Basic Research (grant no. 16-08-00381-a) and by the Presidium of UB RAS Complex Program (grant no. 18-2-2-3).

**PROPERTIES OF THERMODYNAMIC SYSTEMS PARTICIPATING IN THE
PROCESS OF OBTAINING BIODIESEL FUEL IN SUB- AND
SUPERCRITICAL FLUID CONDITIONS**

Zaripov Z. I., Usmanov R. A., Gumerov F. M.*

KNRTU, Kazan, Russia

**zufar_zaripov@mail.ru*

The catalytic transesterification of vegetable oils in the environment of supercritical alcohols becomes one of the promising ways of producing biodiesel fuel [1]. The technological processes taking place in the biodiesel production facilities assume a quantitative analysis of the thermal effects of the transesterification process of vegetable oils in the environment of supercritical alcohols. Along with this, for modeling and optimization of technological processes of production of biodiesel fuel in the course of the transesterification reaction carried out under sub- and supercritical conditions, it is necessary to locate the thermodynamic properties of the initial components (especially at pre- and supercritical states of the reacting alcohol component) and reaction products. The thermophysical properties of the main components of the transesterification reaction and reaction products are presented in sufficient detail in the domestic and foreign literature. At the same time, there are no data on the properties of the mixtures of the reaction components and the thermal effects of the transesterification reaction. Extensive studies of thermodynamic properties, carried out at the Department of Theoretical Foundations of Heat Engineering, FSEI HE KNRTU [2-4], allowed to cover the whole chain of the process of obtaining biodiesel fuel in sub- and supercritical fluid conditions (preparation, mixing, reaction and separation). On the basis of this material, it became possible to proceed to the modeling and optimization of the technological process and to go to the design of an industrial biodiesel fuel plant. 1. Gumerov F. M., and others. Supercritical fluids: Theory and practice. 2006. V. 1. Nom.1. P.66-76. 2. Usmanov RA, Gabitov RR, Biktashev Sh.A. Supercritical fluids: Theory and practice. 2011. V.6. Nom.3, P.45-61. 3. Usmanov R. A., Gumerov F. M., Gabitov F. R., Zaripov Z. I., Scshamsetdinov F. N., Abdulagatov I. M. : Liquid Fuels: Types, Properties and Production. Nova Science Publisher, Inc., New York, 2012, Chapter 3, P. 99-146. 4. Gumerov F.M. Biodiesel fuel. Transesterification in supercritical fluid conditions. Monograph.Kazan.Publishing house. Ltd Innovation - publishing house Butlerov Heritage. 2017. 360p.

**THERMODYNAMIC BASES OF THE PROCESS OF EXTRACTION OF
HYDROCARBONS FROM OIL SLUDGE USING SCF PROPANE-BUTANE
MIXTURE**

Khairutdinov V.F.,^{1,2} Gumerov F.M.,¹ Farakhov M.I.²*

¹KNRTU, Kazan, Russia, ²Inzhekhim, Kazan, Russia

**kvener@yandex.ru*

To date, enterprises of the Russian oil and gas complex have accumulated a huge amount of oil sludge. According to the most conservative estimates, the annual increase in their quantity is about 3 million tons. In recent years, various technological solutions aimed at recycling oil production wastes and oil treatment have been introduced by oil producing enterprises. However, a sufficiently effective and unified way of processing oil sludge for the purpose of neutralizing and utilizing them is still not available.

As part of the study of oil sludge utilization, raw materials are used, characterized by the content of mechanical impurities and water in the amount of 12.05% and 20% by weight. respectively. As an extractant, a mixture consisting of 75 wt. % propane and 25 wt. % butane.

Extraction processes are carried out in the temperature range of 85-160 ° C and a pressure interval of 5-50 MPa. Dedicated oil is characterized by the absence of mechanical impurities, asphaltenes and water. The first (5-6.5 MPa) and the second (11-12 MPa) crossover points of the isotherms of solubility of the petroleum products studied in the propane-butane solvent were determined. Knowledge of crossover points is an important condition for the implementation of extraction and impregnation processes.

To scale the results obtained, it is necessary to model the process, and for modeling it is necessary to investigate the thermodynamic properties of the systems participating in the process. For this purpose, the solubility of pure components of oil sludge, such as naphthalene, anthracene, etc., in the subcritical fluid (SbCF) and SCF propane-butane was studied.

Taking into account the studies of thermodynamic properties and laboratory studies, the modeling of processes was carried out.

Based on the simulation results, a pilot plant has been created that allows the extraction and impregnation processes to be carried out.

The study was carried out through a grant from the Russian Science Foundation (project No. 18-19-00478).

-
1. Khairutdinov V. F., Akhmetzyanov T. R., Gabitov F. R., Zaripov Z. I., Farakhov M. I., Mukhutdinov A. V., Gumerova F. M., and Yarullin R. S. Extraction of oil-products from oil sludge with the use of liquid and supercritical fluid extraction processes with propane-butane extractant. *Petroleum Science and Technology*, V 34. 4. 2016. p. 372-378.

DEW-BUBBLE CURVE DETERMINATION OF NEAR-CRITICAL HYDROCARBON MIXTURES USING LIGHT-SCATTERING METHOD

Kiyachenko Yu.F., Deshabo V.A., Kosov V.I., Yudin D.I., Yudin I.K., Podnek V.E.*

OGRI RAS, Moscow, Russia

**kiyatchenko@mail.ru*

The method of optical determination of the dew-bubble curve and the position of the liquid-gas critical point of near-critical multicomponent hydrocarbon mixtures simulating gas-condensate deposits of the so-called transitional type is presented. The work is a part of a comprehensive study of the phase behavior of model near-critical hydrocarbon mixtures, which includes calorimetry and PVT measurements in addition to experimental light-scattering methods. A high-pressure optical cell was elaborated and an apparatus was designed to measure the intensity of Rayleigh scattering of light in hydrocarbon mixtures at the temperature range from 10 to 120 °C and the pressures up to 50 MPa. The volume of the measuring optical cell is 3.2 cm³. The intensity of light-scattering is measured at an angle of 45°. As a light source, a laser with a wavelength of 635 nm is used. Calibration of the measuring system was carried out at the critical isochore of carbon dioxide. Measurements of the intensity of light scattering were carried out along the isochores at cooling from a single-phase region. The position of the dew-bubble curve of the mixture was determined from the change in the character of the temperature dependence of the scattered-light intensity at the transition from the single-phase to the two-phase state. The position of the critical point was determined from the maximum intensity of the light scattering on the dew-bubble curve. The temperature dependence of the anomaly of the intensity of light scattering in a single-phase region was analyzed in the framework of the generalized "linear model the scaling parametric equation of state of a near-critical fluid. The results of the experimental study of the near-critical phase behavior of methane-pentane binary mixture (50/50 weight percent) are presented. A comparison of the obtained critical

parameters of the mixture with the values determined previously by PVT method (Sage *et al.*, 1942) as well as with the results obtained by means of engineering programs PVTsim (Calsep) and REFPROP (NIST) intended for calculating of thermophysical properties of hydrocarbon mixtures has been also done.

HYDRATE FORMATION IN SUPERSONIC JETS OF VAPOR AND GAS

Faizullin M.Z., Vinogradov A.V., Tomin A.S., Koverda V.P.*

ITP UB RAS, Yekaterinburg, Russia

**andrey.itf.2017@yandex.ru*

The aim of the present work is an experimental study of gas hydrate formation in the condensation of nanoclusters in supersonic molecular beams of rarefied water vapor and gas in vacuum.

Formation of gas hydrate was observed in a vacuum chamber with walls cooled by liquid nitrogen. The pressure in the chamber before the experiment was no more than 10^{-3} mm Hg. Counter-directed molecular beams of rarefied steam and ethane were simultaneously admitted to the chamber through the nozzle of Laval, which accelerated them to supersonic speeds. Adiabatic expansion of the rarefied vapor molecular flow at the nozzle outlet provides temperature decrease and formation of crystalline ice nanoclusters of cubic diamond-like structure. The formation of ice clusters is accompanied by the capture of gas molecules and the formation of a crystal hydrate phase. The change in pressure at the inlet to the supersonic nozzle regulated steam consumption and, as a consequence, the performance of gas hydrate. Cooling of the chamber walls with liquid nitrogen allowed to keep it unlimited time.

When heated, the crystalline condensate remained up to the melting point of the sample. Self-preservation ensured its stability in a metastable state at temperatures well above the equilibrium dissociation temperature of ethane hydrate.

The gas content in the crystallized water and the gas product exceed 50 mass. %. This content was achieved due to the additional sorption of the gas in the formation of crystalline condensate, which was a gas-saturated nanoporous medium containing crystalhydrate phase and crystalline ice.

The results of these experiments are of interest in connection with the development of economical and safe gas storage and transport technologies.

The work was supported by the Russian Foundation for Basic Research (Grant No 18-08-00352-a, No 18-38-00443mol-a) and the Program for Basic Research of the Ural Branch of the RAS (Grant No 18-2-2-3).

THERMOPHYSICAL PROPERTIES OF SYSTEM HIGH-MOLECULAR ORGANIC CONNECTION (ROCK-OIL) - WATER-SCF SOLVENT

Nakipov R.R., Zaripov Z.I.*

KNRTU, Kazan, Russia

**nakip88@yandex.ru*

The current trend in petroleum-refining industry this use heavy rock-oil. Because of higher maintenance of heteroatoms, asphalts and metals, and also more quantities of not divided hydrocarbons, it is more difficult to process it.

Problems of rational use and processing of difficultly taken stocks high-viscosity rock-oil and natural bitumens cannot be solved without introduction of a wide spectrum of modern technologies of extraction and processing.

On this background all become more actual than a problem of rational use and processing of difficultly taken stocks, such, as high-viscosity rock-oil and natural bitumens. These problems cannot be solved without introduction of modern technologies of extraction, such as steam, cold extraction, with use of solvents and catalysts, and also processings of hydrocarbonic raw materials with application supercritical fluid (SCF) technologies.

Thermophysical properties heavy rock-oil and bitumens are the necessary initial data for working out, designing of technological processes, the actions connected with their manufacture, transportation and oil refining. Knowledge of phase behaviour is necessary for working out and optimisation of technological processes of oil refining, thermophysical properties (for heat conductivity, a thermal capacity, density, viscosity and structure) both rock-oil and fractions, and their mixes with solvents. In researches in this direction are engaged much enough, it and works on phase equilibria, to structures and properties.

The purpose of the present research is reception of the new data on thermophysical properties high-viscosity rock-oil of the Ashalchinsk deposit of the Republic of Tatarstan .

Research thermophysical properties (thermal capacity) of systems of heavy rock-oil and water-rock-oil emulsion various concentration - SCF (propane-butane) are spent in the range of temperatures 343K-474K and pressure in a range 4,9-29,4 MPa. The system thermal capacity has been measured on scanning adiabatic calorimeter.

Research is executed at the expense of the grant of the Russian scientific fund (the project 18-19-00478)

EXHAUST COMPOSITION AT LASER IGNITION OF COMBUSTIBLE GAS MIXTURES UNDER CONTROLLED CONDITIONS

*Anishchanka Yu. V., Loktionov E. Yu.**

BMSTU, Moscow, Russia

**stcpe@bmstu.ru*

One of the main advantages of laser ignition is the ability to ignite lean combustible mixtures, resulting in obvious economy and reduction of harmful emissions, primarily NO_x . Experimental data on exhaust composition are presented in the literature very poorly. As a rule, the studies were not of a systematic nature, affected only very specific conditions of combustible mixtures exposure and composition (mainly methane-air) and were obtained for experimental piston engines, the design and operational features of which could significantly affect the result.

A number of models simulate exhaust composition, but they are created either without taking into account the ignition mechanism, or for electric spark or compression ignition. For laser ignition, it is known that the formation of the combustion core occurs faster than from an electric spark. We suggested that in order to obtain a starting point for further optimization, a study of exhaust composition should be carried out under conditions of minimal impact on the engine design. For this purpose, an experimental stand was created, which allows to investigate the laser ignition of combustible mixtures of different composition in wide pressures range. Its peculiarity specific to this work is the presence of volume for combustion products storage after a series of impacts, it is coupled with the combustion chamber through the discharge valve. By means of the latter, the increase of the cylinder operational volume is simulated and the protection against excessive pressure increase is implemented.

We studied the laser ignition of gas mixtures based on hydrogen, methane, propane and butane with air excess coefficient $\alpha \sim 0.5-2$, in pressure range $p \sim 1-3$ bar, ignited by radiation of the 1st-5th harmonics of the nanosecond Nd:YAG laser. The exhaust composition was analyzed by O_2 , CH, CO, CO_2 , NO_x . Correspondence of the obtained results, known from other experimental and theoretical works, is analyzed.

**EXPERIMENTAL INVESTIGATION OF THE PRESSURE OF THE SYSTEM
OF N-HEPTAN-WATER (99:1)**

Mirskaya V.A., Nazarevich D.A., Ibaov N. V.*

IP DSC RAS, Makhachkala, Russia

**naz_77@mail.ru*

At present, there is an urgent need for investigating a collection of thermophysical properties of liquids and gases under the conditions of a single experimental cell. During a single experiment, we can obtain data on a broad spectrum of thermophysical properties of substances. The union of measurements of thermophysical and calorimetric properties within the framework of a single experimental setup is a complicated enough problem.

In order to satisfy the condition of simultaneous measurement of isochoric heat capacity and pressure, in the structure of the experimental setup for investigation of isochoric heat capacity and PVT properties of liquids and gases, we decided to use a digital pressure strain-gage sensor.

The sensor should have the following characteristics: high accuracy, small external dimensions, large measurement ranges for pressures and temperatures of the media being investigated, independence of the measurement results from the state of the surrounding medium (temperature, air moisture, etc.). These characteristics were satisfied by the pressure sensor Kurant DI-V.

Data on the pressure of the system under investigation from the sensor are transmitted to a digital measuring instrument (Keithley 2000 multimeter). The data obtained go from the multimeter to a personal computer with software specially developed by the authors, where this information is processed and kept together with other data.

In this way, we studied the n-heptane-water system (99:1). This system is immiscible under normal conditions. Investigations were carried out on 11 isochores in the density range from 150 kg/m³ to 501 kg/m³ and a pressure range from 0.1 MPa to 16 MPa. Isochores of pressure and dependences of the first derivative of pressure on temperature on temperature are constructed. They indicate phase transitions corresponding to transitions from the three-phase state to the two-phase state and from the two-phase state to the single-phase state.

The work was supported by the Russian Foundation of Basic Research (grant No. 17-08-00800)

**THE EXPERIMENTAL INVESTIGATION OF THE ISOBARIC HEAT
CAPACITY OF THE REACTION MIXTURE "ETHANOL / RAPESEED
OIL" IN THE PRESENCE OF A HETEROGENEOUS CATALYST**

Mazanov S. V., Zaripov Z. I., Gumerov F. M.*

KNITU, Kazan, Russia

**serg989@yandex.ru*

The measurements were made of the isobaric heat capacity of ethanol and a mixture of "ethanol / rapeseed oil" in the presence of a heterogeneous Al₂O₃ catalyst at initial molar ratios of 6 : 1 to 30 : 1 in the pressure range 9,8-29,4 MPa and temperatures from 303K to 563K in an experimental setup, created on the basis of the scanning calorimeter IT-s-400. To more efficiently mix the poorly-miscible reagents, the ultrasonic emulsifier UIP1000hd of the German firm Hielscher was used before they were fed into the measuring cell and the pressure maintenance system. Preliminary treatment of the mixture in an ultrasonic disperser leads to a displacement of the region of the heat capacity jump in lower temperature range. With increasing pressure and oil concentration, the magnitude of the thermal effect of the reaction decreases. The dependence of the change in the isobaric heat capacity over the entire range of the

investigated pressures and the initial mole ratios with increasing temperature. The theoretical justification of the observed growth and fall in the values of the isobaric heat capacity of the initial mixture was analyzed by the Shaw method [1].

1. Lastovka, V. A similarity variable for estimating the heat capacity of solid organic compounds. Part II. Application: Heat capacity calculation for ill-defined organic solids. V. Lastovka, M. Fulem, M. Becerra, J.M. Shaw. Fluid Phase Equilibria.2008.134 p.

VISCOSITY AND DENSITY OF VACUUM WORKING FLUIDS FOR DIFFUSION PUMPS

Sagdeev D.I., Gabitov I.R., Fomina M.G., Alyaev V.A., Minkin V.S., Abdulagatov I.M.*

KNITU, Kazan, Russia

**sagdeev@mail.ru*

Results of a research of viscosity and density of four vacuum oils for diffusive vacuum pumps of domestic and foreign production are presented. Measurement of properties are carried out with an atmospheric pressure: viscosity by a capillary method, and density - methods of the densimeter and hydrostatic weighing. Identification of samples of vacuum oils has been made by method of nuclear magnetic resonance. There is rather good correlation of structure of oils with their viscosity and density. Settlement expressions are presented and density error estimates by a hydrostatic method and viscosity by a capillary method are calculated. The temperature dependence of viscosity is presented by means of the known equation like Arrhenius-Andrade, and for density is used square function on absolute temperature. The research is executed at the expense of a grant of the Russian scientific fund (project No. 18-19-00478).

1. Sagdeev D.I., Fomina M.G., Alyev V.A., Musin R.Z., Abdulagatov I.M. Density of working liquids for diffusion vacuum pumps. J. Chem. Eng. Data, 2018, v. 63, 1698-1705.
2. Lesh A. Nuclear induction. - The lane from German under P.M. Borodin's edition. - M.: Publishing house of foreign literature, 1963. - 684th page.
3. MI of 2083-90 GSI. Indirect measurements. Determination of results of measurements and estimation of their errors. - Vved. from 01.01.92. - 10 pages.

ISOCHORIC HEAT CAPACITY AND PVT PROPERTIES OF BINARY AZEOTROPIC SYSTEM N-HEPTANE-WATER

Ibavov N.V., Mirskaya V.A., Nazarevich D.A.*

IP DSC RAS, Makhachkala, Russia

**nabi79@mail.ru*

The results of the study azeotropy phenomena in complex systems are of interest at the design of technology for the extraction, azeotropic distillation and obtaining from oil the chemicals of high purity. Isolation of high-boiling fractions from hydrocarbons is achieved by an azeotropic distillation using a steam.

The investigated system of n-heptane-water [(1-x)C₇H₁₆+H₂O], (x-content of the polar component) is a complex hydrocarbon-water system consisting of components that differ significantly in molecular structure and properties.

Investigations were carried out on an automated pilot plant that is based on the well-known technique of Amirhanov high-temperature adiabatic calorimetry-piezometer.

The temperature and volume dependences of thermodynamic properties of the system [(1-x)C₇H₁₆+H₂O] were studied for several constant compositions $0.147 \leq x \leq 0.420$ m.f. with different content of the polar component (water) in the intervals from the normal boiling temperature of components up to 570 K. Were made measurements on 7-12 isochores $\rho = \text{const}$, for each system of constant composition $x = \text{const}$.

As a result of researches on the temperature and volume dependences of the isochoric heat capacity and pressure are found the peculiarities in behavior of thermophysical properties of dual exfoliating system n-heptane - water, allowed to identify areas of mutual solubility of components, boundary of phase equilibria, the dependence of composition displacement of the system azeotrope state on the temperature and pressure.

Work was supported by the Russian Foundation for Basic Research (grant 17-08-00800-a)

DATA DRIVEN APPROACHES IN MATERIALS
DESIGN: THEORY MEETS EXPERIMENT
(MISIS)

**ENTHALPIES OF FORMATION OF TRANSITION METAL AND
RARE-EARTH BORIDES. A FIRST PRINCIPLES STUDY.**

*Colinet C.,^{*1} Tedenac J.P.²*

¹*Université de Grenoble Alpes, Saint Martin d'Hères, France,* ²*Université Montpellier II,
Montpellier, France*

^{*}*ccolinet@simap.grenoble-inp.fr*

Calculations based on the density functional theory have achieved considerable reliability for the prediction of the properties of materials. In the present work, we have studied the structural stability of binary intermetallic compounds of boron with transition metals and rare-earth elements. The density functional (DFT) calculations have been performed with the Vienna *ab initio* simulation package (VASP) [1], making use of the projector augmented waves (PAW) technique [2, 3]. For the generalized gradient approximation (GGA) exchange correlation functional, we have used the Perdew-Burke-Ernzerhof parameterization (PBE) [4].

The calculated values of the lattice parameters at $T = 0$ K of the stable compounds agree well with the experimental values [5]. The calculated enthalpies of formation of these compounds are compared to the values obtained with calorimetric methods [6, 7]. In the whole, the calculated values of the formation enthalpies of formation the borides in their ground state are in good agreement with the experimental ones when available. The calculated values have also been compared with those previously published in various publications or data bases. Finally, the evolution of the enthalpies of formation of the borides along the 3d, 4d, and 5d series of the transition metals and the series of rare-earth Sc, Y, La and La to Gd to Lu is discussed.

1. G. Kresse and J. Furthmüller, *Comp. Mater. Sci.* 6 (1996) 15; *Phys. Rev. B* 54 (1996) 11169.
2. P. E. Blöchl, *Phys. Rev. B* 50 (1994) 17953.
3. G. Kresse and D. Joubert, *Phys. Rev. B* 59 (1998) 1758.
4. J.P. Perdew, S. Burke, and M. Ernzerhof, *Phys. Rev. Lett.* 77 (1996) 3865–3868.
5. P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, Release 2014/15, ASM International, Materials Park, Ohio, USA.
6. S.V. Meschel and O.J. Kleppa, *J. Alloys and Compounds*, 321 (2) (2001) 183-200.
7. G. Kim, S. V. Meschel, P. Nash, and W. Chen, *Sci. Data* 4:170162 doi: 10.1038/sdata.2017.162 (2017).

**MODELLING OF PHASES WITH GENERAL NIAS-TYPE STRUCTURE:
WHAT CAN WE LEARN FROM POWDER XRD?**

Richter K. W.

University of Vienna, Faculty of Chemistry, Wien, Austria

klaus.richter@univie.ac.at

The general NiAs structure includes the related structure types CdI₂, NiAs and Ni₂In. It is composed of transition metals T and main group elements B, out of the 13th to 16th group, forming T1+/-xB structures. Due to its ability to include different amounts of transition metal, large homogeneity ranges can be found between T0.5B and T2B. The structure type is widespread among transition metal compounds and therefore present in many different alloy

systems. In higher order systems, little is known about occurrence and homogeneity ranges of corresponding solid solution phases. Extrapolations using the Calphad approach are therefore often the method of choice for the prediction of multicomponent systems. For consistent models, however, a detailed knowledge of the underlying crystal chemistry is necessary.

To contribute to this knowledge, some selected ternary model systems were investigated experimentally in a current research project. The NiAs-type solid solutions were characterized by detailed Rietveld refinements of XRD powder patterns. This data helped to clarify open questions regarding the possibility of transition metal ordering and the maximal extension of a continuous phase field. Based on these results, a modified sublattice model for phases with general NiAs structure is proposed. Three endmembers of this model correspond to the boundary structures of the general NiAs type (CdI₂, NiAs, Ni₂In) so the end member energies can easily be calculated by DFT calculations. This was demonstrated by calculating a small database of energies of formation of (hypothetic) binary Ni-containing NiAs structures with varying main group elements.

EXPERIMENTAL DATABASE DEVELOPMENT FOR DATA-DRIVEN MATERIALS DESIGN

*Kim G., Gu Q., Jia H., Meschel S., Chen W., Nash P.**

Illinois Institute of Technology, Chicago, United States

**nash@iit.edu*

We will describe the program at IIT to develop experimental thermodynamic data on the enthalpies of formation of intermetallic compounds, including B2 and L2₁ structures. The data are incorporated into a database that can be accessed by computer for data mining and machine learning based materials design. These data are compared and benchmarked with first-principles results in multiple Materials Genome databases. As an example we will discuss the application of machine learning to elucidate a relationship between the properties of B2 binary compounds and L2₁ ternary compounds with the aim of developing rules that can be used to predict the stability of L2₁ ternary compounds.

PRECIPITATION SIMULATION ENABLED BY THERMODYNAMIC AND KINETIC DATABASES

*Chen Q.,*¹ Wu K.,² Jeppsson J.,¹ Engstrom A.¹*

¹TCSAB, Stockholm, Sweden, ²TCSInc, Pittsburgh, United States

**qing@thermocalc.se*

Computational tools, such as Thermo-Calc and Dictra, have been developed for several decades and are now routinely utilized in materials research in both academia and industry. Their success is rooted in their capability to provide indispensable phase equilibrium and phase transformation information for simulating microstructural evolution in commercial multicomponent alloys, which was made possible by the adoption of the CALPHAD methodology where the Gibbs energy or atomic mobility of each phase can be modelled hierarchically from low-order systems to high-order ones, and model parameters can be evaluated by considering both ab-initio and various experimental data. A collection of sets of optimal thermodynamic or atomic mobility model parameters for all phases in binary and ternary systems forms a CALPHAD thermodynamic or kinetic database. Over the years, databases containing up to 35 elements for various alloys, such as steels, light metal alloys, Ni-based superalloys, etc., have been developed. By using Thermo-Calc and Dictra together

with such databases, phase equilibria, driving forces, and diffusivities necessary for simulating diffusion-controlled phase transformation in multicomponent systems can be calculated without resorting to ad hoc approaches that require fitting parameters varying from one alloy to another, and therefore diffusion-controlled microstructural evolution in multicomponent systems can be predicted.

Precipitation gives many alloys their desired strength and toughness. A precipitate microstructure consists of dispersed second phase particles embedded in a solution phase matrix and is a product of diffusion-controlled solid state phase transformation fully governed by system (bulk and interface) thermodynamics and kinetics. With the advance of CALPHAD and widely available databases, computer simulation of the precipitate microstructure in multicomponent alloys is readily feasible on the basis of Langer-Schwartz theory and Kampmann-Wagner numerical (KWN) method. In this talk, we present TC-PRISMA, now fully integrated into Thermo-Calc as the Precipitation Simulation module, that extends the Thermo-Calc and Dictra approach with additional thermophysical property data to simulate the concurrent nucleation, growth, and coarsening of second phase particles. Nucleation and growth rate models implemented in the software will be elaborated. Engineering applications of precipitation modelling and challenges will also be shown and discussed as well.

THERMODYNAMIC ASSESSMENT OF THE Al_2O_3 -MgO-TiO₂ SYSTEM

Ilatovskaia M.,^{*1,2} *Fabrichnaya O.*¹

¹TU-BAF, Freiberg, Germany, ²IMMIT, St. Petersburg, Russia

**mariia.ilatovskaia1@iww.tu-freiberg.de*

The Al_2O_3 -MgO-TiO₂ system is of interest for industrial applications: MgAl_2O_4 -based materials have a good combination of physical and chemical properties such as high refractoriness, high mechanical strength and high resistance to chemical attack, while the addition of Al_2TiO_5 improves thermal shock resistance of spinel. The Al_2O_3 -based ceramics are proposed as filter materials for steel and Al-alloy filtration from MgAl_2O_4 and Al_2O_3 inclusions. Thus, thermodynamic modelling of the Al_2O_3 -MgO-TiO₂ system is important for thermodynamic database development to model interactions in filter material.

To provide an experimental base, Al_2O_3 -MgO-TiO₂ samples were prepared by the co-precipitation routine followed by prolong annealing experiments and then characterized using XRD, SEM/EDX, and DTA. Four isothermal sections of the Al_2O_3 -MgO-TiO₂ system at 1000 – 1464°C were constructed based on obtained results which are mainly consistent with the literature data [1-2]. Formation of continuous solid solutions with spinel, Mg_2TiO_4 - MgAl_2O_4 , and pseudobrookite, MgTi_2O_5 - Al_2TiO_5 , structures at high temperatures was confirmed. The solid-state reaction, $\text{Al}_2\text{O}_3 + \text{TiO}_2 + \text{Sp s.s.} = \text{Psbk s.s.}$, was observed at about 1160°C for the first time. On the liquidus surface, the eutectic invariant reaction between MgTiO_3 , Psbk s.s. and Sp s.s. was detected at 1602°C. Another invariant reaction of transitional type, $\text{L} + \text{Al}_2\text{O}_3 = \text{Sp s.s.} + \text{Psbk s.s.}$, was observed at 1733°C. Obtained experimental data for the Al_2O_3 -MgO-TiO₂ systems were used to derive its thermodynamic database. The compound energy formalism was applied to describe solid solutions, while to describe oxide liquid the two-sublattice partially ionic liquid model was implemented. A special attention was paid to reproducing the degree of inversion when the spinel phase changes from inverse Mg_2TiO_4 to normal MgAl_2O_4 and in the pseudobrookite phase from normal MgTi_2O_5 to completely disordered Al_2TiO_5 .

1. Boden, P., and Glasser, F.P., Phase relationships in the system MgO-Al₂O₃-TiO₂, Trans. J. Br. Ceram. Soc., 72(5) (1973): 215-220.

2. Bereznoi, A.S., and Gul'ko, N.V., Investigation of the MgO-Al₂O₃-TiO₂ system, Ukr. Khim. Zh. (Russ. Ed.) 21(2) (1955): 158-166.

EXPERIMENTAL INVESTIGATION AND THERMODYNAMIC MODELING OF THE ZrO₂-TiO₂-MgO SYSTEM

Saenko I., Ilatovskaia M., Fabrichnaya O.*

TU-BAF, Freiberg, Germany

**Ivan.Saenko@iww.tu-freiberg.de*

Composite materials based on high-alloyed steels reinforced by zirconia ceramics are of particular interest due to the wide range of their possible technological applications especially in automotive production. An example of these composite materials is the high-alloyed austenitic stainless TRIP-steel (Transformation Induced Plasticity) reinforced by MgO-stabilized zirconia (Mg-PSZ). That composite material exhibits extraordinary high values of specific energy absorption in compression [1]. The Mg-PSZ shows a martensitic transformation of tetragonal to monoclinic phase during deformation resulting in additional strength increase [2]. Minor addition of TiO₂ improves mechanical properties of the composite due to increase of bonding between the zirconia particles and the TRIP steel [3]. Additionally, materials based on the ZrO₂-TiO₂-MgO system are of particular interest due to their dielectric properties [4]. Therefore, the aims of this work are experimental study of phase relations and thermodynamic database development for the ZrO₂-TiO₂-MgO system.

Preliminary phase diagram of the ZrO₂-TiO₂-MgO system was presented by Coughanour et al. [4] in 1955 and new experimental study was necessary. Samples were prepared using the co-precipitation method. Phase assemblages stable after long heat treatment were identified by X-ray powder diffraction. Temperatures of invariant reactions were determined by differential thermal analysis. Sample microstructures were investigated using scanning electron microscopy combined with dispersive X-ray spectrometry.

Based on the obtained experimental data, isothermal sections of the ZrO₂-TiO₂-MgO system at temperatures 1530, 1680 and 1880 K were established. Wide extension of stability of Zr_{1-x}Mg_xO_{2-x} phase with fluorite structure into ternary system was found. Very limited solubility of MgO was found in beta (Zr_xTi_{1-x})₂O₄ and tetragonal (Zr_{1-x}Ti_x)O₂ phase, while more substantial solubility of ZrO₂ was found in the intermediate compounds of the TiO₂-MgO system (Mg₂TiO₄, MgTiO₃ and MgTi₂O₅). Low temperature ternary compound similar to δ -phase Y₄Zr₃O₁₂ was revealed at 1530 K. Differential thermal analysis indicated that this phase was stable up to 1664 K. Temperatures and compositions of three eutectic reactions were determined. Thermodynamic parameters of the ZrO₂-TiO₂-MgO system were optimized using CALPHAD approach based on the obtained experimental results.

-
1. Biermann, H., et al., Adv.Eng.Mater., Vol.11 (2009):1000-1006
 2. Martin, S., et al., Steel Research int., Vol.82 (2011):1133-1140
 3. Weigelt C., et al., Ceram. Int., Vol.41 (2015):2328-2335
 4. Coughanour L.W., et al., J. Res. Nat. Bur. Stand., Vol.54 (1955):191-199

DATA-MINING APPROACHES TO FIND NEW FUNCTIONAL MATERIALS

Eriksson O.

¹UU, Uppsala, Sweden, ²ÖU, Örebro, Sweden

olle.eriksson@physics.uu.se

Progress in materials science is with few exceptions primarily driven by experimental exploration that is followed by theoretical work. Unfortunately, theory seldom leads the way forward in identifying or predicting materials with desired functionality, albeit a few exceptions to this rule exists. For instance, the observed tunneling magneto resistance in Fe/MgO/Fe sandwich structures, where a few layers of insulating MgO is inserted between thin films of Fe, was an experimental realization that followed theoretical predictions, based on calculations of the electronic structure. Graphene, the celebrated two-dimensional material, where many of the observed exotic properties are the result of a linear dispersion of the electron states around the Fermi level, is another example where theory of the exotic electronic structure preceded experimental measurements.

Unfortunately, the list of examples where theory actually makes predictions of new materials or new properties, is very short. New tools and new ways to work are clearly needed to improve the rate with which new materials may be identified, and theory may play a crucial role. A method that quickly is being established, involve data-mining algorithms and advanced, high-throughput electronic structure theory. The fundamental ideas behind this method [2] are described in this talk, and examples will be given of how it has so far been found to perform.

-
1. RCTP-15 web site, <http://www.ihed.ras.ru/rctp2018/en/contribution>
 2. O.Eriksson, Nature Nanotechnology **13**, 180 (2018)

STUDY OF THE PHASE DIAGRAM OF ZIRCONIUM BY MOLECULAR DYNAMICS METHOD

Gordeev I.S.

¹JIHT RAS, Moscow, Russia, ²MIPT, Dolgoprudny, Russia

gordeevilu@gmail.com

Zirconium is an important structural material, however, its phase diagram has not been fully studied. The method of molecular dynamics allows to calculate phase transition curves by different methods. The purpose of this work is to compare the results of such methods as two-phase and single-phase modeling, calculation of thermodynamic potentials by the vibration density of states for the BCC-HCP and BCC-melt transitions. The calculations are carried out for two potentials: EAM-potential #2 [1] and ADP-potential [2]. The two-phase simulation method is based on the observation of the phase boundary motion in a two-phase system. The single-phase simulation method is based on extrapolation of the transition temperature between the phases at different heating or cooling rates in a single crystal. The calculation of thermodynamic potentials by vibration density of states received from the calculations of the velocity autocorrelation function. All simulations were carried out in LAMMPS.

-
1. M.I. Mendeleev G. J. Ackland // Philosophical Magazine Letters, Vol. 87, No. 5, May 2007, 349-359
 2. D.E. Smirnova, S.V. Starikov // Computational Materials Science 129 (2017) 259-272

DEVELOPMENT OF ATOMISTIC MODEL FOR PREDICTION OF PROPERTIES OF BINARY ZR-NB SYSTEM

Smirnova D.E.,^{1,2} *Starikov S.V.*,^{*1,2} *Gordeev I.S.*¹

¹*JIHT RAS, Moscow, Russia,* ²*ICAMS, Bochum, Germany*

**d.e.smirnov@gmail.com*

Zirconium is a constituent of many alloys, which found their application in substantially different areas: from nuclear engineering to medical prosthetics. As examples, we can mention here corrosion-resistant cladding alloys, namely Zr-2.5%Nb, and a series of Ti-Nb-Zr medical alloys. Characteristics of the given alloy strongly correlate with the properties of zirconium phase on which it is based. Therefore, the determination of the zirconium phase stability conditions is an essential issue for the design of the mentioned materials. At the same time, some controversies exist on the phase transitions in zirconium. The range of questions varies from the uncertainty in the melting line to the disputes about the details of the solid-solid phase transitions and influence of the alloying elements. Here we report a new attempt to study properties of Zr-Nb binary system. For this purpose, we constructed an angular-dependent many-body interatomic potential [1]. The potential functions were fitted towards the *ab initio* data computed for a large set of reference structures. We show that the model reproduces structure and properties of all Nb and Zr phases existing in the Zr-Nb binary system with a good accuracy. Moreover, the model can be applied for prediction of melting and α -Zr \longleftrightarrow β -Zr transition temperatures. The potential provides an opportunity for simulation of Zr-Nb alloys based on α -Zr and β -Zr. This conclusion is illustrated by the results obtained for the alloys with different niobium concentrations: up to 7% in case of hcp alloys and up to 50% for bcc alloys. Besides, we report results of the deformation tests made for the atomistic models of β -Zr-Nb alloys with different niobium content.

-
1. Smirnova D.E., Starikov S.V. // An interatomic potential for simulation of Zr-Nb system. *Comp. Mater. Sci.* 2017 V. 129. P. 259.

METASTABLE EMBEDDED NANOPARTICLES IN METALLIC ALLOYS. GENERAL CONCEPTS AND ATOMISTIC MODELING.

Gornostyrev Yu.N.,^{*1,2} *Korzhvyi P.*,^{1,3} *Gorbatov O.I.*,^{1,3} *Katsnelson M.I.*⁴

¹*IMP UB RAS, Ekaterinburg, Russia,* ²*IQMS, Ekaterinburg, Russia,* ³*KTH, Stockholm, Sweden,* ⁴*RU, Nijmegen, Netherlands*

**yug@imp.uran.ru*

Nanoscale inhomogeneities are typical for numerous metallic alloys and crucially important for their practical applications [1]. This kind of structural state can be formed due to freezing/stabilization of an incomplete stage of the phase transformation or due to formation long-living metastable nanosized-scale precipitates embedded in a host. This a heterogeneous state was observed in many technologically important alloys (Guinier-Preston zones in Al alloys, athermal omega-phase in Ti- and Zr-based alloys, precipitates of Co in Cu and other). However, the mechanism of formation and stabilization such state are still poorly understood.

Here we present an overview of the problem, together with a discussion of the typical examples of heterogeneous states. It is demonstrated, the stability of such precipitates is controlled by competition between short-range (chemical) and long-range (elastic) contributions to the free energy. We show that many-body interactions, including the contributions due to lattice relaxations, are mainly responsible for the formation of metastable planar (GPZ) atomic arrangements [2] and the kinetics of their formation can include several stages [3]. We discussed

possible mechanisms of stabilization embedded nanoparticles and establish that it is controlled by removing long-range stresses due to loss of coherence [1] or/and segregation of alloying elements on the interface.

1. Yu.N. Gornostyrev, M.I. Katsnelson, Phys. Chem. Chem. Phys., **17**, 27249 (2015)
2. O.I. Gorbatov, Yu.N. Gornostyrev, P.A. Korzhavyi, Scripta Materialia, **138**, 130 (2017)
3. A.Yu. Stroev, O.I. Gorbatov, Yu.N. Gornostyrev, P.A. Korzhavyi, Phys Rev Materials, **2**, 033603 (2018)

ELECTROCHEMICAL SURFACE PHASE DIAGRAMS: SOLVATION EFFECTS AND SELECTIVITY

Todorova M., Yoo S., Neugebauer J.*

MPIE, Duesseldorf, Germany

**m.todorova@mpie.de*

Solid/liquid interfaces are at the heart of many problems of practical importance. Improving the life of battery materials, the efficiency of electro-catalysts or the protection against corrosion requires understanding of the processes occurring at the solid/liquid interface. Central to such an understanding is the identification of the structures forming at the surface of a solid immersed in an aqueous electrolyte. Unfortunately, our knowledge how the electrolyte influences their formation and thermodynamic stability is limited.

Ab initio modelling using density functional theory (DFT) has proven immensely successful in providing atomistic insight into various questions of materials science, but its application to electrochemical problems is challenging, due to the presence of the solvent. Utilising concepts from semiconductor physics has enabled us to overcome some of these obstacles [1], which opens, for example, the path to constructing electrochemical surface Pourbaix diagrams using *ab initio* calculations. These are phase diagrams, which depict the stability of surface structures as a function of the relevant environmental conditions of *pH* and electrode potential *U*. Constructing such an *ab initio* surface Pourbaix diagram for the (0001) surface of ZnO, we study the impact an aqueous electrolyte has on the thermodynamic stability of polar oxide surfaces. We find that solvation effects are highly selective. They have little impact on surfaces with metallic character, but favour the stabilisation of semiconducting surfaces experiencing a high electrostatic penalty in vacuum [2]. This high selectivity has direct consequences for the surface phase diagrams and explains why certain structures are preferentially observed in electrochemical environment.

1. M. Todorova and J. Neugebauer, Phys. Rev. Applied **1**, 014001 (2014).
2. S. Yoo, M. Todorova and J. Neugebauer, Phys. Rev. Lett. **120**, 066101 (2018).

THEORETICAL STUDY OF MAGNETIC PROPERTIES OF THE 1:12 ALLOYS

Vekilova O. Yu., Eriksson O., Herper H. C.*

UU, Uppsala, Sweden

**olga.vekilova@physics.uu.se*

Since the discovery of Nd₂Fe₁₄B, the best permanent magnet to date, magnets containing the combination of rare earth elements and Fe attract high scientific interest. The iron-based compounds are specifically attractive as they have large magnetic moments due to the high

concentration of Fe, rather high coercivity and high Curie temperature. One of the best candidates are the 1:12 compounds with the ThMn_{12} -type structure. It has been shown that light rare earths and iron cannot form a stable binary 1:12 compound, so a third element must be added to stabilize the ternary $\text{RE}(\text{Fe},\text{M})_{12}$ phase, where $\text{M}=\text{Ti}, \text{V}, \text{Si}, \text{Mo}$ and etc. Such substitution results in a significant decrease in the saturation magnetization of the compound because the M atom does not carry a magnetic moment and causes a reduction of the magnetic moments of surrounding Fe atoms. Further, the change in the structure due to the substitution of iron by other elements can influence magnetocrystalline anisotropy and Curie temperature of the alloy. A number of attempts to stabilize the compounds with the decreasing concentration of M element have recently been made. Most of the known 1:12 compounds are stable when they have 10 atoms of Fe and 2 atoms of an impurity in the unit cell ($\text{REFe}_{10}\text{M}_2$). An example is $\text{SmFe}_{10}\text{V}_2$. However, $\text{NiFe}_{11}\text{Ti}$ is known to be stable even with one Ti atom per formula unit. Recent experiments show that it is also possible to stabilize the 1:12 phases with reduced concentrations of V or Ti.

In this work the magnetic properties of the 1:12 compounds were studied theoretically from first principles. Starting from the known stable $\text{NiFe}_{11}\text{Ti}$, $\text{SmFe}_{11}\text{Ti}$ and $\text{SmFe}_{10}\text{V}_2$ phases we tried to improve the magnetic properties by reducing the content of Ti and V respectively. The phase stabilities of $\text{NdFe}_{11-x}\text{Ti}_x$ and $\text{SmFe}_{10-x}\text{V}_x$ were calculated and compared to the available experimental data. This work is supported by the European Research Project NOVAMAG (EU686056) and STandUP for energy (Sweden).

DIFFUSION IN IONIC CONDUCTORS FROM AB INITIO MOLECULAR DYNAMICS

Simak S.I.

LiU, Linköping, Sweden

sergeis@ifm.liu.se

Even if diffusion in ionic conductors could be rather fast, to study it from accurate ab initio equilibrium molecular dynamics (MD) is usually impossible due to prohibitively long simulation times. The use of the nonequilibrium color-diffusion algorithm [1] allows one to substantially speed up the simulations. The algorithm has been implemented in the widely used Vienna Ab Initio Simulation Package (VASP) and applied to the problem of oxygen diffusion in doped ceria, a promising electrolyte material for intermediate temperature solid oxide fuel cells (IT-SOFCs). The application of the methodology speeds up the simulated oxygen transport by a factor 60 compared with standard equilibrium MD. The calculated conductivity values agree with the available experimental data, and the experimental temperature trend is well reproduced [2, 3]. If time allows we also discuss the finite-temperature lattice dynamics and superionic transition in ceria and show how they can be treated despite all the difficulties [4].

The project has been supported by the Swedish Government Strategic Research Area in Materials Science on Functional Materials at Linköping University (Faculty Grant SFO-Mat-LiU No. 2009 00971) and the Swedish Research Council (VR) (Project No. 2014-4750).

-
1. P. C. Aeberhard, S. R. Williams, D. J. Evans, K. Refson, and W. I. David, *Phys. Rev. Lett.*, 108(9), 095901 (2012).
 2. J. Klarbring, O. Yu. Vekilova, J. O. Nilsson, N. V. Skorodumova, and S. I. Simak, *Sol. St. Ionics* 296, 47 (2016).
 3. J. O. Nilsson, O. Yu. Vekilova, O. Hellman, J. Klarbring, S. I. Simak, N. V. Skorodumova, *Phys. Rev. B* 93, 024102 (2016).
 4. J. Klarbring, N. V. Skorodumova, and S. I. Simak, *Phys. Rev. B* 97, 104309 (2018).

ATOMIC DIFFUSION MECHANISMS IN TITANIUM CARBIDE

Ehteshami H.,¹ *Smirnova E.A.*,² *Sun W.*,³ *Korzhavyi P.A.**^{1,2,4}

¹*KTH, Stockholm, Sweden*, ²*NUST "MISIS Moscow, Russia*, ³*ORNL, Oak Ridge, United States*, ⁴*IMP UB RAS, Ekaterinburg, Russia*

**pavelk@kth.se*

Transition-metal carbides and nitrides combine ceramic-like properties (high melting point, hardness, and corrosion resistance) with metal-like properties (high electrical and thermal conductivity). These compounds are therefore highly suitable for many existing and emerging high-temperature applications [1]. Understanding atomic defects and diffusion in refractory compounds is important for controlling their properties during manufacturing and service [2]. While monovacancies can fully account for the self-diffusion in Group-IV metal nitrides [3], understanding the diffusion mechanisms of metal atoms in the corresponding carbides represents a challenge due to the extremely high formation energy of a metal vacancy [4, 5]. An overview of recent *ab initio* studies of point defects, defect clusters, and diffusion mechanisms in titanium carbide will be given [4–7]. The focus will be made on the Ti self-diffusion mechanisms in TiC mediated by various defect complexes involving vacancies, self-interstitials, and/or oxygen impurity atoms.

1. Toth L. E. (ed.) Transition Metal Carbides and Nitrides. Academic Press, New York, 1971.
2. Andrievskii R. A. // Powder Metallurgy and Metal Ceramics. 2011. V. 50. Nos.1-2. P. 2; [Russian original: Poroshkovaya Metallurgiya (Kiev). V.50, Nos.1-2. P. 5].
3. Gambino D., Sangiovanni D. G., Alling B., Abrikosov I. A. // Phys. Rev. B. 2017. V.96. Art. No. 104306.
4. Razumovskiy V. I., Ruban A. V., Odqvist J., Korzhavyi P. A. // Phys. Rev. B. 2013. V. 87. Art. No. 054203.
5. Razumovskiy V. I., Popov M. N., Ding H., Odqvist J. // Comput. Mater. Sci. 2015. V. 104. P.147.
6. Sun W., Ehteshami H., Korzhavyi P. A. // Phys. Rev. B. 2015. V.91. Art.No. 134111.
7. Sun W., Ehteshami H., Kent P. R. C., Korzhavyi P. A., to be published.

DEVELOPMENT OF NEW MATERIALS USING AN INTEGRATED APPROACH OF DFT CALCULATIONS, CALPHAD MODELING AND KEY EXPERIMENTS

Pisch A.

SIMaP, Grenoble, France

alexander.pisch@simap.grenoble-inp.fr

ICME (Integrated computational materials engineering) is a modern approach to develop new materials with tailored properties for a given application. Chemical thermodynamics is a cornerstone of this method, because it is always the first step to evaluate if new materials and their synthesis routes are feasible. To perform thermodynamic calculations, the Calphad method is generally employed because it is the only method to allow simulations in higher components systems (3 or more) taking into account complex solids, liquids and the gas phase. Calphad thermodynamic modeling is a phenomenological method, i.e. the underlying Gibbs energy functions for the phases are obtained by least square fitting using available theoretical and experimental data. Therefore, the need for the generation of high quality theoretical and experimental data is obvious. This integrated thermodynamic approach will be illustrated in this contribution on three different examples: the solubility limit of Nb in liquid Al and the consequences for the Al-rich equilibria in the Al-Nb binary system, Mg-Al-carbides as new

option for grain refinement in magnesium alloys and the development of novel low CO₂ cements.

The solubility and heat of dissolution of Nb in Al was measured by isothermal drop calorimetry at 1126 K. In addition, the heat capacity of NbAl₃ was measured and calculated as a function of temperature. The obtained results contradict the peritectic nature of the Al-NbAl₃-liquid three phase equilibrium. In the case of Mg-Al-C, ab-initio DFT and phonon calculations were performed and compared to new heat capacity measurements. Based on this new data, a new Calphad modeling of this ternary system was performed and will be discussed. Typical Portland cement is at least a nine component system (CaO-SiO₂-Al₂O₃-Fe₂O₃-MgO-K₂O-Na₂O-SO₃-P₂O₅-TiO₂). Cement clinker, the main component of cements, is obtained by high temperature solid-liquid reaction using natural raw materials. It will be shown how a pragmatic approach to set-up a new multicomponent thermodynamic database using ab-initio calculations and experimental equilibrium data allowed a consistent thermodynamic description of the full clinker system. Based on this database, a simulation model for the clinker burning was set-up and compared to industrially obtained data with excellent agreement. The application of this new model to improve OPC clinker properties will be discussed.

THERMODYNAMIC PROPERTIES OF RE-CONTAINING TBC MATERIALS

Gavrich K.S., Guskov V.N., Nikiforova G.E.*

IGIC RAS, Moscow, Russia

**gavrich@igic.ras.ru*

Focusing to the study of thermal and thermodynamic properties of thermal barrier coating (TBC) materials explains by the possibility to advance, sufficiently, the parameters of gas turbine or aero-engine parts. Requirements for such materials (such as high melting point, absence of phase transformations, low thermal conductivity, low ionic conductivity, compatibility with the metallic material of the part (superalloy)) significantly limit the range of substances that can be used as TBC materials.

Heat capacity of different RE-containing substances with the high melting point (REPO₄, RENbO₄, RE₂Zr₂O₇, RETaO₄; RE=Sc, Y, Ln), acceptable for TBC, was studied in the temperature range from 2 K to 1300 K. Thermal properties were investigated from 350 to 1800 K using the differential scanning calorimetry (DSC). Different types of calorimetric measurements were used (quasi-adiabatic (relaxation) (from 2 to 100 K), adiabatic (from 6 to 340 K), DSC (from 350 to 1300 K), and drop calorimetry (from 400 to 1500 K)) in this study.

Lanthanide compounds undergo a set of phase transitions due to the electronic structure in f-level. As a rule, these transitions (magnetic, Jahn-Teller, Schottky anomaly) do not cause the change of crystal structure, but affect a shape of heat capacity curve, and, consequently, lead to additional contributions in a heat capacity and in related thermodynamic functions (entropy, enthalpy change and change of Gibbs energy).

Joint application of different calorimetric methods allows to increase the reliability of obtained results, especially for high-temperature region because of the high possibility of systematic errors in DSC and drop-calorimetric measurements.

Different variants of joint fitting of low and high temperature heat capacity data were used to receive the consistent data.

This work was supported by the Russian Science Foundation (project 18-13-00025).

THIRD-GENERATION THERMODYNAMIC DESCRIPTION OF SiO₂

*Bajenova I. A.,*¹ Kondratiev A. V.,¹ Khvan A. V.,¹ Dinsdale A. T.^{2,3}*

¹SRC Thermochemistry of materials, Moscow, Russia, ²Hampton Thermodynamics Ltd, Hampton, United Kingdom (Great Britain), ³BCAST, Uxbridge, United Kingdom (Great Britain)

**irabajenova00@mail.ru*

Modern assessments of thermodynamic properties of elements and substances require more physically based models that provide accurate and reliable predictions in a wide range of temperatures from 0 K to temperatures above the melting point. In the present work the extended Einstein model [1] and the two-state model [2] were used to describe thermodynamic properties of silicon dioxide. The extended Einstein model, which includes harmonic vibrations into the heat capacity, was used for the thermodynamic description of α - and β -quartz and α - and β -cristobalite. The two-state model that assumes a liquid phase to consist of two kinds of atoms was used to describe the amorphous and liquid SiO₂, which were treated as the same phase. The optimization of the model parameters was based on the critical review of the experimental thermodynamic data available for SiO₂ and was carried out using ThermoCalc software [3]. In a number of studies the two-state liquid model was applied for thermodynamic description of the pure elements (e.g. metals). However, a rather limited data on the heat capacity of the supercooled liquid phase available for pure metals makes it difficult or even impossible to evaluate consistency of the calculated results with the experimental data. It should be pointed out that application of the model for the thermodynamic description of oxide melts (e.g. pure SiO₂) with extensive experimental data available for both the amorphous and supercooled liquid states has not yet been carried out and therefore is a challenging task. The thermodynamic assessment presented in this work provides a good description and high reproducibility of the low-temperature and high-temperature heat-capacity data and is consistent with the standard S₂₉₈ and enthalpy increment data.

-
1. Chase M., Ansara I., Dinsdale A., Eriksson G., Grimvall G., Hoglund H., Yokokawa H. // Calphad 19(4) (1995) 437-447
 2. Agren // J., J. Phys. Chem. Liq. 1988;18:123-139.
 3. J.-O. Andersson, T. Helander, L. Hoglund, P. Shi, and B.Sundman // Calphad 26, (2002), 273-312

ATOMISTIC SIMULATION OF PHASE TRANSITIONS AND STRUCTURE TRANSITIONS UNDER IRRADIATION IN U-MO ALLOYS

Kolotova L.N., Starikov S. V.*

JIHT RAS, Moscow, Russia

**lada.kolotova@gmail.com*

Uranium is the main component of nuclear fuel. Due to high values of thermal conductivity and density, a metal nuclear fuel based on uranium alloys is the promising fuel for generation IV reactors. In addition, U-Mo fuels has high thermal conductivity, low thermal expansion, and high melting point.

The investigation found that structure of γ^0 -lattice is similar to body-centered tetragonal (bct) lattice with a displacement of central atom at basic cell into [001] direction. The lattice parameters fulfil the following condition: $a = b > c$. Moreover, high temperature γ -phase of uranium and uranium alloys has quasi-bcc lattice. At such state, local positions of atoms correspond to bcc lattice with displaced central atoms in basic cell. Also, the various mechanisms of structure changes in irradiation are examined. In particular, the simulation results indicate

that the defects formation may be produced without melting and subsequent crystallization. Threshold stopping power of swift ions for the defects formation in irradiation in the various conditions are calculated.

EMPLOYING AB INITIO THERMODYNAMICS TO DESIGN STRUCTURALLY COMPLEX MATERIALS

Neugebauer J., Zhu L., Körmann F., Grabowski B., Hickel T.*

MPIE, Düsseldorf, Germany

**neugebauer@mpie.de*

Ab initio approaches provide in principle perfect tools for the design of new materials, but face serious challenges: Free energies which are the key quantity to compute thermodynamic phase diagrams, deformation paths or defect formation energies require formalisms that accurately capture all relevant entropic contributions due to electronic, vibrational or magnetic excitations, as well as their coupling such as phonon-phonon, magnon-phonon interactions or spin-quantization. Calculating these contributions is conceptionally challenging and computationally expensive. The talk gives an overview over the developed approaches and their ability to accurately describe thermodynamic quantities and phase transitions. Based on these studies the performance of popular DFT functionals in describing these quantities will be discussed. To demonstrate the practical applicability of these approaches examples will be given showing how they helped discovering a new class of light-weight metallic alloys with improved mechanical properties.

EFFECTIVE BOSONIC MODELS FOR COLLECTIVE ELECTRONIC FLUCTUATIONS

*Stepanov E.A.,*¹ Lichtenstein A.I.,² Katsnelson M.I.¹*

¹Radboud University, Nijmegen, Netherlands, ²UHH, Hamburg, Germany

**e.stepanov@science.ru.nl*

Collective electronic fluctuations in correlated materials give rise to various important phenomena, such as charge ordering, superconductivity, Mott insulating and magnetic phases, and plasmon and magnon modes. Description of these correlation effects requires a significant effort, since they almost entirely rely on strong local and nonlocal electron-electron interactions. Some collective phenomena, such as magnetism, can be sufficiently described by simple Heisenberg-like models that are formulated in terms of bosonic variables. This fact suggests that other many-body excitations can also be described by simple bosonic models in the spirit of Heisenberg theory. Here we derive an effective bosonic action for charge and spin degrees of freedom for the extended Hubbard model. Also, we define a physical regime where the obtained model action reduces to a classical Hamiltonian of an effective Ising and Heisenberg models for charge and spin variables, respectively. The derived formalism is reminiscent of Anderson's idea of the effective exchange interaction and takes into account nonlocal correlation effects. The results for the exchange interaction and susceptibility are expressed in terms of single-particle quantities, which can be obtained efficiently in realistic calculations of multiband systems.

FLUCTUATING LOCAL FIELD APPROACH TO STRONG CORRELATIONS

Rubtsov A.

Russian Quantum Center, Moscow, Russia

ar@rqc.ru

A quantitative description of developed collective fluctuations in correlated media remains one of the main challenges for the theoretical and computational physics. The essentially nonlocal nature of the collective modes makes the mean-field schemes inappropriate. The advanced diagrammatic schemes such as Dual boson approach built on top of the Dynamical mean field theory require an enormous numerical effort, and even their accuracy can be questioned. In our talk, we will report a new approach targeting the problem of strong collective fluctuations. Unlike the mean-field paradigm, where the effective field obeys a constant value to determined in a self-consistent way, we perform an integration over the value of the effective field. The mean field solution corresponds to the saddle point in this integration, whereas a grid-integration over all values of the effective field allows to handle the fluctuations. The method is benchmarked for small Ising and Heisenberg classical clusters, as well as for the half-filled Hubbard one, and shows a superior accuracy against the mean-field approach.

THEORETICAL PHYSICS APPROACHES FOR UNDERSTANDING OF MATERIALS: LESSONS FROM Yu. Kh. VEKILOV

Abrikosov I.A.

¹Linköping University, Linköping, Sweden, ²NUST "MISIS", Moscow, Russia

igor.abrikosov@liu.se

Electronic structure theory is now recognized as highly useful tool for prediction of materials properties, for their understanding, as well as for determination of parameters employed in higher-level modeling. In this talk, novel methodological solutions and exciting applications, which have been inspired by my interactions with Yuri Vekilov will be presented. In particular, development of theoretical tools for simulations of chemical disorder and studies of matter at extreme conditions will be discussed.

DETERMINATION OF TEMPERATURE AND COMPOSITION AREAS OF SOLID SOLUTION IN Fe-Ni-Co-(Cu,Cr) SYSTEM

Sinyova S.,^{*1,2} Starykh R.,^{1,2} Vasil'eva A.,³ Boduen A.³

¹SPbSPU, Saint-Petersburg, Russia, ²LLC Gipronickel Institute, Saint-Petersburg, Russia,

³SpbMU, Saint-Petersburg, Russia

**svetlana.sinyova@gmail.com*

The work is devoted to the determination of temperature and composition area of solid solution, existed at Fe-Ni-Co-(Cu,Cr) system. It is well-known, that alloys of this system are the new type of materials, characterized by high entropy of mixing. Design of high entropy alloys (HEAs) with desired properties is modern trend in materials science nowadays, and number of articles, related to the discussed topic, is constantly increasing. Authors of the current work came down to the design and analysis of HEAs from the thermodynamic point of view, based on the own experience in experimental investigation of phase diagrams of multicomponent metallic systems [1,2].

Research is provided with the use of classical physico-chemical methods of phase diagram construction, namely, differential thermal analysis, electron probe microanalysis, X-ray diffraction analysis and scanning electron microscopy. During the first step of research the liquidus and solidus surface projections of the Fe-Ni-Co-Cu quaternary system have been constructed. There were defined the limits of solid-state miscibility gap and tie-lines location within the discussed miscibility gap. In such a way we defined the area of quaternary solid solution, within the volume of that the HEAs can be synthesized. The next step of research is determination of temperature and composition areas of solid solution in Fe-Ni-Co-(Cu,Cr) system. The effect of addition of Cu and Cr on the structure, phase composition and properties of obtained alloys has been shown. Obtained information could be useful as basis for design of HEAs.

The work was supported by RFBR grants 16/03/00987 and 17/08/00875.

1. Ilatovskaya M.O., Starykh R.V., Sinyova S.I. Liquidus and Solidus Surfaces in the Quaternary Fe-Cu-Co-S System. Part II: The Ternary Fe-Cu-Co System// Metallurgical and Materials Transactions B, vol. 46B, 2015, pp. 243-249.
2. Starykh R.V., Sineva S.I. Study of the liquidus and solidus surfaces of the quaternary Fe-Ni-Cu-S system: V. Refinement and addition of the data on the ternary Fe-Ni-S and Fe-Ni-Cu phase diagrams // Russian Metallurgy, vol.2012. 3 pp.189-194.

OPTIMIZATION OF THE CELL UPTAKE OF GADOLINIUM OXIDE NANOPARTICLES BY CAPPING WITH SORBITOL FOR CELL TRACKING IN MRI

Abrikosova N.A.,^{*1,2} *Brommesson C.*,² *Larsson E.*,² *Eriksson P.*,² *Zhangjun H.*,² *Uvdal K.*²

¹NUST "MISIS", Moscow, Russia, ²LiU, Linköping, Sweden

**natabrikos@gmail.com*

Design of novel nanoparticles with antioxidant capabilities for MRI contrast enhancement is an active field of research [1]. In the optimization of the cell uptake of contrast agent for cell tracking in MRI, it is important to make compromises between the optimal contrast in MRI and metabolic cell activity. In this work, we investigated if the Sorbitol aids the uptake of Gd₂O₃ nanoparticles (GdNP) by the cells. In order to test this hypothesis, GdNP were both capped to and immersed in Sorbitol. Micro Magnetic Resonance Imaging was used to investigate the contrast enhancement and the uptake of the MRI contrast agents by mouse alveolar macrophages. The samples were scanned with a 9.4 Tesla (400 MHz) micro MRI scanner, with a vertical bore high-resolution superconducting magnet (Japan Superconductor Technology, Inc., Kobe, Japan). The immortalized mouse alveolar cell line MH-S (1x10⁶ cells/ml) were incubated with a GdNP and GdNP were both capped to and immersed in Sorbitol.

Longitudinal relaxation rates and the corresponding calculated regression slopes for filtered DEG-Gd₂O₃ nanoparticle samples (GdNP) and GdNP, both capped to and immersed in Sorbitol were measured experimentally. Chemiluminescence recordings of the reactive oxygen species (ROS) production from neutrophil granulocytes (2x10⁶ cells/ml) after an exposure the NP was carried out. Effect of addition of capping or immersion of Sorbitol to GdNPs to change of the T₁-contrast in MRI has been investigated.

The cell optimization strategies presented in this work may be of importance to several fields aiming at imaging inflammatory diseases, based on the utilization of contrast agent-loaded macrophages.

1. P. Eriksson, A. A. Tal, A. Skallberg, C. Brommesson, Z. Hu, R. D. Boyd, W. Olovsson, N. Fairley, I. A. Abrikosov, X. Zhang and K. Uvdal, Cerium oxide nanoparticles with antioxidant capabilities and gadolinium integration for MRI contrast enhancement, *Sci. Rep.* 8, 6999 (2018).

ELASTIC CONSTANTS FOR ALLOYS WITH MECHANICAL INSTABILITY: AB INITIO INVESTIGATION OF BCC Ti

*Skripnyak N. V.,^{*1} Ponomareva A. V.,² Belov M. P.,² Abrikosov I. A.¹*

¹*LiU, Linköping, Sweden, ²MISIS, Moscow, Russia*

**natali.skrp@mail.ru*

The influence of the amount content of V on the mechanical phases stability of body-centered cubic (bcc) based Ti-V alloys was studied. The elastic properties of the binary system of bcc Ti-V alloys were investigated using the non-empirical method of pseudopotentials and the method of exact MT orbitals in the entire concentration range of V. Disorder substitution was modeled using a special quasi-random structure (SQS) technique and in the coherent potential approximation (CPA). The concentration V dependence of the elastic constants of the single crystal $C_{\alpha\beta}$, obtained by calculating the total energy for the corresponding deformations, and also family of material characteristics E, B, G, Pc, k, v for the TiV system were introduced and discussed. In the case Ti-V alloys, a comparative analysis of efficiency of the PAW and EMTO methods to obtain data of the elastic properties of Ti-V alloys from the first-principle modeling over a wide range of the concentration V was presented. It was found that Ti-rich TiV alloys are mechanically unstable in the bcc phase, but at higher concentration V in the system the mechanical stability is increased. The efficiency of using different calculation methods in the study of the elastic properties of disordered alloys are discussed.

THE IMPORTANCE OF THE LATTICE DYNAMIC IN THE MAGNETIC PHASE TRANSITION IN FERH

*Belov M. P.,^{*1} Syzdykova A. B.,¹ Ponomareva A. V.,¹ Smirnova E. A.,¹
Abrikosov I. A.^{1,2}*

¹*NUST "MISIS Moscow, Russia, ²LiU, Linköping, Sweden*

**maksपालych@gmail.com*

FeRh undergoes an unusual antiferromagnetic-to-ferromagnetic (AFM-FM) transition just above room temperature. This magnetic transition was discovered for the first time in the late 1930s [1] but the origin of this transition is still a source of active debate. There are basic questions about what drives this transition, and usually the driving force is discussed in terms of magnetic, lattice and electronic entropy differences between the phases. In this work we have carried out calculations in the framework of Temperature Dependent Effective Potential method (TDEP) [2] based on molecular dynamic simulations at different temperatures and obtained full phonon spectra and corresponding lattice entropies of AFM and FM FeRh at different temperatures. In this way we have demonstrated strong temperature dependence of phonon spectra for both phases and consequently the importance of temperature on lattice entropy difference which calculated value is 16 J/kg/K at 350 K.

-
1. M. Fallot, *Ann. Phys. Serie 11* 18, 291 (1938).
 2. O. Hellman, I.A. Abrikosov, S.I. Simak, *Phys. Rev. B* 84, 180301 (2011).

CALCULATION OF SOLUTION ENTHALPY OF CARBON IMPURITY IN FE – MN PARAMAGNETIC ALLOYS

Ponomareva A. V.,* Mukhamedov B. O., Abrikosov I. A.

NUST MISIS, Moscow, Russia

**alenaponomareva@yahoo.com*

In the framework of electronic density functional theory, we calculated a solution enthalpy of carbon impurity into paramagnetic fcc $Fe - Mn$ alloy. Properties of $Fe - Mn - C$ alloys were described with using the model that takes into account the contribution of thermal magnetic fluctuations in paramagnetic matrix with point defects. This model is generalized for the cases of magnetic and chemical disorder. It was found that in alloys containing Mn , the solution enthalpy of carbon decreases compared to pure gamma- Fe . Also, we analyze various possible factors that can increase the carbon solubility in $Fe - Mn$ alloys.

DATA DRIVEN DESIGN OF AL ALLOYS

Smirnova E. A.,* Mosyagin I. Yu., Vorobuev D. A.

NUST MISIS, Moscow, Russia

**ekaterina.smirnova@misis.ru*

Modern High-throughput methods make it possible to obtain large volumes of data. This "Big Data" approach allows not only to find trends and dependencies, but also opens up fundamentally new methods of research.

Today less than 200,000 materials are known, but only for a few of these "known" materials basic properties have been studied, and in fact there is an infinite number of compounds that need further research.

Therefore it is likely that new materials with excellent and still unknown properties exist that could help to solve fundamental problems in energy, transportation, security, information and health.

One of the most widely studied and practically useful problems is the creation of new aluminum alloys. Therefore binary aluminum alloys with 1% impurity concentration were selected for our High-throughput analysis. To do this we have developed a comprehensive automated system for physical properties computation. The software handles creation of configuration files, executes calculations, processes and visualises the results.

We had reviewed binary aluminum alloys with 63 alloying components. For each alloy we built its equation of state, determined the lattice parameters and the bulk modulus, computed the elastic constants, the Young's modulus and the shear modulus. Finally we had compared these results with the available experimental data.

AUTHOR INDEX

- Abdulagatov I., 59
Abdulagatov I.M., 34, 92, 107, 156
Abdulagatova Z.Z., 92
Abdullaev R.N., 16
Abrikosov I.A., 69, 76, 112, 170, 172, 173
Abrikosova N.A., 171
Aetov A. U., 75
Agazhanov A.Sh., 16
Ahmetzyanov T.R., 37
Akhmedov E.N., 24, 110
Akhtyamov E.R., 95
Alchagirov B.B., 64, 66, 106, 108
Alekseev S.G., 136
Alexandrov I.S., 18
Alikhanyan A.S., 66
Aliverdiev A.A., 24
AlyaeV V.A., 156
Andbaeva V.N., 18
Andrusova N.N., 76
Anishchanka Yu.V., 154
Antonov V.A., 46, 52
Apfelbaum E.M., 97
Apfelbaum M.S., 131
Aristova N.M., 68, 136
Artamonov A.V., 123
Babich A.Yu, 55
Baidakov V.G., 18
Bajenova I.A., 168
Bakmaev A.G., 92
Barbin N.M., 136
Barinov A.A., 113, 130
Batryshev D.G., 117
Batyrova R.G., 107
Bazaev A.R., 33, 34, 92, 145
Bazaev E.A., 33, 34, 145
Beliavskiy A.E., 46
Belikov R.S., 47
Belonoshko A. B., 17
Belousov O.K., 123
Belov G.V., 20, 68, 136
Belov M.P., 69, 172
Beltyukov A.L., 44, 56
Belyaev G.E., 125
Belyakov M. Yu., 28
Belyavsky E.A., 52
Beybalaev V.D., 24
Bezgomonova E.I., 42
Bezverkhii P. P., 23
Bgasheva T.V., 85
Bilalov T.R., 26
Blagonravov L.A., 126
Boduen A., 170
Bogatishcheva N.S., 149
Bogatyrev A.F., 49
Bogdanov A.V., 149
Bogdanov E.N., 97
Borisenko D.I., 60
Borshchev N.O., 52
Borshev N.O., 46
Bozhko S.I., 112
Brommesson C., 171
Brykin M.V., 80, 82
Bukhmirov V.V., 124
Buleiko V.M., 144
Chen Q., 159
Chen W., 159
Chernoskutov M. Yu., 83
Chernoskutov M.Yu., 118
Chigvintsev A.Yu, 33
Chinnov V.F., 100, 142
Chirkov A.Yu., 113
Chudanov V.V., 132
Chusov I.A., 141
Colinet C., 158
Dadashev R.Kh., 64
Davydov A.G., 36, 42
Demirov N.A., 90
Deshabo V.A., 152
Didenko V.I., 141
Ding L., 51
Dinsdale A.T., 168
Director L.B., 147
Divin A.G., 122
Dmitriev A.S., 21
Doludenko A.N., 131
Dolzhenko A.V., 115
Doronin Ya.I., 74
Dosbolayev M.K., 117
Druzhinina A.I., 74
Dudarev V.A., 102, 104
Dunaev A.M., 80, 87
Dyachkov S.A., 20
Dzhapparov T.A-G., 92
Dzhumagulova K.N., 100
Dzugurova L.K., 71
Efimov A.V., 142

- Efimov S., 96
Efremov V.P., 110
Egorov G.I., 61
Ehteshami H., 166
Eletskiy I.A., 54
Elimkhanov D.Z., 106
Emelyanov A.N., 30
Engstrom A., 159
Eriksson O., 162, 164
Eriksson P., 171
Erkimbaev A.O., 103
Ermishkin V.A., 119, 123
Evdokimov S.A., 90
Ezhov V.M., 147
Fabrichnaya O., 160, 161
Fabrichnaya O.B., 76
Faizullin M.Z., 61, 149, 153
Falyakhov T.M., 82, 87
Farakhov M.I., 151
Fleita D.Iu., 30
Fokin L.R., 63, 106
Fomina M.G., 156
Fortova S.V., 134, 135, 139
Frolov A.M., 85, 87, 89
Gabdullin M.T., 37, 117
Gabitov F.R., 37
Gabitov I.R., 45, 156
Gadzhiev M.Kh., 90, 131
Gadzhimagomedov S.Kh., 90
Galimova A.T., 38
Galkin D.A., 50
Gaskov A.K., 124
Gatin R.S., 38
Gavrichev K.S., 167
Gerasimov A.A., 18
Golyshev A.A., 53, 99
Gorbatov O.I., 163
Gorbatov V. I., 120
Gorbatov V.I., 95
Gordeev I.S., 162, 163
Gornostyrev Yu.N., 163
Gorokhov L.N., 105
Grabowski B., 169
Granchenko P.P., 25
Gribchenkova N.A., 66
Grigorenko A.V., 125
Grigoriev B.A., 18, 144
Grigoriev E.B., 149
Gryaznov V.K., 98
Gu Q., 159
Guluzade A., 59
Gumerov F. M., 151
Gumerov F.M., 26, 35, 37, 151, 155
Guskov V.N., 167
Halkin V.N., 41
Hassel E., 59
Hazipov M.R., 38
Herper H.C., 164
Hickel T., 169
Ibavov N.V., 155, 156
Igolnikov A.A., 150
Il'ina M.A., 146
Il'ina1 M.A., 147
Ilatovskaia M., 160, 161
Ilichev M.V., 120
Inogamov N.A., 135
Ionov A.M., 112
Iosilevskiy I.L., 15, 29, 33, 98
Isakaev E.Kh., 90
Iskhakov M.E., 47
Ismagambetova T.N., 37
Issanova M.K., 101
Ivanov P.P., 134
Ivanova D.D., 121
Ivliev A.D., 118
Ivliyev A. D., 83, 120
Janickovic D., 72
Jeppsson J., 159
Jia H., 159
Körmann F., 169
Kachalov V.V., 93, 125
Kalazhokov K.K., 71, 109
Kalazhokov Z.K., 71, 109
Kalinichev A.G., 129
Kallaev S.N., 92
Kaplun A. B., 23
Kaptilnyi A.G., 31
Kapustin D.I., 120
Karamurzov B.S., 71
Kashapov L.N., 143
Kashapov N.F., 143
Kashapov R.N., 143
Katsnelson M.I., 163, 169
Kaverin A.M., 18
Kavirshin D.I., 142
Kavyrshin D.I., 100
Kazakov A.I., 147
Kedik S.A., 76
Khairulin R.A., 16
Khairutdinov V.F., 151

- Khasanova R.R., 114
 Khayrutdinov V.F., 37
 Khokonov Kh.B., 66
 Khomkin A.L., 22
 Khotienkova M.N., 18
 Khromov M.A., 142
 Khvan A.V., 168
 Khvesyuk V.I., 111, 130
 Kim G., 159
 Kiselyova N.N., 102, 104
 Kiyachenko Yu.F., 152
 Kobelev M.A., 73, 78
 Kobzev G.A., 103
 Kochanova S.A., 115
 Kochurov D.S., 54
 Kodanova S.K., 101
 Kokov Z.A., 106
 Kolotova L.N., 168
 Komarov P.S., 96, 127
 Kondratiev A.V., 168
 Kondratyev A.M., 31, 86
 Kondratyuk N.D., 44
 Konovalov P.A., 120
 Konyukhov S.A., 89
 Korepanov A.Yu., 56
 Korobenko V.N., 98
 Korotkov P.K., 106
 Korotkovskii V.I., 65
 Korshunov I.G., 95
 Korzhavyi P.A., 166
 Korzhvyi P., 163
 Kosakovich E.O., 116
 Kosinov A.V., 103
 Kosov V.I., 152
 Kosova D.A., 74, 77
 Kostanovskaya M.E., 70, 124
 Kostanovskiy A.V., 70, 124
 Kostanovsky A.V., 133
 Kotov A.N., 146
 Kotova E.S., 54
 Koverda V.P., 61, 153
 Kovtun D.M., 105
 Kozlov G.A., 97
 Kozlovskii Yu.M., 16
 Krasik Ya.E., 96
 Kuanishev V.T., 138
 Kucherenko M.A., 49
 Kuchina J.A., 148
 Kudin L.S., 80, 87
 Kudryavtsev E.M., 91, 119
 Kudryavtseva I.V., 28, 38, 40
 Kulakov A.A., 79
 Kulikov V.D., 28
 Kulyamina E. Yu, 63
 Kunakov S.K., 57
 Kurichenko A. A., 120
 Kurichenko A.A., 95
 Kuryakov V.N., 121
 Kutuzov D.S., 100
 Kuznecov K.I., 60
 Kuznetsov K.I., 25, 121
 Kyasova O.Kh., 64, 108
 Lad'yanov V.I., 56
 Ladyanov V.I., 44
 Laptev Yu.A., 53, 55, 57
 Larsson E., 171
 Lebedev A.V., 91
 Legon'kova O.A., 76
 Lepeshkin A.R., 52
 Lesev V.N., 64
 Levashov P.R., 20, 84
 Lichtenstein A.I., 169
 Likhanskii V.V., 140
 Lipatova I.A., 125
 Liu B., 113
 Loktionov E.Yu., 154
 Lukyanov K.V., 146
 Lyakhovitskii M.M., 91
 Lyubimova D.A., 122
 Maevskii K.K., 24
 Magomedov M. N., 108
 Magomedov R.A., 24
 Makarov D.M., 61
 Makeenkova O.A., 49
 Malkin A.I., 91
 Maltsev M.A., 84
 Maltseva S.A., 79
 Martynets V. G., 23
 Martynova I.A., 29
 Matskevich N.I., 77
 Mazanov S.V., 155
 Mazilin I.V., 88, 123
 Mazilkin A.A., 112
 Medvedev A.B., 97
 Meilanov R.R., 24
 Melent'ev V.V., 73
 Mendelejev V.Ya., 125
 Menshikova S.G., 56
 Meschel S., 159
 Meshalkin A. B., 23

- Meshkov E.A., 132
Meshkov V. V., 83
Meshkov V.V., 118
Mezinov N.S., 20
Mikhailov V.A., 94
Mikhaylov D.L., 123
Milyutin V.A., 32
Minakov A.V., 115
Minakov D.V., 20, 84
Minina N.A., 91, 119, 123
Minkin V.S., 156
Miroshnichenko E.A., 67
Mirskaya V.A., 155, 156
Mitropov V.V., 55
Modenov A.A., 126
Molodets A.M., 40, 53, 99
Molokanov A.A., 146, 147
Monaenkova A.S., 77
Moroz A.I., 72
Morozov I.V., 20, 68, 84
Mosyagin I.Yu., 173
Motalov V.B., 80, 87
Muboyadzhyan S.A., 90
Mukhamedov B., 112
Mukhamedov B.O., 76, 173
Murlieva Zh.Kh., 47
Nagmutdinova A.I., 88
Nakipov R. R., 75
Nakipov R.R., 153
Nakonechny Gh.V., 148
Nash P., 159
Nazarevich D.A., 155, 156
Nedyalkov Yu.V., 133
Neruchev Y.A., 62
Neruchev Yu.A., 65
Neugebauer J., 164, 169
Nikiforova G.E., 167
Nikitin E.D., 149
Nikolaev D.N., 32, 48
Noginova L.Yu., 33
Norman G.E., 22, 30
Novikov A.N., 74
Novikov G.E., 141
Novoselov I.I., 132
Obraztsov N.B., 148
Obysov N.A., 141
Ochkov V.F., 31, 102
Olyanina N.V., 44
Omarov Z.M., 92
Onufriev S.V., 82, 89, 90
Orazbayev S.A., 117
Osadchii S.M., 118
Osin S.B., 105
Osina E.L., 84, 105
Osmanova B.K., 33, 34
Ostrik A.V., 32, 48
Ovchinnikov V.V., 79
Pakhomov E.P., 65
Palchaev D.K., 49, 90
Palchayev D.K., 47
Palyi N.A., 123
Pashchenko L.L., 67
Paukova A.E., 137
Peshkichev I.V., 137
Peshkina K.G., 39
Petrik G.G., 27
Petrov V.A., 16
Petukhov S.V., 87
Petukhov S.V., 82
Pisarev V.V., 30, 44, 129, 132
Pisch A., 166
Pletnev A.E., 31
Plishkin N.A., 147
Podnek V.E., 152
Podnek V.P., 35
Pokrasin M.A., 91, 119
Polev V.F., 95
Polikhronidi N.G., 107
Ponomarev S.V., 122
Ponomareva A.V., 112, 172, 173
Popel P.S., 94
Popov A.P., 149
Popov D.A., 91
Popov I.M., 147
Popov S.D., 148
Popov V.E., 148
Postnikov E.B., 133
Potapov B.G., 118
Povolotskiy I.I., 46
Povolotsky I.I., 50
Prima A.I., 51
Prokofjev S.I., 112
Pronkin A.A., 124
Pronyaev V.G., 141
Prorokova M.V., 124
Prostorova F.O., 57
Pryazhnikov M.I., 115
Pugachev V.Yu., 137
Pyatakov G.L., 53
Qiao W., 130

- Röpke G., 100
Rabadanov M.Kh., 47
Rabadanova A.E., 90
Radchenko A.K., 62
Ragimkhanov G.B., 90
Rakhel A.D., 31, 86, 98
Rakhmanova P.A., 74
Ramazanov T.S., 37, 100, 101, 117
Raschektaeva E.P., 55
Reinholz H., 100
Richter K.W., 158
Rodionov A.V., 97
Roshchupkin V.V., 91
Rososhek A., 96
Rozhdestvensky A.V., 138
Rubtsov A., 170
Rudyak V.Ya., 106, 115
Rusanov B.A., 72, 94
Rusin S.P., 127
Rutin S.B., 140
Ryazantseva A.A., 91
Rykov S.V., 26, 28, 31, 38, 40, 102
Rykov V.A., 26, 28, 31, 38, 40, 102
Ryshkova O.S., 65
Sachkov I.N., 138
Saenko I., 161
Saenko I.S., 76
Safarov J., 59
Safarov M.M., 68
Safonov A.V., 116
Safronov A.A., 148
Sagdeev A.A., 38
Sagdeev D.I., 156
Saidov S.M., 42
Saitov I.M., 22
Samoshkin D.A., 16, 77
Sargsyan M.A., 142
Savchenko I.V., 16
Savinykh A.S., 53
Savvatimskiy A.I., 82, 89, 90
Scherbakov V.M., 142
Senchenko V.N., 47, 120
Senchikhin I.N., 114, 116
Serba E.O., 148
Seredkin N.N., 90
Shabatin A.V., 114
Shakhov A.V., 62
Shalenov E.O., 100
Shapiyeva A.Ye., 57
Shebzukhova I.G., 66
Sheindlin M.A., 19, 81, 82, 85, 87, 89
Shepelev V.V., 135
Sherieva E.K., 71
Shish A.I., 60
Shkolnikov E.I., 115
Shults O.V., 131, 137
Shulyatev D.A., 112
Shumikhin A.S., 22
Shutov A.V., 48
Shvets I.V., 112
Sidash I.A., 136
Sidnov K., 69
Sidorov V.E., 72, 94
Simak S.I., 165
Sinelshchikov V.A., 147
Sineva M.A., 68
Sinyova S., 170
Skorba V.R., 74
Skorodumov S.V., 25, 121
Skripnyak N.V., 172
Skripov P.V., 46, 50, 51, 140, 146, 150
Skryabin A.S., 113
Skurikhin A.V., 133
Smirnov A.S., 66
Smirnov V.N., 20
Smirnova D.E., 163
Smirnova E.A., 166, 172, 173
Smirnova I.A., 112
Sobirov J.F., 68
Sobol O.V., 63
Sobolev D.V., 99
Sokolov N.A., 118
Sokotushenko V.N., 149
Solovyov S.N., 74
Son E.Ye., 57
Sorogin I.G., 138
Sorogina T.I., 138
Spodobin V.A., 148
Stankus S.V., 16, 55, 77
Starikov S.V., 163, 168
Starostin A.A., 146
Starykh R., 170
Stepanov E.A., 169
Stepanov V.P., 73
Stolyarenko A.V., 104
Struleva E.V., 96, 127
Subbotin D.I., 148
Sukhikh A.A., 25, 60, 121
Suleymanov M.G., 124
Sulimov A. V., 77

Sulimov A.V., 74
 Sun W., 166
 Surov A.V., 148
 Svec P., 72
 Sverdlov A.V., 26
 Sviridenko V. I., 128
 Syzdykova A.B., 69, 172
 Taova T.M., 66
 Tatarinov A.S., 73
 Tedenac J.P., 158
 Terentev D.I., 136
 Ternovoi V.Ya., 32, 48
 Tewari S., 96
 Tiflova L.A., 74, 77
 Tkachev N.K., 36, 39, 42, 78
 Todorova M., 164
 Tomin A.S., 61, 153
 Tsvetkov O.B., 53, 55, 57
 Tsygankov P.A., 113
 Usmanov R. A., 75, 151
 Ustyuzhanin E.E., 31, 102
 Utkin P.S., 139
 Uvdal K., 171
 Uzdenova A.N., 64, 108
 Valiano G.E., 85
 Varlamova N.I., 147
 Vasil'eva A., 170
 Vasilyov V.A., 74
 Vasin A.A., 89
 Vasserman A.A., 41
 Vekilova O.Yu., 164
 Verba O.I., 55
 Verveiko M.V., 59
 Verveiko V.N., 59
 Vervikishko D.E., 115
 Vervikishko P.S., 81, 85
 Vesnin V.R., 113
 Vinogradov A.V., 61, 153
 Vinzarevich A.V., 57
 Vlaskin M.S., 125, 134
 Volosnikov D.V., 46
 Vorobuev D.A., 173
 Voronov V.P., 35
 Vorotilo S., 69
 Vyazovkin I.V., 77
 Walls B., 112
 Wolf T.A., 77
 Wu K., 159
 Yanilkin A.V., 132
 Yanovskiy L.S., 146
 Yanovsky L.S., 147
 Yanuka D., 96
 Yarullin L.Y., 35
 Yatsuk O.S., 16
 Yoo S., 164
 Yudin D.I., 152
 Yudin I.K., 152
 Zainullina E.R., 53
 Zaitsev N.G., 123
 Zakatilova E.I., 110
 Zakharov S.A., 132
 Zakiryanov D.O., 78
 Zaripov Z. I., 75, 151
 Zaripov Z.I., 35, 45, 153, 155
 Zaycev N.G., 88
 Zeodinov M.G., 124
 Zhang Q., 51
 Zhang Z.C., 51
 Zhangjun H., 171
 Zhanimova D.A., 71
 Zhavoronok E.S., 114
 Zhavoronok E.S., 76, 116
 Zhernokletov M.V., 97
 Zhu L., 169
 Zhuk A.Z., 125, 134
 Zhukov S.A., 146
 Zhumadylov R.E., 117
 Zhunisbekov A.T., 117
 Zitserman V.Yu., 63, 103
 Znamensky B.E., 31, 102