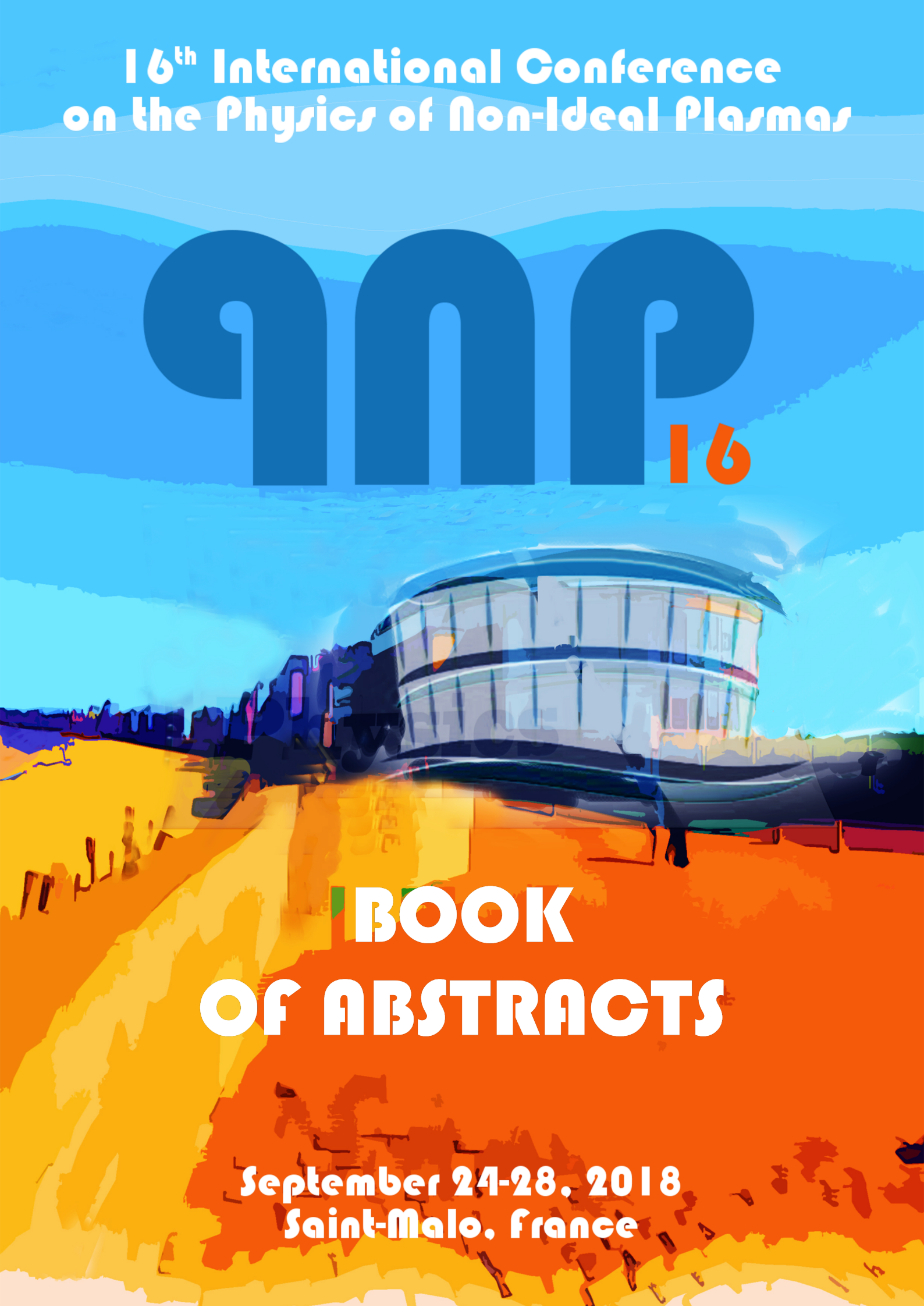
Book of Abstracts,16th International Conference on the Physics of Non-Ideal Plasmas (PNP16)

Jean Clerouin, Claude Deutsch, Michel Koenig, Gilles Maynard, Maxime Mikikian, Vanina Recoules, Nimet Deutsch

16th International Conference on the Physics of Non-Ideal Plasmas



BOOK OF ABSTRACTS

September 24-28, 2018
Saint-Malo, France

16th International Conference on the Physics of Non-Ideal Plasmas

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BOOK OF ABSTRACTS

Edited by: J. Clérouin, C. Deutsch, M. Koenig, G. Maynard, M. Mikikian, V. Recoules, N. Deutsch

PNP

16 th International Conference on the Physics of Non-Ideal Plasmas

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FOREWORD

It is a great pleasure to open this new edition of the Physics of Non-Ideal Plasmas (PNP) conference here in Saint-Malo, France, at Palais du Grand Large.
PNP conference series are held every 3 years in alternation with the Strongly Coupled Coulomb Systems conference. Last venues were in Binz (1995), Rostock (1998), Greifswald (2000), Valencia (2003), Darmstadt (2006), Chernogolovka (2009), Rostock (2012) and Almaty (2015). We have been solicited by the International Board to organize the 2018 session.

Topics are covering

- Dense and strongly coupled plasmas for inertial fusion and astrophysics,
- Equilibrium, transport properties and equations of state
- Hydrogen and mixtures of astrophysical interest
- Dusty plasmas
- Experimental vindication of strong coupling
- Production and diagnostics of non-ideal plasmas (XFELs, heavy ions beams, X ray Thomson scattering …)

We thank all the scientists from 14 countries attending this edition. We received 123 abstracts, all of very good quality, making the choice difficult, since we have only plenary sessions to preserve the format of our conference. With the help of the Program Committee we built a program with 10 invited talks and 42 contributed orals covering all the fields. Posters sessions will be an important moment combined with an oyster's degustation, known here, in Saint-Malo since 1999, as the POYSTERs session.
I hope you will enjoy Saint-Malo, just walking in the old city or joining the excursion to the Mont Saint-Michel.

We would like to thank the sponsors who allowed to organize the conference in Saint-Malo: CEA, CNRS and Labex PALM, LULI, University of Paris-Saclay and the Naval Research Laboratory.

Special thanks to the Palais du Grand-large and his organization staff, in particular Sophie Fontaine and Aurélie Paris.

We are also grateful to Nicolas Dessaint who facilitated the interactions with CNRS.

Ronald Redmer and the whole Program Committee are also warmly acknowledged for helping us in the organization of the scientific program.

We wish you an intense conference and a pleasant stay in Saint-Malo.

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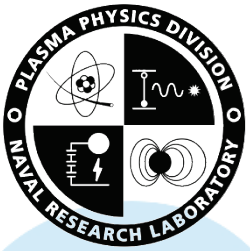
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TOPICS

1. **Statistical physics and ab-initio simulations**
2. **Production of non-ideal plasmas (using optical lasers, free electron lasers, heavy-ion beams, Z machine, high explosives etc.)**
3. **Diagnostics of non-ideal plasmas (using x-ray scattering, line shapes, stopping power, emission and absorption, etc.)**
4. **Equilibrium properties, equations of state and phase transitions**
5. **Kinetics, transport and optical properties**
6. **Dense astrophysical and ICF plasmas**
7. **Ultra-intense laser-matter interaction**
8. **Dusty plasmas**

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Recent results in dense astrophysical plasmas

Gilles Chabrier[1,2]

[1]CRAL, ENS-Lyon, Lyon, FRANCE
[2]University of Exeter, Exeter, UK

In this talk, I will review recent results concerning the properties of dense astrophysical plasmas, some of them being also of interest for the domain of Inertial Confinement Fusion. I will first present a new equation of state for hydrogen/helium mixtures aimed at describing the structure and evolution of a wide range of astrophysical bodies, from solar-type stars to low-mass stars, brown dwarfs and (solar and extrasolar) gaseous planets. An application to the derivation of a new internal structure model for Jupiter, constrained by the recent observations of the Juno mission, will be highlighted, as well as comparisons with recent high-pressure Hugoniot experiments for H and He. Then, I will briefly present recent equations of state for heavy elements of interest for stellar and planetary physics, notably water, iron and silicates. Finally, I will present new results concerning the quantum crystallization of the One Component Plasma at finite temperature, a problem of interest not only from the fundamental physics point of view but also for compact astrophysical objects such as massive white dwarfs and neutron stars

Miscibility gap of hydrogen-helium mixtures

Manuel Schöttler*[1], Ronald Redmer[1]

[1]*Universität Rostock, Germany*

We calculate the high-pressure demixing phase diagram of hydrogen-helium mixtures [1], which is important for applications in planetary physics, in particular, for calculating the interior and evolution of gas giants. The separation of hydrogen and helium has long been proposed as a possible source of Saturn's excess luminosity: The initially hot planet cools down with increasing age and when the planetary isentrope intersects with the demixing region [2], helium-rich droplets can form and sink toward the planetary core, thus, acting as an additional source of heat; see, e.g., [3].

The region of demixing is observed from thermodynamic relations by computing the free enthalpy G(x,P,T) at constant pressure P and temperature T for different helium fractions x. We use finite-temperature density functional theory molecular dynamic simulations to obtain the equation of state for given volumes and temperatures. The non-ideal entropy of mixing is calculated using a combination of coupling-constant integration and thermodynamic integration of the equation of state.

The choice of an appropriate exchange-correlation (XC) functional is of paramount importance. It has been shown that standard approximations such as PBE lack the ability to adequately describe the metallization transition in hydrogen [4], which is directly connected to the H-He demixing. Functionals that take into account non-local correlations such as vdW-DF [5] are in better agreement with recent experiments [4]. Benchmarking studies with many XC functionals against QMC calculations suggest vdW-DF as an appropriate functional also for hydrogen-helium mixtures [6].

Here, we present a demixing phase diagram of H-He mixtures calculated with vdW-DF and compare with previous calculations derived with the PBE functional [7,8]. Differences and implications for planetary physics are discussed, in particular, for the gas giants Jupiter and Saturn.

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*E-Mail address: manuel.schoettler@uni-rostock.de

Properties of Magnesium Oxide in Super-Earths

F. Soubiran[1,2], B. Militzer[2,3]
[1] *LGLTPE - ENS de Lyon, Lyon, FRANCE*
[2] *Earth and planetary science department, University of California, Berkeley, USA*
[3] *Astronomy department, University of California, Berkeley, USA*

The Kepler spacecraft led to the discovery of numerous Super-Earth-type planets. Little is known about them, as there is no equivalent in the Solar System. For instance, it is uncertain whether they have a convective mantle like the Earth. It is also unclear if their mantle is insulating or conducting. In the latter case the mantle could generate a magnetic field via dynamo processes. In order to better understand the properties of silicate materials under pressure-temperature conditions relevant for Super-Earth interiors, we studied MgO, one silicate end-member, with *ab initio* simulations based on density functional theory. We explored its phase diagram and complete equation of state. We also determined its electronic transport properties, conductivity and reflectivity, to characterize its behavior in the different phases. We find that liquid and solid MgO behave differently and discuss the consequences for the planetary interiors.

Using equations of state to construct Jupiter models

F. Debras[1,2], G. Chabrier[1,2]

[1]*ENS de Lyon, Lyon, France*
[2]*University of Exeter, Exeter, United Kingdom*

In 2016 the NASA satellite Juno entered in orbit around Jupiter, leading to observations of the gravity field of the planet with extreme precision. The previous models of Jupiter have all been invalidated by these new data, and our understanding of the planet has been challenged.

A new global picture of the planet has been drawn, including a diluted core and composition gradients, but we still don't understand the internal structure of Jupiter precisely. The total mass of metals for example is poorly constrained.

In this talk, I will show how important are precise equations of state of hydrogen, helium [1] and heavier elements (such as water) to construct Jupiter models. I will show the degeneracy of interior structures from the sole observations of gravitational data, and discuss the impact of equations of state on the physical parameters. A particular emphasis will be made on how to construct models of the planet [2], and notably the possible presence of layered convection, creating entropy and composition gradients in the planet.

Following this discussion, I will present our new models of Jupiter [3] and their physical implication on the metallization pressure of hydrogen and the hydrogen-helium phase separation.

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Band gap closure under pressure in phase III and phase IV of molecular hydrogen by Quantum Monte Carlo.

Vitaly Gorelov[1], Markus Holzmann[2,3], D.M. Ceperley[4], D. Domin[1], Carlo Pierleoni[1,5]

[1] *Maison de la Simulation, CEA, CNRS, Univ. Paris-Sud, UVSQ, Université Paris-Saclay, 91191 Gif-sur-Yvette, France*
[2] *LPMMC, UMR 5493 of CNRS, Université Grenoble Alpes, France*
[3] *Institut Laue-Langevin, BP 156, F-38042 Grenoble Cedex 9, France*
[4] *Department of Physics, University of Illinois Urbana-Champaign, Illinois, USA*
[5] *Department of Physical and Chemical Sciences, University of L'Aquila, Italy*

We investigate the closure of the fundamental band-gap under pressure in the phases III and IV of crystalline molecular hydrogen beyond 250GPa. We apply Grand-Canonical Reptation Quantum Monte Carlo (GC-RMC) with twisted-boundary conditions to analyze energies of systems of N_p protons and a number of electrons in the range $[N_p\text{-}n;N_p+n]$ with n=2,4,6. Finite temperature effects are considered by averaging over nuclear configurations obtained by Coupled Electron-Ion simulations at finite temperature [1]. Nuclear quantum effects are considered by representing nuclei by Path Integral.

We investigate two candidate structures of Phase III, namely C2/c and Cmca12, and the structure Pc48 candidate for phase IV [1]. For ideal crystalline structures (classical nuclei in the perfect crystal configuration) the band gap closes above 400GPa, slightly earlier for the Cmca12 than for the C2/c structure. Nuclear quantum and thermal effects are found to reduce considerably the amplitude of the gap, shifting the closing pressure between 350GPa and 400GPa. By a directional analysis of our data we find a strong directional character of the gap amplitude which suggests the presence of an indirect gap and the semimetallic character of the system at the closing pressure and at pressure just above. This scenario is in agreement with predictions based on Density Functional Theory [1] and with recent experiments [2].

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Metastable states of warm dense hydrogen

Norman G.E[1,2,3], Saitov I.M[2,1,3], Sartan R.A[2,3]

[1] *National Research University Higher School of Economics, RUSSIA*
[2] *Joint Institute for High Temperatures of the Russian Academy of Sciences, RUSSIA*
[3] *Moscow Institute of Physics and Technology, RUSSIA*

The first-order fluid–fluid phase transition is observed in warm dense hydrogen in shockwave [1] and diamond anvil cell [2] experiments. However, Z-machine experimental observations [3] confirm only an abrupt insulator-to-metal transition. In [4], the interpretation of the experimental data points to the continuous transition to the conducting state of hydrogen, ruling out even the possible existence of the first-order phase transition in the range studied. The jump of density is reproduced by *ab initio* calculations [3,5,6].
The existence of accompanying metastable states of warm dense hydrogen could be used as a criterion, that the transition is of the first order.
This research focuses on obtaining the metastable states of warm dense hydrogen by means of density functional theory and quantum molecular dynamics. The supercell contains 512 atoms. The exchange correlation functional chosen is PBE. The structure of hydrogen is analyzed by pair-correlation functions (PCFs). To obtain the molecular metastable state, the initial configuration should correspond to the molecular state beforehand. We take coordinates and velocities of ions from the equilibrium states or from the obtained metastable ones. Changing the size of the supercell, it is possible to calculate another density and save the state. We reproduce the metastable branch of the isotherm by consequently changing the supercell volume and relaxing configurations at every new density without the thermostat, since under the influence of it the hydrogen less likely remains metastable.
Two isotherms of 700 and 1000 K are investigated. The pressure and the density of the transition are the same as ones obtained in [5], since the calculation parameters are similar. Although the region of the phase transition strongly depends on temperature, the equilibrium and metastable branches of two molecular phase isotherms are located approximately along one and the same curve. The ionized phase branches fit another curve. The metastable region obtained is 470 and 320 kbar by pressure for 700 and 1000 K respectively; the difference between pressure of the metastable and equilibrium states at the same density is approximately 150 kbar for both isotherms. The PCFs have high first peaks along the metastable branch, that confirms hydrogen saving molecular phase. The main results are as follows: (a) the procedure of modeling of the metastable states is developed, (b) the existence of metastable states points out that the phase transition is a first order transition.
The work is supported by the grant 18-19-00734 of the Russian Science Foundation.

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The Deuterium Hugoniot: Pitfalls of Beyond-DFT Thermodynamic Sampling

Raymond C. Clay, III[1], Luke Shulenburger[1], Michael P. Desjarlais[1]

[1]*HEDP Theory Department, Sandia National Laboratories, USA*

Density functional theory is the workhorse of ab initio equation of state calculations at extreme conditions due to its reasonable computational cost and significantly improved accuracy over chemical models. However, the often unquantified errors arising from the choice of exchange-correlation functional make thermodynamic sampling based on many-body methods appealing. One proposed beyond-DFT method is “coupled electron-ion Monte Carlo” (CEIMC), which explicitly treats many-body electronic exchange and correlation effects with ground state projector Monte Carlo. Troublingly, the principal Hugoniot of deuterium calculated with CEIMC deviates significantly from both density functional theory calculations and experiments [1]. In particular, CEIMC predicts too soft of a Hugoniot, which both fails to match well established gas gun data and predicts a peak compression roughly 7% larger than experiment [2]. In this talk, we demonstrate that in the absence of all other sources of error, the commonly employed fixed-node approximation in projector QMC can introduce energy and pressure errors large enough to account for the discrepancy between the CEIMC Hugoniot and experiment. We demonstrate this by deriving a first-order equation for the dependence of the density of a predicted Hugoniot point on energy, pressure, and volume errors. Using configuration interaction type wave functions with projector QMC in small simulation cells, we estimate the size of the fixed-node error for the class of wave functions used in CEIMC at pressure and temperature conditions relevant for the principal Hugoniot. These estimated errors in conjunction with our formula for the first-order density change allow us to account for the vast majority of the discrepancy between CEIMC and experiments [1]. In contrast, we find that several functionals that achieve excellent agreement with experiment do so through error cancellation, which we contend accounts for their observed poor performance in predicting the reshock measurements [2]. While this talk focuses primarily on CEIMC, most of the issues discussed are general to all wave function based methods for treating the electronic structure.

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Equation of state of warm dense matter: Reproducing quantum molecular dynamics results at high temperature

J.-F. Danel[1], L. Kazandjian[1], and R. Piron[1]

[1]CEA, DAM, DIF, F-91297 Arpajon, FRANCE

In the thermodynamic domain of warm dense matter (WDM), there is no clear definition of the chemical species present and various effects like bonding, exchange-correlation or electron degeneracy must generally be taken into account. Quantum molecular dynamics (QMD), a first-principles approach in which the system is regarded as a mixture of electrons and nuclei and in which the quantum nature of electrons is taken into account [1], is appropriate for addressing the equation of state (EOS) of WDM. However, QMD is limited at high temperature by computational cost. In the present work, our aim is to construct an approach allowing to reproduce the QMD EOS at high temperature.

If an orbital-free approximation of the kinetic electronic free energy is used, QMD is made into orbital-free molecular dynamics, an approach which can be implemented at high temperature [2,3]. In the present work, we consider orbital-free-Weizsacker molecular dynamics (OFWMD) [4] and we define the ionic excess pressure for QMD and OFWMD as the difference between the excess pressure and an average atom pressure. We present the case of deuterium in the domain above 1 eV and 0.2 g/cc, and we show that we have been able to perform QMD calculations at sufficiently high temperature to demonstrate that the OFWMD ionic excess pressure is the limit of the QMD ionic excess pressure as temperature increases at given mass density. As a result, the QMD ionic excess pressure can be reproduced at high temperature. And, since the quantum average atom model can be implemented at high temperature, the QMD pressure can be reproduced at high temperature. The same is true for internal energy. The EOS which allows to reproduce the QMD results at high temperature is denoted OFWHMD.

With the approach described above, we have constructed an EOS table for deuterium in the domain above 1 eV and 0.2 g/cc [5]. Although the QMD and OFWHMD results are obtained independently, the convergence of QMD to OFWHMD is observed within statistical error or within a few tenths of a percent of total pressure [5]. The sensitivity of the EOS constructed to the exchange-correlation functional is shown.

In conclusion, we note that, while the QMD EOS cannot be reproduced at high temperature by the OFWMD EOS because of a non-monotonic convergence due to shell effects, it is reproduced by the OFWHMD EOS we have constructed [5]. We also evoke the applicability of our approach to atoms of higher atomic numbers and we consider what future work could consist in.

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Probing C-H mixtures at conditions relevant to the interiors of giant planets and Brown Dwarfs

Dominik Kraus[1,2]

[1]*Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany*
[2]*Technische Universität Dresden, Germany*

Carbon-hydrogen (C-H) mixtures at extreme pressure and temperature conditions are highly relevant for the interiors of icy giant planets like Neptune and Uranus where pressures of several Mbar are present in their deep interiors. Moreover, various warm dense matter and dense plasma states up to the Gbar regime can be found inside Brown Dwars. Experiments at state-of-the-art facilities allow for insights of unprecedented quality into such extreme states of matter. At the Linac Coherent Light Source (LCLS), we have investigated C-H mixtures at conditions comparable to planetary interiors [1], showing structural transitions and chemical activity applying various X-ray diagnostic techniques in one experiment. In other experiments, performed at the National Ignition Facility and using spectrally resolved X-ray scattering in combination with radiography, we have investigated the ionization balance of warm and hot dense C-H at conditions that are comparable to the interiors of Brown Dwarfs or small stars. These results indicate that, particularly for mixtures, standard ionization models may require revisions in the regime of warm and hot dense matter [2].

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Material properties for the interiors of massive giant planets and brown dwarfs.

Andreas Becker[1], Mandy Bethkenhagen[1,2], Clemens Kellermann[1], Johannes Wicht[3], Ronald Redmer[1]

[1]University of Rostock, Institute of Physics, D-18051 Rostock, GERMANY
[2]Lawrence Livermore National Laborytory, Livermore, CA 94550, USA
[3]Max-Planck-Institute for Solar System Research, D-37077 Göttingen, GERMANY

We present thermodynamic and transport properties for the extreme conditions prevalent in the interiors of massive giant planets and brown dwarfs [1]. They are obtained from extensive molecular dynamics simulations based on density functional theory for hydrogen-helium mixtures along the isentropes of three representative objects: KOI-889b (M~10 M_J), Corot-3b (M~22 M_J), and Gliese-229b (M~46 M_J). In particular, we determine the heat capacities, the thermal expansion coefficient, the isothermal compressibility, and the sound velocity. Important transport properties such as the electrical and thermal conductivity, electronic opacity, and shear viscosity are calculated as well. Further results for associated quantities including magnetic and thermal diffusivity, kinematic shear viscosity, the static Love number k_2, and the equidistance are discussed.
Overall, the behavior inside massive giant planets and brown dwarfs is stronger dominated by degenerate matter than in Jupiter mass planets, see [2]. Based on our *ab initio* data we discuss the possible dynamics and magnetic field structure in massive giant planets and brown dwarfs. The consistent data set presented here may serve as starting point to obtain material and transport properties for other substellar H-He objects with masses above one Jovian mass M_J.

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This work was supported by the DFG via the SFB 652. The DFT-MD simulations were performed at the North-German Supercomputing Alliance (HLRN) and at the IT and Media Center of the University of Rostock. Mandy Bethkenhagen acknowledges support by the U.S. Department of Energy at the Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344.

Thermal conductivity of water plasmas from *ab initio* simulations

Martin French[1]

[1]*Universität Rostock, GERMANY*

The determination of thermal conductivities of dense plasmas is a great challenge for both experimental and theoretical approaches. In partially ionized plasmas, not only electrons contribute to the thermal conductivity but also ions. Here we use *ab initio* molecular dynamics (MD) simulations based on density functional theory (DFT) to calculate the ionic contribution to the thermal conductivity of dense partially ionized water plasmas. The required heat current of the ions is determined by matching the forces from each of the DFT-MD simulations onto effective pair interaction force fields. These force fields are then used to evaluate the Green-Kubo relation for the thermal conductivity using the ion trajectories of the same DFT-MD simulation run. This approach is generally applicable to various multi-component plasmas as well as to materials in liquid, solid, or superionic phases.
For water plasmas the ionic contribution to the thermal conductivity is found to be equal to or greater than the electronic contribution [1] up to temperatures of 20 000 K, depending on the density. The presence of characteristic contributions from thermal dissociation reactions of the water molecules can be traced back to the shapes of the derived force fields between the ionic species. These contributions enhance the ionic thermal conductivity between 3000 and 10 000 K noticeably and are more pronounced toward low densities. Additional benchmark calculations for ice VII and liquid water show good agreement with experimental data and with an *ab initio* study in which the ionic heat current was determined with a generalized variant of density functional perturbation theory for the electronic ground state [2].
Our results are of general significance for understanding thermal transport properties in dense, partially ionized plasmas and other states of matter. The generated thermal conductivity data for water are particularly important for the development of non-adiabatic evolution models for the water-rich giant planets like Uranus and Neptune.
This work is supported by the DFG within the FOR 2440 "Matter under Planetary Interior Conditions - High Pressure, Planetary, and Plasma Physics."

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Plasma phase transition (*by the fiftieth anniversary of the prediction*).

Norman G.E. [1,2,3], Saitov I.M. [2,1,3]

[1]*National Research University Higher School of Economics, RUSSIA*
[2]*Joint Institute for High Temperatures of RAS, RUSSIA*
[3]*Moscow Institute of Physics and Technology (State University), RUSSIA*

The plasma phase transition was predicted in 1968 by analogy with the van der Waals equation [1]. Besides, for isotherms of pressure dependences on density, strong overlapping in the density of the equilibrium branch of one phase with a metastable branch of another phase are predicted [2], in contrast to the van der Waals equation. The third prediction [3] is a triple point on the melting curve [4]. Estimates [1-3] are obtained within the framework of the chemical model, where the ionization equilibrium equation is used with the corrections for the nonideality of the system of free charges. Over the next decades, this approach was developed: on the one hand, new components were included in the chemical model, in addition to electrons and ions, considering interactions between all components, on the other hand, the nature of accounting for these interactions was clarified. See brief reviews in [5,6].
The first experimental results, which could be interpreted as an experimental detection of the plasma phase transition, appeared only in the last decade (see references in [6]). The measurements are carried out with warm dense hydrogen in both shock waves and diamond anvil cells. At the same time, the theory began to use methods based on the theory of density functional. The properties of warm dense hydrogen are investigated by ab initio methods of molecular dynamics and quantum modeling using the density functional theory and quantum Monte Carlo theory. A first-order phase transition is observed. The coexistence curve is close to the measured one. There are different approaches for the description of the nature of the transition. The first assumption is related to the metallization of hydrogen under the influence of the work of Wigner and Huntington in 1935. The alternative one is the pressure dissociation of $H_2 \rightarrow 2H$. The plasma phase transition is also mentioned.
In [6], the idea is introduced that during the fluid-fluid phase transition in the warm dense hydrogen, the H_2 molecules are ionized to form the molecular ions H_2^+ and H_3^+. Thus, a plasma phase transition occurs with partial ionization of H_2 molecules and the formation of H_2^+ ions. H_3^+ ions are formed because of the reaction of H_2^+ ions with H_2 molecules. The nature of the transition combines ionization with structural changes. Strong ionization during the fluid-fluid phase transition in warm dense hydrogen makes this transition close to the prediction of the plasma phase transition [1]. Strong overlapping of metastable states corresponds to prediction [2]. The triple point is expected to be on the melting curve as in [3].
The work is supported by the grant 18-19-00734 of the Russian Science Foundation.

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Warm Dense Matter studies relevant for planetary science

A. Ravasio [1], M. Guarguaglini [1], J-A. Hernandez [1], T. Vinci [1], A. Benuzzi-Mounaix[1], R. Bolis [1], E. Brambrink [1], M. Koenig [1,]

[1]LULI, CNRS, Ecole Polytechnique, CEA, Route de Saclay, 91128 Palaiseau, FRANCE

The study of planetary interiors is a key concern to provide a unified framework about planets' formation, evolution and structure. Today this purpose acquires new significance because of the active discovery of extrasolar planets. Planets of our Solar System are thus studied for both their specific interest and their role as better-known prototypes for classification and modelling of exoplanets. A major issue for this kind of study is represented by the substantial impossibility to directly probe the planets interiors. While the internal structure of our Earth can be inferred by means of analysis of seismic waves, for the other solar planets probing is limited to the surface (Mars) or even to a fly-by in the upper atmosphere (giant planets). In the last case, the only data in our possession are measurements of mass, magnetic and gravitational field, luminosity, radii etc.Therefore, a model is needed to couple these observables in a self-consistent way with the interior structure and dynamics.
In this context, an accurate modelling requires a precise knowledge of structural and transport properties of some key elements (e.g. iron for our Earth), such as the equation-of-state, phase transitions, conductivity, etc. These properties at regimes typical of planetary interiors (few Mbar, few 1000 K) can today be measured in long pulse (ns) laser driven shock experiments. In this talk, we will present the experimental results that our group has obtained on key materials and will show the impact that they have on the planetary science.

Investigating the insulator to metal transition in dense fluid hydrogen with laser-driven dynamic compression

Peter M. Celliers,[1] Marius Millot,[1] Stephanie Brygoo,[2] R. Stewart McWilliams,[3] Dayne E. Fratanduono,[1] J. Ryan Rygg, [1,4] Alexander F. Goncharov,[5] Paul Loubeyre,[2] Jon H. Eggert,[1] J. Luc Peterson,[1] Nathan B. Meezan,[1] Sebastien Le Pape,[1] Gilbert W. Collins,[1,4] Raymond Jeanloz,[6] Russell J. Hemley[7]

[1] *Lawrence Livermore National Laboratory, Livermore, CA 94550, UNITED STATES*
[2] *CEA, DAM, DIF, F-91297 Arpajon, FRANCE*
[3] *School of Physics and Astronomy and Centre for Science at Extreme Conditions, University of Edinburgh, Peter Guthrie Tait Road, Edinburgh, EH9 3FD UNITED KINGDOM*
[4] *University of Rochester, Rochester, NY 14623, UNITED STATES*
[5] *Carnegie Institution of Washington, Washington, DC 20015, UNITED STATES*
[6] *University of California, Berkeley, CA 94720, UNITED STATES*
[7] *The George Washington University, Washington, DC 20052, UNITED STATES*

Despite extensive theoretical and experimental advances in the past decades, the properties of fluid hydrogen remain challenging to understand in the vicinity of the predicted first-order insulator-to-metal (IM) transition - also known as the plasma phase transition (PPT). In particular, there are apparent discrepancies between different experimental platforms and techniques regarding the character and the thermodynamic states at which the insulator-to-metal transition is observed to occur.

We will describe two new experiments employing laser-driven dynamic compression to create and diagnose high pressure, low entropy states of dense fluid hydrogen. We will report the results of experimental campaigns at the National Ignition Facility and at the Omega Laser Facility that span the IM transition with different dynamic compression schemes and discuss their implications for our understanding of the metallization of dense fluid hydrogen for planetary, astrophysical and high energy density science.

Part of this work was performed at LLNL under Contract DE-AC52-07NA27344.

Numerical simulation of experiments with non-ideal plasma at 247-MeV proton microscope

V.B.Mintsev[1], N.S.Shilkin[1], D.S.Yuriev[1], A.V.Kantsyrev[2], A.V.Skoblyakov[2], A.V.Bogdanov[2], A.A.Golubev[2]

[1]Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, RUSSIA
[2]State Scientific Center of the Russian Federation "Institute for Theoretical and Experimental Physics", National Research Center "Kurchatov Institute", Bolshaya Cheremushkinskaya 25, Moscow 117218, RUSSIA

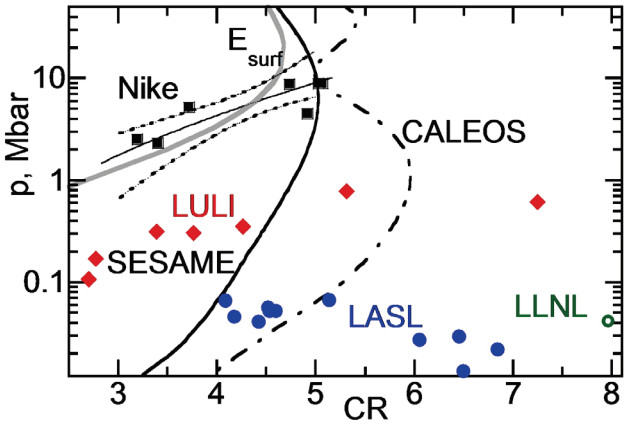
A radiographic facility for an investigation of fast dynamic processes with areal density of targets up to 5 g/cm2 is under development on the basis of high-current proton linear accelerator at the Institute for Nuclear Research (Troitsk, Russia). A virtual model of the proton microscope developed in a software toolkit Geant4 is presented. Fullscale Monte-Carlo numerical simulation of static radiographic experiments at energy of a proton beam 247 MeV was performed. The results of simulation of proton radiography experiments with the shock-compressed non-ideal xenon are presented. The results of visualization of copper and polymethyl methacrylate step wedges static targets also described.

Absolute Hugoniot measurements of CH foams in the 2-9 mbar range and future plans*

T.A. Mehlhorn[1], A. L. Velikovich[1], Y. Aglitskiy[1], K.R. Cochrane[2], J. Giuliani[1], A. Dasgupta[1], N. Ouart[1], M. Karasik[1], A. J. Schmitt[1], V. Serlin[1], J. L. Weaver[1], J. Oh[1], and S. P. Obenschain[1]

[1]*Plasma Physics Division, Naval Research Laboratory, Washington DC, USA*
[2]*Sandia National Laboratories, Albuquerque, NM, USA*

Foams can be used in ICF and HEDP as low-density, high-adiabat ablators; as wetted foam liquid fuel layers; as radiating sources to heat and backlight materials in z-pinch dynamic hohlraums for opacity measurements; and many other ways. There is, however, a long history of surprises with the Hugoniot curves of porous materials. This paper will report on absolute Hugoniot measurements for empty plastic foams at~10% of solid polystyrene density and supporting rad-hydro simulation results. Planar foam slabs, ~400 μm thick and ~500 μm wide, some of which were covered with a 10 μm solid plastic ablator, were directly driven with 4 ns long Nike krypton-fluoride 248 nm wavelength laser pulses that produced strong shock waves in the foam. The shock and mass velocities in our experiments were up to 104 km/s and 84 km/s, respectively, and the shock pressures up to ~9 Mbar. The motion of the shock and ablation fronts was recorded using side-on monochromatic x-ray imaging radiography. The steadiness of the observed shock and ablation fronts within ~1% has been verified. The shocked foam plasma is strongly coupled, with plasma parameter $\Gamma \approx 1$. The Hugoniot data inferred from our velocity measurements agree with the predictions of the SESAME and CALEOS equation-of-state models near the highest pressure ~9 Mbar and density compression ratio ~5. In the lower pressure range 2 to 5 Mbar, a lower shock density compression is observed than that predicted by the models, see the Figure. Possible causes for this discrepancy are discussed. We will also report on planned experiments on lower density foams, such as those relevant to dynamic hohlraum systems, as well as the design of spectroscopic measurements to determine temperature for further comparisons of thermodynamic properties with various EOS models.



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The High Energy Density (HED) instrument at the European XFEL – status and perspectives

Ulf Zastrau[*1], K. Appel[1], C. Baehtz[2], S. Göde[1], H. Höppner[2], Z. Konôpková[1], H.-P. Liermann[3], M. Makita[1], M. Nakatsutsumi[1], A. Pelka[2], T. Preston[1], C. Strohm[3], T. Toncian

[1] *European XFEL, Schenefeld, Germany*

[2] *Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany*

[3] *DESY, Hamburg, Germany*

The advent of the first free-electron X-ray lasers (XFELs), FLASH in 2004 and LCLS in 2009, may prove to be the most profound development since the invention of the laser and, equally, the synchrotron. Sharp improvements in a number of laser parameters, most notably intensity and pulse duration, support this expectation. This brings scientific dreams within reach. Indeed, the unprecedented opportunities and expectations have triggered considerable research activities worldwide.

In 2019, the High Energy Density Science (HED) instrument at the European X-ray Free-Electron Laser Facility in Schenefeld, Germany, will allow investigations of a wide range of materials and systems at extreme conditions. For sample excitation a variety of high energy drivers will be installed [1]. In particular, a 100 J ns and a 200 TW fs optical laser will be available for warm- to hot-dense-matter creation, dynamic compression and laser-plasma interaction in electron-relativistic regime. These drivers will allow studying various phase space parameters with time-resolution down to 10 fs, pressures into the TPa regime, and electric field strength up to 10^{20} W/cm. This unique instrument is designed to enable the application of various x-ray probes including spectroscopic, diffraction and imaging methods [2]. It will operate in the photon energy range from 5 to 25 keV and will feature a variety of platforms facilitating the usage of different techniques in user-driven experiments. The capabilities of the HED instrument, which is built in strong symbiosis with the HIBEF user consortium [3], will be presented along with selected science cases.

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[*] email: ulf.zastrau@xfel.eu

The effect of magnetic field on plasma particles in dusty plasma

Karasev V.Yu., Dzlieva E.S., Pavlov S.I., Novikov L.A., Ermolenko M.A.

Saint Petersburg State University, 199034, Universitetskaya nab., 7/9, St. Petersburg, e-mail: plasmadust@yandex.ru, RUSSIA

There is considerable interest in the study of complex plasmas in a magnetic field [1-2], including a fairly strong one [3-5]. Iit is important to understand how the presence of a dust component can affect the properties of a plasma in magnetic field. By analogy with the effect on the operation of electrical probes, the presence of dust particles complicates the magnetization of the plasma components and, affects the charging and dynamics of the particles.

The change in the characteristics of motion and diffusion of charged particles in a magnetic field occurs when critical values are reached by several parameters. When $\omega_e\tau_e$ = 1, the electron circulates around the cyclotron circle of radius $r_{ce} = \frac{m_e v_e}{eB}$ and is considered magnetized. Under typical conditions in experiments with a complex plasma, $\omega_e\tau_e$ = 1 already in a field of the order of 10^{-2} T. In the presence of a dust particle with radius *a*, the determination of the magnetization becomes more complicated. To effectively hit electrons on the surface of dust particle, the condition $r_{ce}=a$ is required. The magnetic field corresponding to this condition does not depend on the pressure. For particles with a size of about 10 μm, it is performed in fields of the order of 1 T. The criterion for the magnetization of ions depends on their type. For neon, the condition $\omega_i\tau_i$ = 1 is satisfied in fields of the order of $2\cdot10^{-1}$ T. The total magnetization of an ion in a complex plasma is realized when the condition $r_{ci}=a$ is satisfied. In helium, the field of about B = 2.4 T is required for the magnetization of the ion

In this paper, the results of the studies of dust formations are presented with the magnetization of the plasma component in the lightest inert gases. The experiment with neon is carried out on a superconducting magnet at pressures typical for dusty plasma in the dust trap in stratum. The experiment with helium is carried out in standard magnetic coils under reduced pressure in the trap near the narrowing of the current channel. In preliminary observations, the conditions of magnetization are achieved.

Investigation of the magnetization in helium was supported by RFBR grant № 18-02-00113, the study of the magnetization in neon is carried out within the framework of the project RSF grant № 18-12-00009.

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Molecular Dynamics approach to plasma nanoparticle growth and reactivity.

Pascal Brault[1], W. Chamorro-Coral[1], A. Caillard[1], C. Coutanceau[2], S. Baranton[2]

[1]GREMI, UMR 7344, CNRS-Université d'Orléans, BP6744, 45067 Orléans cedex 2, France
[2]IC2MP UMR7285 CNRS Université de Poitiers, TSA 51106, 86073 Poitiers cedex 9, France

Controlling catalyst nanoparticle growth is of paramount importance for improving catalyst size distribution, structure and morphology to achieve high activity and selectivity. Experimentally, Magnetron Sputtering - Gas Aggregation Source is a new tool for designing nano(alloy)catalysts [1] based upon plasma sputtering at high pressure in an inert plasma (Ar) or reactive plasma (Ar with O_2, N_2) which is carrying the grown cluster to a substrate through a nozzle.

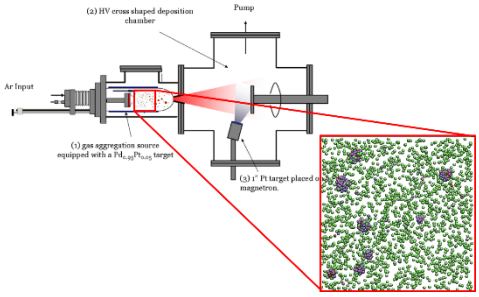

Fig. 1 : Schematics of a plasma condensation source. Inset gives the nanoalloy growth process in the condensation chamber. (after Ref. 1)

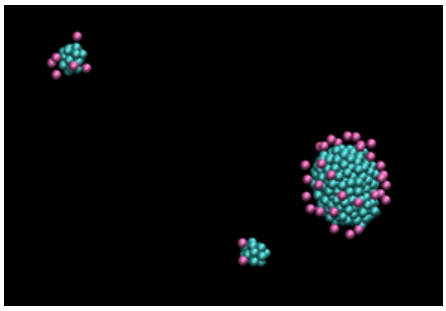

***FIG. 2:** Example of Pt_9Bi_1 nanoparticle growth in plasma condensation source. Background Ar gas atoms are removed for clarity.*

Initial conditions of MD simulations are selected for matching experimental chemical and physical Magnetron Sputtering - Gas Aggregation Source parameters. This takes into account the sputtering properties for determining the initial ratios between sputtered and background gas (reactive or not) atoms. Results concerning the growth of $Pt_xNi_yAu_z$, Pt_xBi_y (Fig. 2) and Pd_xO_y nanoparticles under such conditions will be presented. Radial distribution functions and X-Ray Diffraction patterns are systematically computed for enabling direct comparison with experiments.

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Measuring Plasma Parameters of Warm Dense Matter from X-Ray Thomson Scattering at the LCLS and the NIF

B.B.L. Witte[1,2], M. Bethkenhagen[1,3], V. Recoules[4], P. Sperling[2,5], M. French[1], T. Döppner[3], S.H. Glenzer[2], R. Redmer[1]

[1]*Institut für Physik, Universität Rostock, Germany*
[2]*SLAC National Accelerator Laboratory, USA*
[3]*Lawrence Livermore National Laboratory, USA*
[4]*CEA, DAM, DIF, France*
[5]*European XFEL, Germany*

A The thermal and electrical conductivity, equation of state and the spectral opacity in warm dense matter (WDM) are essential properties for modeling, e.g., fusion experiments or the evolution, interior and magnetic field generation of planets. In the last decade, it has been shown that x-ray Thomson scattering (XRTS) is an effective tool to determine plasma parameters like temperature and density in the WDM regime [1]. Recently, the electrical conductivity was extracted from XRTS experiments for the first time [2]. The spectrally resolved scattering data of aluminum, isochorically heated by the Linac Coherent Light Source (LCLS), show strong dependence on electron correlations. Therefore, the damping of plasmons, the collective electron oscillations, has to be treated beyond perturbation theory. Furthermore, an ongoing experimental campain at the National Ignition Facility (NIF) measures XRTS spectra of imploding beryllium capusules for the first time in forward direction under extreme conditions, i.e. beyond 20 times compression.

Here, we present results for the dynamic transport properties in warm dense aluminum and beryllium using density-functional-theory molecular dynamics (DFT-MD) simulations.
The choice of the exchange-correlation (XC) functional, describing the interactions in the electronic subsystem, has significant impact on the ionization energy of bound electrons and the dynamic dielectric function.
Our newly developed method for the calculation of XRTS signals including plasmon and bound-free transitions is based on transition matrix elements together with ionic contributions using uniquely DFT-MD simulations. The results show excellent agreement with the LCLS data if hybrid functionals are applied [3]. The experimental finding of nonlinear plasmon damping is caused by the non-Drude conductivity in warm dense aluminum. Here, we show further validation by comparing with x-ray absorption data [4]. These findings enable new insights into the impact of XC functionals on calculated properties of WDM and allow detailed predictions for ongoing experiments at the extreme densities reached at the NIF.

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Modelling Time-Resolved X-ray Absorption Measurements

R.A. Baggott[1], B. Kettle[1], S.J. Rose[1,2] and S.P.D Mangles[1]

[1] *The Blackett Laboratory, Imperial College London, UK*
[2] *Department of Physics, University of Oxford, UK*

Methods to create warm and hot dense matter in the laboratory typically generate non-equilibrium conditions, with energy being deposited initially in either the electron or ion populations [1]. An understanding of energy transfer mechanisms is therefore required in order to interpret and design such experiments. Furthermore, measurements of equilibration rates can inform our understanding of the physics governing wider transport processes in dense plasmas. However, our understanding of this area remains incomplete. Experiments have yielded widely differing results, suggesting a dependence on both material and the initial heating mechanism [2]. Theoretically, a number of approaches within both plasma and solid-state frameworks have been applied [3,4].

The bright betatron x-rays produced by laser wakefield accelerators can have durations of order 10fs and are therefore ideally suited to probe non-equilibrium processes in dense plasmas [5]. The broadband spectrum produced is smooth over a wide range of energies up to tens of keV and therefore lends itself well to x-ray absorption measurements. Measurements of structure near to absorption edges (XANES) can yield information about the electron and ion temperatures [6], allowing betatron radiation to probe temperature equilibration on sub-picosecond timescales.

Here, we present modelling and preliminary experimental results demonstrating the feasibility of measuring temperature equilibration using a betatron x-ray probe. Using *ab initio* simulations alongside theoretical predictions, we examine to what extent a proposed experimental setup should be able to distinguish between existing models for electron-ion coupling (e.g. Spitzer, coupled-mode [3], two-temperature *ab initio* [4]). Furthermore, we discuss developments in modelling electron-ion energy transfer at the boundaries between plasma and solid-state.

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Thomson scattering from dense non-equilibrium plasmas.

Thomas Bornath[1], Tim-Niklas Beuermann[1], Ronald Redmer[1]

[1]*Institute of Physics, University of Rostock, Rostock, GERMANY*

X-ray Thomson scattering (XRTS) experiments in the soft and hard X-ray regime yield information on fundamental parameters of high-density systems [1]. Pump-probe experiments with variable time delay provide insight into the excitation and relaxation dynamics in dense plasmas on short time scales. Often, a theoretical description of states is applicable in which the electrons and ions are thermalized to different temperatures. At even shorter time scales, states arise in which the electron distribution function (EDF) cannot be described by local equilibrium functions and a more detailed kinetic description is necessary.

Besides non-equilibrium effects on the EDF, there is an influence of spatial inhomogeneities on the scattering signal. The simplest approximation is to sum the contributions of the different volume elements assuming local equilibrium conditions [2]. Belyi [3] showed that the inclusion of gradients might have a great influence on the field and density fluctuations in a non-equilibrium plasma. Kozlowski et al. [4] discussed implications for Thomson scattering spectra for inhomogeneous plasmas in the warm dense matter regime based on a gradient expansion within real-time Green's functions theory. They used, however, some simplified approximations, see also [5].

Giving a derivation with some more rigor, we discuss density and field fluctuations in non-equilibrium systems as well as the relation to the fluctuation-dissipation theorem in equilibrium [6]. Especially in the collective scattering regime, Thomson scattering spectra are modifed substantially by spatial inhomogeneities. Within a first-order gradient expansion, the dispersion relation for plasmons is determined. Further the ratio of the heights of the plasmon peaks is changed, preventing, e.g., a simple estimation of the plasma temperature from a detailed balance relation.

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Signals of Ionization Potential Depression in X-Ray Thomson Scattering Spectra

D.O. Gericke[1], T. Doeppner[2], R.A. Baggott[3] and D.A. Chapman[4]

[1] *CFSA, Department of Physics, University of Warwick, UK*
[2] *Lawrence Livermore National Laboratory, USA*
[3] *Plasma Physics, Imperial College London, UK*
[4] *First Light Fusion, Oxford, UK*

X-Ray Thomson Scattering has evolved into an important diagnostic method for dense matter revealing a number of important properties from the atomic scale structure of strongly interacting ions to modified plasmon shifts in electron-ion systems [1]. It is well known that the scattering signals also highlights changes in the ionization energies. The most basic effect is the changing ionization degree that is reflected in the changing ratio of the elastic to inelastic scattering feature as these parts of the spectrum are roughly proportional to the number of bound and free electrons, respectively. Moreover, the contribution from bound-free scattering shows a cut-off at the effective ionization energy and its shape is thus directly related to the IPD. Both effects have been already exploited in the analysis of experiments [2,3].

There are however also changes to the elastic scattering feature due to IPD that will become increasingly prominent as more extreme conditions are probed, e.g., at the OMEGA or NIF facilities. First we demonstrate that the screening cloud describing the free-electron contribution to the elastic scattering can be directly related to the electronic contribution of the IPD. The ionic part to the IPD is also included as it can be expressed by the ion-ion structure factor. Thus, a complete measure of the elastic Rayleigh weight for all wavenumbers gives a direct measure of the IPD. We demonstrate this effect with different models for the screening cloud [4]. Secondly, the bound states are also modified by the interactions with the environment. The changing binding energies are the IPD while the changes in the wave functions modify the elastic scattering in XRTS. Thus, we have found another direct link between the IPD an ion experiences and its scattering strength that can be measured by XRTS. Of course, the latter effect is small for most conditions investigated so far. However, we demonstrate with a simple hydrogen-like model that it becomes significant for the extreme conditions that can be created and probed by NIF.

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Polarized angular-dependent reflectivity and density-dependent profiles of shock compressed xenon plasmas

Yu. Zaporozhets[1], V. Mintsev[1], V. Fortov[1], H. Reinholz [2,3], G. Roepke[2], S. Rosmej[2], Yu. Omarbakiyeva[4]

[1]*Institute of Problems of Chemical Physics, Chernogolovka, Moscow Reg., 142432 Russia*
[2]*Universitaet Rostock, Institut fuer Physik, 18051 Rostock, Germany*
[3]*University of Western Australia School of Physics, WA 6009 Crawley, Australia*
[4]*International IT University, 050040, Almaty, Kazakhstan*

New data for the reflectivity of shock-compressed xenon plasmas of different target densities at pressures of 10-12 GPa at large incident angles are presented. These data allow to analyze the free electron density profile across the shock wave front. Assuming a Fermi-like density profile, the width of the front layer is inferred. The reflectivity for the s and p - polarized waves are calculated. The influence of the scattering on the atoms which has been taken into account at the level of the dynamical collision frequency prove to be essential for the understanding of the reflection process. Subsequently, as expected, a unique density profile is sufficient to obtain good agreement with the experimental data at different incident angles and at all investigated optical laser frequencies. Reflectivity measurements for different densities allow to determine the dependence of shock-front density profiles on the plasma parameters. As a result, it was found that the width of the front layer increases with decreasing density.

Ionization potential depression and in-medium wave equation in dense plasmas

Chengliang Lin[1], Gerd Roepke[1], Wolf-Dietrich Kraeft[1], Heidi Reinholz[1,2]

[1]*Universitaet Rostock, Institut fuer Physik, 18051 Rostock, Germany*
[2]*University of Western Australia School of Physics, WA 6009 Crawley, Australia*

The properties of a bound electron system immersed in a plasma environment are strongly modified by the surrounding plasma. The modification of an essential quantity, the ionization energy, is described by the electronic and ionic self-energies including dynamical screening within the framework of the quantum statistical theory. Introducing the ionic dynamical structure factor as the indicator for the ionic micro-field, we demonstrate that ionic correlations and fluctuations play a critical role in determining the ionization potential depression [1]. This is in particular true for mixtures of different ions with large mass and charge asymmetry. The ionization potential depression is calculated for dense aluminum plasmas as well as for CH plasmas and compared to the experimental data and more phenomenological approaches used so far. The solution of the two-particle in-medium wave function gives also access to calculate the optical properties such as spectral line profiles. In this way the unified description of the Inglis-Teller effect and ionization potential depression is possible [2].

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Checking Salpeter's enhancement factor of nuclear reactions in asymmetric mixtures

Philippe Arnault[1], Jean Clérouin[1], Nicolas Desbiens[1], Alexander J. White[2], Lee A. Collins[2], Joel D. Kress[2], and Christopher Ticknor[2]
[1]CEA, DAM, DIF, 91297 Arpajon, France
[2] Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

ABSTRACT

Since the seminal work of Salpeter [1], it is recognized that fusion reaction rates in stars are enhanced by the plasma environment, in every stage of their evolution: from main sequence stars to red giants, and eventually for the cooling of white dwarfs and the explosions of supernovae. This enhancement depends strongly on the Coulomb coupling and on the composition which varies from hydrogen-rich to degenerate carbon-oxygen cores. Even more asymmetric mixtures are found in Inertial Confinement Fusion and Warm Dense Matter experiments. Using orbital free molecular dynamics (OFMD) simulations we study mixtures of hydrogen-copper and hydrogen-silver as prototypes of a light-heavy plasma mixtures at 100 eV, various concentrations and constant pressure. We show that the ionic structure obtained by OFMD simulations is accurately reproduced by a multi-component hyper netted chain (MCHNC) calculation. In particular, the hydrogen-hydrogen correlation bump, which is a crowding effect caused by the collisions with the highly charged heavy component, is well reproduced. This adequacy of the MCHNC approach allows for a straightforward evaluation of the enhancement factor for nuclear reactions between light elements. This procedure is faster and more accurate than the Widom expansion used in previous work [2]. Being standalone and independent of simulations, the MCHNC approach allows to extend the range of thermodynamic conditions to very low concentrations in the heavy component (5% or less) and to very high temperatures (few keV). Enhancement factors for nuclear reactions rates are found close to Salpeter's strong coupling formulation below 2 keV and to the weak coupling formulation beyond 2 keV [3].

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Study of plasma microfield properties in highly magnetized plasmas.

S. Ferri, L. Dakroub and A. Calisti

Aix-Marseille Université, CNRS, PIIM, UMR 7345, Marseille, FRANCE

Highly magnetized media have been a great deal of interest in recent years. They occur in the high-energy-density (HED) environments characteristic of intense laser-matter interactions and astrophysical compact objects. Kilotesla magnetic fields can be generated in plasmas in which the temperature can reach several hundreds of eV and densities are up to $10^{21}cm^{-3}$. In such extreme conditions, the atoms of the medium are partially ionized resulting in a mixture of ions, electrons and neutrals. The emitted radiation from those ionized species is closely related to the atomic physics and the plasma environment. The presence of B-field leads, among other phenomena, to bending trajectories of the charged particles into a helical path. Such trajectories can have an effect on the Stark-Zeeman broadening mechanisms of spectral line shapes.

The present study is to investigate the influence of the bending trajectories of the charged particles on the statistical properties of the plasma microfields. To do so, Molecular Dynamics simulations, [1], in presence of B-field is used for plasma conditions related to laser driven capacitor-coil targets experiments, [2,3,4].

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Interpretation of thermodynamic quantities in ab-initio non-equilibrium molecular dynamics

Stegailov V. V.[1,2]

[1] *Joint Institute for High Temperatures of the Russian Academy of Sciences, RUSSIA*
[2] *Moscow Institute of Physics and Technology, RUSSIA*

Irradiation of solids with ultrashort laser pulses opened an exciting field of research. New emerging physics is connected with formation of warm dense matter (WDM) at the initial transient state of material evolution after energy deposition into electron subsystem. WDM in such ultrafast phenomena is a non-equilibrium state that makes it very challenging for theory, modelling and simulation, especially in two-temperature (2T) systems when electron and ion subsystems can be considered in quasi-equilibrium at $T_e > T_i$. Laser ablation is one of the major phenomena where WDM properties are crucially (e.g. [1,2]).

Both in continuum and in atomistic models of ablation it is assumed that the quasi-equilibrium 2T-WDM can be described using thermodynamic concepts. The free energy is represented as $F(\rho;T_i;T_e) = F_e+F_i$, where $F_e = E_b+F_{fe}$, where E_b is the binding energy, F_{fe} is the free energy of free (ionized, delocalized), F_i is the free energy of the ion subsystem. The corresponding representation of pressure is

$$P = P_e + P_i = P_b + P_{fe} + P_i \,. \qquad (1)$$

Usually the first term is called the cold or binding pressure and depends on density $P_b = P_b(\rho)$, the second term is the kinetic electronic pressure $P_{fe} = P_{fe}(n_{fe};T_e)$ and the third term is the thermal ionic pressure $P_i = P_i(\rho;T_i)$. It is the total pressure P that defines the mass transfer in continuum 2T-WDM models. In the atomistic 2T-WDM models sometimes the so-called blast force is introduced in order to describe the influence of kinetic pressure of electrons on the ion subsystem. The kinetic pressure of electrons is assumed to be a manifestation of free electrons. The difficulty connected with P_{fe} calculations stems from the fact that for this purpose one needs the number density of free electrons n_{fe} (i.e. the degree of ionization).

In this work we discuss two connected questions [3,4]. On examples of aluminum and gold using the finite temperature Kohn-Sham density functional theory we are making an attempt to analyze the electronic contribution to the total pressure in 2T-WDM metals and to clarify the representation (1). Another question is the separation of electrons into bound and free that is a general problem for non-ideal plasma physics.

The comparison of this approach with other techniques [5,6] will be discussed. As well as possible alleviation of these problems within the wave packets models for WDM [7,8].

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DFT-MD simulations of mixing properties in warm dense hydrocarbons

J. Vorberger & K. Ramakrishna

Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany

Mixtures of carbon and hydrogen at megabar conditions and at temperatures up to one electron volt can be found in a variety of planets of our solar system like Uranus and Neptune and are believed to feature prominently in extrasolar planets. The microscopic structure, the equation of state, as well as transport and mixing properties of hydrocarbons thus strongly influence the inner structure and evolution of these astrophysical objects. We present results of density-functional molecular dynamics simulations for the structure and equation of state of dense CH. We include the non-ideal entropy of mixing in order to calculate mixing properties of hydrocarbons at such conditions. The results of these simulations explain recent experimental findings showing the demixing of carbon and hydrogen and the formation of nano-diamonds at double shock conditions [1]. In addition, we analyze theoretical capabilities and limitations to predict the inelastic x-ray scattering signal off warm dense hydrocarbons with particular focus on the carbon and diamond part, respectively.

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Fast Non-Adiabatic Warm Dense Matter Simulation

B. Larder[1] , S. Richardson[1,2], D. Gericke[3], G. Gregori[1]

[1]Department of Physics, University of Oxford, UK
[2]AWE, UK
[3]Centre for Fusion, Space and Astrophysics, Department of Physics, University of Warwick, UK

When constructing modern simulations of Warm Dense plasma, one must make compromises in accuracy so that the calculations are computationally accessible. One of the many difficulties inherent in these simulations is the vast difference in the time scales of electron and ion motion. To access long-time ion correlations, then, the Born-Oppenheimer approximation is usually relied upon so that simulations can be performed at the time scale of the ions[1,2].

However, the neglect of electron dynamics associated with the Born-Oppenheimer approximation has been shown to produce systematic errors in the ion dynamics, and hence the ion-ion dynamic structure factor, that are difficult to quantify and correct[3]. Further, existing non-adiabatic/non-Born-Oppenheimer approaches require significant computational expense, to the point that they can become impractical for calculating long-term ion correlations[4].

Here, we present a new simulation method for modelling the dynamics of quantum plasmas that goes beyond the Born-Oppenheimer approximation, by treating electrons and ions as thermally-averaged Bohmian trajectories. Beginning with the standard description of Bohm's theory of quantum mechanics[5], we systematically construct a set of classical trajectories capable of accurately reproducing static and dynamic properties of Warm Dense Matter.

Our method complements existing state of the art Density Functional Theory methods. Due to a greatly reduced computational expense, we are able to treat long-time ion dynamics of large systems while also treating electrons fully dynamically. We thereby fill a void where current methods require a prohibitive computational cost.

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Ab-initio shock states and thermodynamic properties of liquid silicates

Joshua P Townsend[1], Luke Shulenburger
[1]High Energy Density Physics Theory, Sandia National Laboratories, Albuquerque, New Mexico, USA

We present *ab-initio* calculations of the principal Hugoniot states, entropy, sound velocity, as well as transport properties for liquid silicate Mg_2SiO_4. Our investigations heavily employ density functional theory-based molecular dynamics (QMD) calculations to self-consistently compute thermodynamic quantities. In this presentation, we discuss the Hugoniot states and possible de-mixing of liquid Mg_2SiO_4. We then turn to new calculations of entropy on the Hugoniot of Mg_2SiO_4 using the 2PT method [1] and compare to results from more traditional thermodynamic integration. Wherever possible, we compare our results to experiment. The results highlight the utility and predictive power of QMD methods for high energy density physics.

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The Uniform Electron Gas at Warm Dense Matter Conditions.

Simon Groth[1], Tobias Dornheim[1], and Michael Bonitz[1]

[1]*Kiel University, GERMANY*

The availability of an accurate parametrization of the exchange-correlation energy of the uniform electron gas (UEG) on the basis of ground state quantum Monte Carlo simulations has been crucial for the success of density functional theory (DFT) calculations within the local density approximation. However, it is widely agreed [1] that the description of recent experiments with inertial confinement fusion and laser-excited solids within the DFT framework requires to go beyond the ground state. While an explicitely thermodynamic DFT approach is long known, it requires an accurate parametrization of the exchange-correlation free energy of the UEG at warm dense matter conditions. Here we present a novel parametrization that is based on our recent ab initio simulations [2,3,4,5] and compare to various other parametrizations.

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Dynamical and transport properties of dense plasmas on the basis of Coulomb logarithm and effective potentials

T.S. Ramazanov, S.K. Kodanova, Zh.A. Moldabekov, M.K. Issanova, M.T. Gabdullin, S.M. Amirov

Al-Farabi Kazakh National University, Institute for Experimental and Theoretical Physics, 71 Al-Farabi ave., 050040, Almaty, KAZAKHSTAN

We have carried out an extensive research on studying both static and dynamic screening in non-ideal dense plasmas. As the result, the model for the accurate calculation of the stopping power as well as other transport properties is presented. In the former case, the main idea is to use a cold plasma model with thermal and quantum effects taken into account in a screened pair interaction potential, where screening is due to partially or totally degenerate (possibly non-ideal) electrons [1]. By comparison with other more involved calculations, which clearly shows a very good agreement at low velocities, the applicability range of the model is discussed. The main advantage of the model is that the strong ion-electron scattering is treated accurately and, hence, applicable for the description of the stopping power at the critical velocity, i.e. when the stopping power has its maximum value. The Coulomb logarithm obtained within this model is used for the computation of the dynamical and transport properties of dense plasmas. In the range of the applicability of the model, our data is in close agreement with the DFT-MD and OFDFT-MD results. Therefore, our model makes the calculation of the aforementioned effects much easier and sheds a light on the most important plasma features which govern a relevant microscopic process. Additionally, the impact of the electronic non-ideality in a quantum regime on the static and dynamic screening of an ion charge, obtained in collaboration with the Kiel group, is discussed [2]. Further, the screened ion potential was used to study the structural properties of the strongly coupled ions in a quantum plasma with correlated electrons [3]. Finally, the recent results of the investigation of the screening of an ion by the electrons oscillating in an external alternating field are presented [4].

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Quantum fluid description of non-ideal dense plasmas

Zh.A. Moldabekov[1,2], M. Bonitz[1], T.S. Ramazanov[2]

[1] *Institut für Theoretische Physik & Astrophysik, Christian-Albrechts-Universität, Kiel, Germany*
[2] *Institute of Experimental and Thepretical Physics, Al Farabi Kazakh National University, Almaty, Kazakhstan*

A large scale simulation of quantum plasmas with correlated electrons is challenging and, currently, a formidable task. *Ab initio* methods such as Quantum Monte-Carlo and Kohn-Sham density functional theory (DFT) are severely limited by the number of electrons and ions which can be simulated [1]. Hence, the orbital-free formulation of DFT has undergone rapid development in recent years [2]. However, the OFDFT is limited to the static case. Therefore, in this work, we present our recent result on the development of quantum hydrodynamics (QHD) of correlated electrons in dense plasmas; which e.g., can be used for the description of the dynamics of the electrons around a mean distribution obtained from the OFDFT and, thereby, can be a reliable tool for a large scale simulation of a quantum plasma dynamics [3].
We have derived the closure relations which allow to go beyond of previously used QHD models. The main features of the developed QHD theory are the following: it can be used at finite temperatures, the agreement with the random phase approximation is guarantied in the non-interacting limit, the effect of correlations is taken into account via the local filed corrections, and can be used for the weakly non-uniform case. On the basis of the obtained closure relations, previous results on the fluid description of the non-interacting quantum electrons have been revised and, in part, improved. The non-ideality effect is discussed for both static and dynamic cases employing local field corrections [4-7]. Finally, the extension to the case of a quantum plasma in an external magnetic field is presented.

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Radar studies of ionospheric dust - plasma phenomena

Ingrid Mann[1]

[1]Dept. Physics & Technology, UiT, the Arctic University of Norway, Tromsø, NORWAY

Dust plasma phenomena occur in the Earth ionosphere in particular in the meteor ablation zone at altitudes ~50-95 km and above where radar meteors form. Radar also detect coherent polar mesospheric radar echoes (PME), i.e. radar echoes that are caused by spatial variations in the plasma refractive index at around 80 to 90 km altitude in the Earth's mesosphere. During summer, PM(S)E form in the presence of ice particles and are linked to the electric surface charge of the particles. Straightforward quantitative descriptions of PME are however still missing as well as the role of turbulence in their formation. In addition, radar can under certain conditions, detect incoherent scatter. Incoherent scatter results from electromagnetic waves scattering at electrons that are coupled to ions and charged dust through plasma oscillations and to the neutral particles through collisions. The contribution of dust to incoherent scatter is small, but possibly an important tool for future studies. When illuminated with electromagnetic waves of frequency ω_0 the waves back scattered from electrons would form a broad distribution around ω_0 due to the Doppler shift caused by the electron thermal motion. If the radar wavelength, λ_{radar} is large in comparison to the plasma Debye length, λ_{Debye} where $\lambda_{Debye} \approx (T_e/n_e q_e)^{1/2}$ the plasma oscillations that couple the electrons to other charged components become important. Resonances occur and in the absence of bulk motion are at frequency shifts corresponding to the frequencies, ω_{wave} of the plasma oscillations $\omega = \omega_0 \pm \omega_{wave}$. The two predominant resonances are from plasma (Langmuir) waves with the plasma frequency ω_p, where $\omega^2_p \approx \omega_e^2 \approx n_e e^2/m_e$ and from ion acoustic waves with frequency ω_{ia}, where $\omega^2_{ia} \approx (T_e + 3\,T_i) / m_i$ with T_e and T_i being electron and ion temperature, respectively and m_i the ion mass. In addition, for $T_i \approx T_e$, which is the case in the lower ionosphere, Landau Damping occurs for the ions and ion acoustic waves and the resonances around $\omega = \omega_0 \pm \omega_{ia}$smear out toward ω_0 forming a central peak, often denoted as the ion line. Incoherent scatter is observed when $(\lambda_{Debye} / \lambda_{Radar})^2 << 1$ and at a sufficiently large transmit power. As the charged dust acts analogous to the ions but with larger mass, it influences the inner part of the ion line. So far, the dust component could only be reliably derived from the observations in a few cases, because at the altitudes of interest the incoherent scatter signal is weak and in addition influenced by ion-neutral collisions, negative ions and positive molecular ions. The differences in electron, ion and dust temperatures also play a role and the scattering varies with frequency. Based on dust parameters derived from models and observations with rocket instruments the radar signals are estimated.

Dynamical properties of dust particles in a background gas and external magnetic field

Dzhumagulova K. N. [1] , Masheyeva R.U. [1], Ramazanov T.S. [1], Donkó Z.[2]

[1] *IETP, al Farabi, Kazakh National University, 71, al Farabi av., Almaty, 050040, Kazakhstan*
[2] *Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary*

In this work, we investigate the simultaneous effects of a static homogeneous external magnetic field and the background gas environment on the dynamical properties of dust particles in strongly coupled two-dimensional Yukawa systems. We use the Langevin dynamics computer simulation method. The equations of motion of the particles with taking into account both effects mentioned above, can be written as:

$$m\ddot{\mathbf{r}}_i(t) = \sum_{i \neq j} \mathbf{F}_{ij}(r_{ij}) + Q[\mathbf{v}_i \times \mathbf{B}] - vm\mathbf{v}_i(t) + \mathbf{F}_{Br}, \quad (1)$$

where the first term on the right hand side gives the sum of inter-particle interaction forces, the second is the Lorentz force, the third term represents the friction force (proportional to the particle velocity), is due to of the presence of the background gaseous environment, while the fourth term accounts for a randomly fluctuating “Brownian” force that is caused by the random kicks of the gas atoms on the dust particles. To integrate the equations of motion (1), a new numerical scheme is used, in which the time step is not limited by the magnitude of the magnetic field [1]. This scheme was obtained similarly to the scheme proposed in Ref. [2], but takes into account the friction force as well.

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Collective excitations in fluids of soft interacting particles

Sergey Khrapak[1,2]

[1] *Institute for Materials Physics in Space, German Aerospace Center (DLR), 82234 Wessling, Germany;*
[2] *Joint Institute for High Temperatures, Russian Academy of Sciences, 125412 Moscow, Russia*

The purpose of this presentation is to introduce very simple practical analytical expressions, which describe dispersion relations of collective modes in fluids composed of soft interacting particles, including strongly coupled plasmas. The expressions are derived within the framework of the quasi-crystalline approximation (QCA) also known as the quasi-localized charge approximation (QLCA), combined with a simple excluded-volume-based approximation for the radial distribution function *g(r)*.

Fully analytical expressions without free parameters have been derived for strongly coupled Yukawa and Coulomb (one-component plasma) systems in three dimensions, as well as one-component plasma fluids with Coulomb and logarithmic interactions in two-dimensions [1-3]. The accuracy of these expressions will be demonstrated using the comparison with the results from numerical simulations (available numerical results have been complemented by new simulations).

The approach appears to be particularly useful for soft long-ranged interactions operating in plasma-related systems, but is not limited to the plasma-related context. As an example, its application to dipole-like interactions in two-dimensions [4] will be demonstrated.

Possible applications of the obtained results will be briefly discussed.

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Mode-coupling instability in 2D complex plasma crystals: The role of damping rate

V. Nosenko[1,2], J. K. Meyer[1], S. K. Zhdanov[1], H. M. Thomas[1], J. Carmona-Reyes[2], and T. W. Hyde[2]

[1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 82234 Weßling, Germany
[2]Center for Astrophysics, Space Physics, and Engineering Research, Baylor University, Waco, Texas 76798-7310, USA

Complex, or dusty plasma is a regular plasma where small particles of solid mater are dispersed. Dust particles collect electrons and ions from the plasma, become charged, and interact with each other via a screened Coulomb (Yukawa) potential. As a result, complex plasmas are often strongly coupled and can be in a liquid form or even crystallize. Since dust particles are relatively massive and individually observable, many processes in complex plasmas can be studied in real time at the level of individual particles. An interesting phenomenon which occurs in two-dimensional (2D) complex plasma crystals and lends itself to direct experimental observation and theoretical analysis is the mode-coupling instability (MCI) [1]. It occurs when the dispersion relations of the two dust-lattice wave modes, longitudinal in-plane (L) mode and transverse vertical (TV) mode intersect. In the vicinity of their intersection, a new hybrid mode appears which is unstable. If not suppressed by the neutral gas friction, it will grow exponentially with time and can result in the crystal melting. Therefore, the gas damping rate is very important for the development of MCI. In this contribution, we will present our recent experiments performed across a wide range of the neutral gas damping rates. Here, the damping rate ν_E is normalized by the frequency scale of 2D plasma crystals ω_0 [1].

In experiments with low damping rate, $\nu_E/\omega_0=0.01$, the coupling of the L and TV wave modes was observed even in the absence of their crossing; in fact, the modes were separated by a gap 4 Hz wide [2]. The coupling manifested itself in the traces of the TV mode appearing in the measured longitudinal spectra, i.e., *mixed polarization*. This observation was facilitated, besides low damping, by relatively large particle charges and respective plasma wake charges in these experiments.

In contrast, in experiments with high damping rate, $\nu_E/\omega_0=0.48$, MCI was observed when the deep crossing of the L and TV modes occurred, resulting in the high growth rate of the hybrid mode which was necessary to overcome strong gas damping [3].

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High intensity action of femtosecond and picosecond x-ray and optical lasers onto ruthenium and molybdenum films

N.A. Inogamov[1,2], Y.V. Petrov[1,3], V.V. Zhakhovsky[2,1], V.A. Khokhlov[1], K.P. Migdal[2,1], V.V. Shepelev[4,1], I. Milov[5], I.A. Makhotkin[5], J. Winter[6], H.P. Huber[6]

[1]Landau Institute for Theoretical Physics of the Russian Academy of Sciences, 142432 Chernogolovka, Moscow region, Russian Federation
[2]Dukhov Research Institute of Automatics (VNIIA), 127055 Moscow, Russian Federation
[3]Moscow Institute of Physics and Technology, 141700 Dolgoprudny, Moscow region, Russian Federation
[4]Institute for Computer-Aided Design of the Russian Academy of Sciences, 123056 Moscow, Russian Federation
[5]Industrial Focus Group XUV Optics, MESA+ Institute for Nanotechnology, University of Twente, 7522 NB Enschede, The Netherlands
[6]Munich University of Applied Sciences, 80335 Munich, Germany

Refractory ruthenium (Ru) is a perspective material used as an extreme ultraviolet/soft x-ray (EUV/SXR) oblique reflectors or as a protective film capping multilayer mirrors preventing their damage under high radiation fluxes typical for next generation lithography machines and from particle debris. Molybdenum (Mo) is another example of widely employed refractory metal. Here we mean applications of Mo films in solar photovoltaics cells and experiments with ultrathin films – thinner than a skin layer for optical electromagnetic wave. Our studies unveil extremely high survivability of molten films made from these refractory metals.

Properties of the refractory metals Ru and Mo are purely known in a warm dense matter regime. In this regime the densities are comparable to the solid state densities while temperatures are ~1 eV. Their properties in the two-temperature warm dense matter regime are even less known. For considered here cases of ultrashort durations of laser pulses the two-temperature effects are very significant. Electron temperature is higher than ion temperature in the two-temperature states created by ultrashort illumination.

The straight-through description from two-temperature (2T) to one-temperature (1T) warm dense matter states is necessary for quantitative calculations because pulse duration is shorter than duration t_{eq} of the 2T to 1T transit process while the electron-ion temperature equilibration time t_{eq} is shorter than acoustic time scale $t_s = d_T/c_s$ defining the rate of hydrodynamics processes; here d_T is thickness of a heat affected zone, c_s is speed of sound. This straight-through description of thermodynamics and kinetics of 2T and 1T states is presented in the report for PNP16. We develop two-temperature equations of state for Ru and Mo, calculate by DFT (density functional theory) their electronic spectra, find their electron-ion coupling parameters, and define two-temperature thermal conductivities; it is shown that the electronic spectra rather weakly react to exciting of electron subsystem. With this input we run our two-temperature hydrodynamic code. Another important achievement is creation of reliable embedded atom model (EAM) interatomic potential for Ru. This potential is used for defining of strength of Ru and molecular dynamics description of nucleation and ablation under laser action. Results are compared with experimental data.

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Particle charge in PK-4 dc discharge from ground and microgravity experiments

T. Antonova[1], S.A. Khrapak[1], M. Pustylnik[1], M. Rubin-Zuzic[1], H.M. Thomas[1], A.M. Lipaev[2], A.D. Usachev[2], V.I. Molotkov[2], M.H. Thoma[3]

[1]*Institut fur Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Weßling, GERMANY*
[2]*Joint Institute for High Temperatures, Russian Academy of Sciences, Moscow, RUSSIA*
[3]*I. Physikalisches Institut, Justus-Liebig Universität, Gießen, GERMANY*

The complex plasma facility Plasmakristall-4 (PK-4) was installed in the Columbus module of the International Space Station (ISS) in November 2014. This is an experimental laboratory developed to provide a range of various experiments in the direct current (dc) or/and radio-frequency (rf) low temperature gas discharge. It allows to use different manipulation technics (e.g. laser manipulation, thermal and electrical disturbances, etc) [1].
Because of the gravity force the positions of microparticles in discharge on ground differ from those under microgravity conditions. The comparison of both cases gives the possibility to resolve discharge parameters as well as main microparticle characteristics in radial direction of the discharge tube. The aim of the current work is to estimate the radial distribution of the particle charge within the discharge tube from the measurements of the particle drift velocity in PK-4 set-up.
The experiments have been performed in the Flight Model (FM) onboard ISS as well as in Science Reference Model 1 (SRM 1) of PK-4 in ground based laboratory, which is functionally identical to the FM. The pressure ranged from 20 to 100 Pa in argon and neon gases with the variation of the discharge current from 0.5 to 1.5 mA. The particles of three different diameters of 1.3, 2.5 and 3.4 μm have been injected into the chamber. They were illuminated by the laser beam and their motion was filmed by video cameras with 35 fr/sec and 14,2 μm/pixel resolution. The velocities have been estimated by measuring the velocity of the whole particle cloud as well as from the intensity slope on the so-called space-time diagram.
The experimental data from ISS show that under microgravity conditions the velocities of microparticles are always lower than those measured on ground, as it already has been observed in parabolic flight experiments [2]. The difference is more pronounced in the lower pressure range (20-30 Pa). Drift velocities from experimental data have been compared with the results of analytical model, which yielded the estimation of the particle charge for chosen experimental conditions on ground and under microgravity. In the developed model variations of the discharge parameters in radial direction of the discharge tube have been taken into account. The experimentally measured and theoretically estimated particle velocities as well charges show different pressure behavior in argon and neon gases.
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Large-scale *O*(N) DFT calculations for carbon at high temperature

Mandy Bethkenhagen[1,2], Abhiraj Sharma[3], Phanish Suryanarayana[3], John E. Pask[1], Babak Sadigh[1], Lin H. Yang[1], Sebastien Hamel[1]

[1]*Lawrence Livermore National Laboratory, USA*
[2]*University of Rostock, GERMANY*
[3]*Georgia Institute of Technology, USA*

Kohn-Sham Density Functional Theory (DFT) implementations based on planewaves have been successfully applied for various materials in the warm dense matter regime. However, the tractable number of particles is rather limited due to the method's $O(N^3)$ scaling and it becomes challenging to employ at high temperatures, where the number of partially occupied states increases significantly. Both problems are addressed with the novel SQDFT code [1], which is a large-scale implementation of the Spectral Quadrature (SQ) method for O(N) Kohn-Sham DFT calculations [2,3]. Here, we present extensive benchmark calculations for selected equation of state points for carbon in comparison to the widely-used planewave Kohn-Sham DFT codes VASP [4] and QUANTUM ESPRESSO [5]. Finally, we calculate the Hugoniot curve for carbon at temperatures up to 500 000 K.

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Dynamic electron-ion collisions and non-local effects on the structures of warm dense matter

Jiayu Dai, Dongdong Kang, Qian Ma, Binbin Lu, Zengxiu Zhao and Jianmin Yuan
Department of Physics, National University of Defense Technology, CHINA

ABSTRACT.

The structural, thermodynamic and transport properties of warm dense matter (WDM) are crucial to the fields of astrophysics and planet science, as well as inertial confinement fusion. WDM refers to the states of matter in a regime of temperature and density between cold condensed matter and hot ideal plasmas, where the density is from near-solid up to ten times solid density, and the temperature between 0.1 and 100 eV. In the WDM regime, matter exhibits moderately or strongly coupled, partially degenerate properties. Therefore, the methods used to deal with condensed matter and isolated atoms need to be properly validated for WDM. It is therefore a big challenge to understand WDM within a unified theoretical description with reliable accuracy. Here, we review the progress in the theoretical study of WDM with state-of-the-art simulations, i.e. quantum Langevin molecular dynamics and first principles path integral molecular dynamics. We study the electronic, ionic structures of warm dense matter from H to Fe, and comparing the equation of states from shock-compressed experiments. Also, we discuss the non-local effects such as van der Waals interactions and nuclear quantum effects on the equation of states and the phase transition of dense hydrogen, showing the consistent results with quantum Monte Carlo method. Finally, the method of calculating electrical conductivity directly from electron molecular dynamics will be shown and the effect of electron-ion collisions could be discussed, which will reduce the conductivity in warm and hot dense matter.

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Non-local electron kinetics around the cloud of dust particles.

A.V. Fedoseev[1], G.I. Sukhinin[1], N.A. Demin[1], M.V. Salnikov[1]

[1]*Institute of Thermophysics SB RAS, Lavrentyev Ave. 1, Novosibirsk, 630090, RUSSIA*

In laboratory conditions, dusty plasma is often observed in the form of dust particles clouds which levitate in the strong electric field of near-electrode region of rf discharge or striations of dc glow discharge. The influence of dust particles on gas discharge plasma is negligible only for low dust particle concentration and charge. With the increase of dust particles charge number, local plasma parameters change in the region containing dust particles, which in turn leads to a change of the average charge of the dust particles and all properties of dusty plasma [1]. It was understood that electron and ion losses on dust particle surface should be compensated for in ionizing collisions, and an averaged electric field should increase in the region containing dust particles. It was also shown [1] that the increase of dust particle density leads to the increase of electron temperature and ionization rate in the dust cloud, to the decrease of the dust particle charge, and to the decrease of electron density compared to the ion density inside the dust cloud. However, the number of dust particles was a fixed parameter and their influence on discharge plasma was considered in the local approximation.

At high dust particle density, the influence of the dust cloud on the plasma parameters can be non-local and governed by the plasma conditions around the cloud [2]. For example, dust particle charging is provided by the electron and ion fluxes into the cloud from the surrounding plasma. In many papers the behavior of dust particles is investigated in fixed plasma parameters without taking into account the influence of a dust component on these parameters. In particular, the electric field providing the confinement of dust particles is usually taken as a given one.

The aim of this work is to highlight the mutual influence of a dust cloud and a dc discharge plasma in a self-consistent non-local approach based on the proposed model [3]. The non-local effects are considered on the example of radial distributions of plasma parameters in non-stratified positive column of a glow discharge with a dust cloud. The model includes the non-local Boltzmann equation for non-equilibrium EEDF, drift-diffusion equations for ions and dust particles, and the Poisson equation for a self-consistent electric field.

The results show that the ionization balance in the discharge with a dust cloud definitely has a non-local behavior. The production of electrons and ions occurs mainly in the region between the dust cloud and the discharge tube wall, while their recombination takes place in the region of the dust cloud and on the discharge tube wall. A self-consistent distributions of the plasma parameters inside the dust cloud are the following: (1) the ionization rate is equal to the rate of electron and ion recombination on the surface of the dust particles, (2) the radial components of electron and ion fluxes are almost equal to zero, and (3) the radial electric field is expelled from the dust cloud.

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Heating Effect of the Surface of the Dust Particle in Cryogenic Complex Plasmas

M. M. Muratov[1,2] , T. S. Ramazanov[1], and Zh. A. Moldabekov [1,3]

1 Institute for Experimental and Theoretical Physics, Al-Farabi Kazakh National University, 71 Al-Farabi ave., 050040 Almaty, KAZAKHSTAN

2 National NanotechnologicalLaboratory of Open Type , Al-Farabi Kazakh National University, 71 Al-Farabi ave., 050040 Almaty, KAZAKHSTAN

3 Institute of Applied Sciences and IT, 40-48 Shashkin str., 050038 Almaty, KAZAKHSTAN

Mukhit.muratov@gmail.com

This work is devoted to the investigation of a heating effect of a surface of a dust particle in cryogenic complex plasmas at low gas pressure. A relation that represents the temperature ratio of the dust particle surface to that of the surrounding gas, in low-pressure weakly ionized complex plasmas, was used to study a dust particle heating at cryogenic conditions [1]. Orbit motion limited theory was used to compute the electron as well as ion flux to the dust particle surface in a weakly collisional case [2].

It is shown that comparing with background gas, the dust particle surface temperature at low pressure is significantly higher (up to ten times). The gas temperature near the grain surface is a slowly decreasing function of distance with asymptotic ~ 1/r behavior. Therefore, the dust particle surface heating is important for near space around dust particle. At distances comparable with average inter-dust distance, the neutral shadowing interaction appearing due to large temperature difference between the grain surface and surrounding gas can lead to a significant changes in the structural properties of a cluster of dust particles [3].

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Effect of ion mean free path length on plasma polarization behind a dust particle in an external electric field.

G.I. Sukhinin[1], M.V. Salnikov[1], A.V. Fedoseev[1]

[1]*Institute of Thermophysics SB RAS, Lavrentyev Ave. 1, Novosibirsk, 630090, RUSSIA*

In this paper, the effect of an external electric field on plasma polarization around dust particles with different radii and for different ion mean free path lengths is considered for the process of resonant ion-neutral charge exchange collisions using a self-consistent numerical simulation method. Plasma parameters around a dust particle, both in an external field and in a plasma flow, are usually modeled with the help of two methods: LR (Linear Response) [1] and PIC ("particle-in-cell") [2]. However, in most works that use these methods, the influence of ion collisions is usually neglected [2]. In this work, a recently developed [3] self-consistent iterative method is applied for determining plasma parameters in collisional plasma for different ions mean free path lengths. It is shown that a positive potential peak is formed in polarized plasma behind the dust particle (in the wake). It is also demonstrated that for different parameters (dust particle radius or charge, ion mean free path length) a dipole moment formed in plasma can be fitted with a single curve. The received data are found to be in good agreement with recently obtained results for the collisionless case [2].

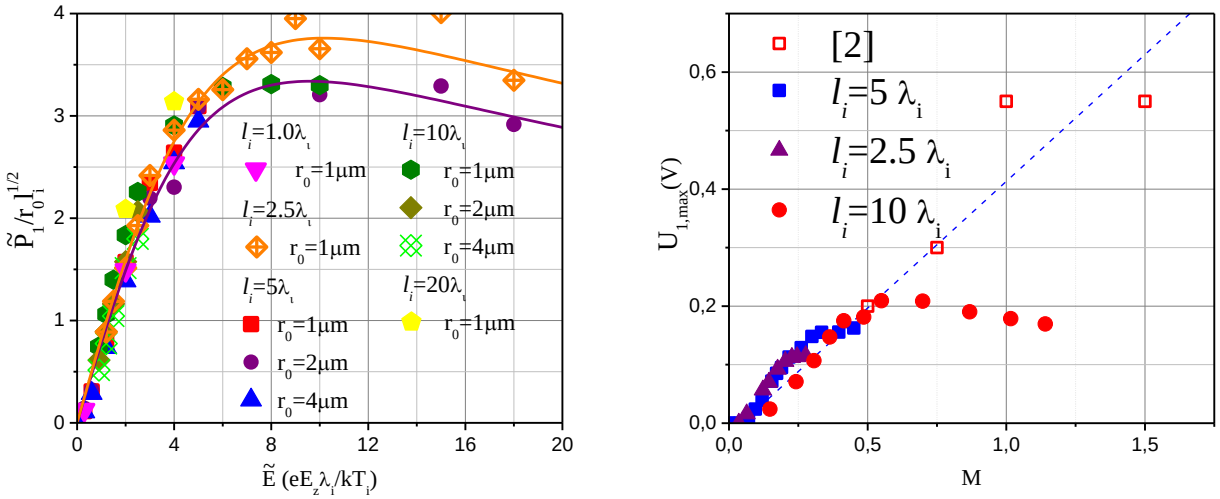

Fig.1. (Left) A normalized dipole moment of an ion-electron cloud around a dust particle in an external electric field. (Right) Dependence of the first potential peaks in the wake behind the dust particle on the Mach number obtained in this paper and in [2].

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Non-linear screening and thermodynamics of complex plasma.

Martynova I.A.[1,2], Iosilevskiy I.L.[1,2]

[1]*Joint Institute for High Temperatures of the Russian Academy of Sciences, RUSSIA*
[2]*Moscow Institute of Physics and Technology (State University), RUSSIA*

The present work is devoted to the analysis of the applicability range of a basic assumption in the phase diagram [1] of complex plasma in the κ–Γ plane (κ is the structural parameter, Γ is the coupling parameter), i.e., linearized (Debye) screening of macroions by microions which leads to the Yukawa form of effective interactions between macroions. Parameters of non-linear screening of macroions were obtained within the direct Poisson-Boltzmann approximation [2]. Two effects were revealed as a result of such calculations: (i) decomposition of all microions into two subclasses, bound and free ones, and (ii) significant reduction of an effective charge Z^* of the initial bare charge Z under non-linear screening by a small high-density envelope of the bound microions. The effective charge Z^* grows in the direct proportion to Z first and then, the change of the effective charge Z^* is negligibly thin. This renormalization of the initial Z and macroion concentration at the border of the cell leads to corresponding renormalization of initial parameters κ and Γ into κ^* and Γ^* ($\kappa^* < \kappa$ and $\Gamma^* < \Gamma$) [2]. The corresponding calculated shifts of excess internal energy are discussed and calculated. Moreover, we used three modifications of the excess internal energy calculated in [3] where the Debye-Hückel-hole approximation was used. We took the non-linear screening effect into account, first, in microion distribution inside the hole and, second, in reduction of the effective macroion charge in comparison with the bare one outside the hole. Third, we considered not point-like macroions, but finite-sized ones. The value of the resulting modified excess internal energy is bigger than the one which can be obtained from [3] where the non-linear screening effect was not taken into account. This work was supported by the Russian Science Foundation, grant No. 14-50-00124.

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Consistent interpretation of experimental data for dense metallic plasma near the liquid-gas coexistence curve.

P.R. Levashov

Joint Institute for High Temperatures, Izhorskaya 13 Bldg 2, Moscow 125412, RUSSIA
Tomsk State University, 36 Lenin Prospekt, Tomsk 634050, RUSSIA

Dense metallic plasma is a complicated object for both theoretical and experimental study. Due to very high coupling and degeneracy parameters traditional chemical picture and perturbation approaches are of questionable applicability for such plasma. Strong correlation effects hamper the usage of average atom models. Expanded states of a liquid metal can be obtained in shock-wave experiments with porous samples. In this case a porous sample unloads into some obstacle after the shock-wave compression and the expansion velocity can be registered. Such experiments are quite complicated and rare. Another example is an isobaric expansion (IEX) of wires under heating by a powerful current pulse. IEX experiments are also sparse and contradictory. The challenge of the current work is to describe both isobaric and isentropic expansion experiments for a number of metals by one and the same theory. Also it is of importance to estimate the liquid-gas phase transition boundary and critical point.

We use quantum molecular dynamics to calculate thermodynamic properties of expanded liquid aluminum, molybdenum and tungsten. Various shock-compression experiments are reproduced for porous tungsten and molybdenum as well as subsequent isentropic expansion. Special attention is paid to available isobaric expansion experimental data for theoretical estimations of critical points. We succeeded in reconciliation of several types of experiments for refractory metals. Thorough analysis of experimental data will be presented. A special Monte Carlo procedure is applied for the estimation of the liquid–gas coexistence curve and critical point parameters of tungsten and molybdenum. The result is close to estimation obtained with Likalter's similarity relation.

Dynamic characteristics of strongly coupled plasmas

Yu.V. Arkhipov[1], A. Askaruly[1], A.E. Davletov[1], D.Yu. Dubovtsev[1], I.M. Tkachenko[2]

[1]Al-Farabi Kazakh National University, Almaty, KAZAKHSTAN
[2]Universitat Politècnica de València, Valencia, SPAIN

A self-consistent version of the method of moments was suggested recently in [1], where it was applied to the direct determination of dynamic properties of one-component classical strongly coupled Coulomb and Yukawa systems in terms of their static characteristics reduced to two frequencies defined by the power frequency moments of the inverse dielectric function. The first of them is related to the static dielectric function by the Kramers-Kronig relations, while the second one is rigorously determined by the system static structure factor charge-charge *S(k*), which can be calculated for each case independently. The aim of the presentation is to expand the approach to partly degenerate multicomponent Coulomb systems. To this end a novel expression is derived for the static dielectric function in terms of *S(k)* that simultaneously takes into account degeneracy and satisfies known asymptotic expansions. Thus, the knowledge of the dynamic characteristics is effectively reduced to that of S(k) without any further adjustment to the dynamic data. The validity of the present approach is confirmed by favorable comparison with available theoretical and simulation data and its robustness is ultimately verified by engaging several schemes for evaluating the static structure factor.

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Application of intense ion beams to planetary physics research at the FAIR facility

N.A. Tahir[1], A. Shutov[2], I.V. Lomonosov[2], A.R. Piriz[3], P. Neumayer[1], V. Bagnoud[1] and S.A. Piriz[3]

[1]*GSI Darmstadt, Germany*
[2]*IPCP Chernogolovka, Russia*
[3]*UCLM, Ciudad Real, Spain*

Discovery of thousands of extrasolar planets of different type including gas giants, water rich as well as rocky planets has led to a much greater interest in planetary physics research. Existing planetary models predict that extreme physical conditions including ultra-high pressures (5-30 Mbar), super-solid density, but relatively low temperatures (5000-20000 K) exist in the planetary interiors. To have a better understanding of the processes of planetary formation and evolution, it is necessary to study the thermophysical and transport properties of matter under such extreme conditions in the laboratory. Theoretical work has shown that intense heavy ion beams are a very efficient tool to implode material samples to induce planetary core conditions.

The heavy ion synchrotron, SIS100, which is under construction at the Facility for Antiprotons and Ion Research [FAIR] at Darmstadt, will deliver strongly bunched, well focused energetic intense ion beams with unprecedented intensities. Numerical simulations have shown that using the FAIR beam parameters, it is possible to generate core conditions of hydrogen rich planets like Jupiter and Saturn [1], water-rich planets like Uranus and Neptune [2] as well as rocky planets like Earth and more massive Earth-like extrasolar planets, the Super-Earths [3]. Based on these simulation results, a dedicated experiment named LAPLAS [Laboratory Planetary Sciences] has been proposed as part of the FAIR High Energy Density program. An overview of this work is presented in this presentation.

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Ab initio simulation of ion stopping in strongly correlated materials

M. Bonitz, K. Balzer*, M. R. Rasmussen, N. Schlünzen, I. Meinke, and E. Pehlke

Institut für Theoretische Physik und Astrophysik, Universität Kiel
**Rechenzentrum, Universität Kiel*

The interaction of ions with solid surfaces is of crucial importance for many technological applications, in particular for nonideal plasmas. Ion stopping has been computed for a long time, and there exist many analytical models and code packages. However, these approaches typically neglect correlation effects in the solid material. We have recently developed first-principle simulations that are based on Nonequilibrium Green functions (NEGF) within an Ehrenfest approach for the ion [1]. First NEGF results for ion stopping were presented in Ref. [2]. Here we compare these results to time-dependent density functional simulations. Furthermore we present results of a recent extension of the NEGF simulation to a study of a special correlation effects: the ion-induced doublon formation in graphene-type nanoclusters [3]. Doublons are doubly occupied lattice sites in strongly correlated materials and have an important effect on the electronic properties and conductivity of these materials. Here we show that ion impact can effectively induce doublons giving rise to interesting applications.

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Time-dependent Density Functional Theory determination of stopping-power and conductivity in warm, dense matter environments

A.J. White[1], O. Certik[1], and L.A. Collins[1], Y.H. Ding[2], S.X. Hu[2]

[1] *Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[2] *Laboratory for Laser Energetics, University of Rochester, Rochester, NY 14623, USA*

ABSTRACT

We have explored a variety of warm dense matter (WDM) and hot plasma systems with a quantum molecular dynamics (QMD) approach. In the QMD, we solve the many-body Schrodinger equation for a large, representative sample of atoms, periodically replicated through space to effect the characteristics of a fluid, which may include a mix of atoms, molecules, ions, and free electrons. For the electrons, we employ density-functional theory (DFT) in two guises: an orbital-based in the Kohn-Sham (KS) form and an orbital-free (OF), usually in a Thomas-Fermi-Dirac approximation. This dual capability permits thorough coverage of these extreme conditions and provides a set of consistent static, dynamic, and optical properties such as equation of state (EOS), mass transport (viscosity/diffusion), opacity, and conductivity (thermal/electrical).

We have also developed time-dependent (TD) versions of both the KS and OF approaches in order to treat primarily electron conductivities and stopping power. The advantages of the time-independent KS for the perturbative determination of these properties quickly vanishes with rising temperatures due to the large numbers of required eigenstates. The nonperturbative TD schemes offer a more viable path into the upper ranges of the WDM regime. They also permit the examination of the interaction of intense laser pulses with a plasma, as well as other nonlinear and nonequilibrium interactions.

We have investigated the electron stopping power for proton stopping in deuterium and beryllium and alpha particles in deuterium-tritium mixtures. The computational efficiency of Orbital-Free TD-DFT allows for the large simulation sizes. This is required for the direct calculation of stopping power for MeV projectiles, relevant to ICF plasma heating. We have compared OF and KS stopping powers, showing excellent agreement for high velocities, and derived a current-dependent kinetic energy functional that improves agreement with the KS results at low velocities while significantly improving propagation stability.

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Stopping power in warm dense targets from first principles

Attila Cangi[1], Daniel S. Jensen[1], Andrew D. Baczewski[1]

[1]*Sandia National Laboratories, Center for Computing Research, Albuquerque, NM, USA*

Recent experimental advances enabled the precise measurement of the stopping power of fusion products in warm dense targets. Time-dependent density functional theory coupled with Ehrenfest molecular dynamics is the standard method to predict stopping power in cold targets. We assess its ability to reproduce these experimental measurements in warm dense targets[1], illustrate the computational challenges with this method, and introduce an alternative framework based on time-dependent density functional theory coupled with average-atom models. Our approach facilitates the prediction of the stopping power in future experiments from first principles and advances our empirical and phenomenological understanding of transport properties in this technologically challenging thermodynamic regime.

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Stopping power of electron gas

Yu.V. Arkhipov[1], A.B. Ashikbayeva[1], A. Askaruly[1], A.E. Davletov[1], D.Yu. Dubovtsev[1], S.A. Syzganbayeva[1], I.M. Tkachenko[2]

[1] *Al-Farabi Kazakh National University, Almaty, KAZAKHSTAN*
[2] *Universitat Politècnica de València, Valencia, SPAIN*

The polarizational stopping power of heavy ions in fully ionized plasmas is described by the Lindhard formula [1]:

$$\left[-\frac{dE}{dx}\right]^{pol} = \frac{2\left(Z_p e\right)^2}{\pi v^2}\int_0^\infty \frac{dk}{k}\int_0^{kv}\omega^2\left(-\mathrm{Im}\left[\frac{\varepsilon^{-1}(k,\omega)}{\omega}\right]\right)d\omega,$$

whose high-velocity asymptotic form was found by Bohr, Bethe, and Larkin [2]:

$$\left[-\frac{dE}{dx}\right]^{pol}_{v\to\infty} \cong \left(\frac{Z_p e\omega_p}{v}\right)^2 \ln\left[\frac{2m_e v^2}{\hbar\omega_p}\right].$$

The plasma inverse dielectric function (IDF), $\varepsilon^{-1}(k,\omega)$, was determined in [3] within the moment approach [4], complemented by some physical observations in terms of two characteristic frequencies ω_1 and ω_2, which are the ratios of the frequency power moments of the IDF imaginary part, in the following form:

$$\varepsilon^{-1}(k,\omega) = 1 + \frac{\omega_p^2\left(\sqrt{2}\omega_1\omega + i\omega_2^2\right)}{\sqrt{2}\omega_1\omega\left(\omega^2-\omega_2^2\right) + i\omega_2^2\left(\omega^2-\omega_1^2\right)}.$$

The frequencies ω_1 and ω_2 can be rigorously evaluated using the static structure factor (SSF) of the system. Nevertheless, here we employ the following interpolating expressions [5,6]:

$$\omega_1^2 = \omega_1^2(k) = \omega_p^2\left(1 + k^2k_D^{-2} + k^4k_q^{-4}\right), \qquad \omega_2^2 = \omega_2^2(k) = \omega_p^2\left(1 + \frac{\left\langle v_e^2\right\rangle k^2}{\omega_p^2} - \frac{v_{\mathrm{int}}^2 k^2}{\omega_p^2}\right),$$

The interpolation and fitting parameters introduced are chosen as follows:

$$v_{int}^2 = -\frac{4}{15}\frac{\Gamma^{3/2}}{\beta m_e}\left(\frac{-0.9052}{\sqrt{0.6322+\Gamma}} + \frac{0.27243}{1+\Gamma}\right),\ \Gamma = \beta e^2/a,\ k_q^4 = 12r_s/a^4,\ r_s = a/a_B,$$

a and a_B are the Wigner-Seitz and Bohr radii, respectively, $\beta = 1/(k_B T)$, k_D^{-1} is the Debye radius, k_B stands for the Boltzmann constant with T being the plasma temperature.

The numerical results obtained for the energy losses of heavy ions moving in an electron gas are found in good agreement with the PIC simulation data [7].

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DFT+U equation of state for iron oxide

Daniel Cebulla[1], Mandy Bethkenhagen[1], Ronald Redmer[1]

[1]*University of Rostock, GERMANY*

The number of detected exoplanets and the capabilities of identifying small, Earth-sized planets have grown tremendously over the last two decades. Yet many of those Earth-sized planets are only characterized in mass and radius. Therefore, interior structure models rely heavily on equations of states (EOS) for rock material to characterize the planetary properties. One particular interesting material is iron oxide, which is very challenging to treat with standard Density Functional Theory (DFT) methods. Here we investigate the DFT+U approach to obtain the correct electronic and structural properties for the FeO phases typically predicted at the high pressures within the planetary interiors. The Hubbard U is obtained self-consistently from spin-polarized DFT calculations with QUANTUM ESPRESSO [1,2] using the linear response approach [3]. The resulting optimized ground state is used as a starting point for phonon calculations within the quasi-harmonic approximation. Based on these calculations we investigate the impact of the Hubbard U on the EOS providing a step forward to incorporating more realistic rock material into interior structure models of super-Earths.

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Electron emission from laser produced nanoplasma.

R.G. Bystryi

Joint Institute for High Temperatures of the Russian Academy of Sciences, RUSSIA
National Research University Higher School of Economics, RUSSIA

Nowadays interaction strong laser fields (10^{13} – 10^{16} W/cm^2) with nanosized objects is a very popular issue. As in the bulk case, the electromagnetic radiation can interact only with the electrons and causes their rapid heating and ionization of atoms. The result is the nanosized object with a relatively high electron temperature density and degree of ionization. It's called nanoplasma. A more precise definition and the associated limitations can be found in the article [1].
One of the distinguishing features of the nanoplasma is the violation of the plasma neutrality [1]. Due to the laser ionization and further thermionic emission from the plasma surface, the object gains an uncompensated positive charge. Concerning a small number of particles in the plasma under consideration ($10 - 10^6$), this charge determines the rate of plasma expansions affects the rate of ionization-recombination processes, electron density profile, and optical properties of the cluster plasma [1-3].
This paper presents a theoretical model of emission current from nanoplasma. The model consists of a system of ordinary differential equations. The derived expression is based on results of molecular dynamic modeling [4-5]. The paper discusses the details of applicability of the model and its advantages and disadvantages. Comparison with a series of experiments [6-9] is presented. The suggested system of equations allows generalizing the experimental results and giving a new explanation of some of them.
Some of the presented results can be found in the article [10].
This work is supported by the Russian Science Foundation, grant No. 18-19-00734.

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Improvement of the EoS of Hydrogen and its isotopes based on reflectivity measurements.

L.Caillabet[1], S. Brygoo[1] and P. Loubeyre[1]

[1] *CEA, DAM, DIF, F-91297 Arpajon, FRANCE*

The occurrence of metallization induced by pressure in dense hydrogen was first discussed by Wigner and Hungtington in 1935 [1] for the solid at T=0K. Metallization was also proposed to exist in dense fluid hydrogen [2,3]. The location of the liquid-liquid transition and the magnitude of the volume discontinuity at the transition is still actively debated, both theoretically and experimentally. The nature and location of the transition of dense fluid hydrogen from the molecular state to the plasma state is an essential input in the building of the equation of state of warm dense hydrogen, impacting notably the prediction of the structure of gas giant planets.

Few years ago, we built an equation of state of dense fluid hydrogen using a chemical model to fit ab-initio data provided by Born-Oppenheimer Molecular Dynamic (BOMD) [4]. Even though the improvement over existing EoS tables was significant, the location of the metallization of dense fluid hydrogen remains uncertain. In the fluid phase, the Insulator to Metal Transition (IMT) location strongly depends on the physics that are taken into account in the simulations (long range forces, choice of the xc approximation in BOMD, nuclear quantum effects), leading to an uncertainty of around 300 GPa. Our current project is to use existing experimental data to overcome this uncertainty and so improve the warm dense hydrogen EoS. We will essentially use the data of the shock Hugoniot data in a large range of density-temperature phase space of the IMT, provided by laser-driven shock wave on hydrogen and deuterium precompressed in diamond anvil cells, from 0.1 to 18 GPa [5, 6, 7] and the reverberating bgas gun experiment [8]. We will first show a bentchmark between this new data and our previous BOMD EoS [5], which exhibits some discrepancies, mainly in temperature, at highest precompressions. Reflectivity measurements at 532 nm are also provided in this data, and we show how we infer the ionization rate (Z*) of the material from these measurements, using a mix Drude-Lorentz model for the electrical conductivity. As BOMD simulations always overestimate Z*, we show how we improve our BOMD EoS, using the Z* inferred from the experiments as a new value for the dissociation rate in our chemical model.

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Study of microfield statistical properties by using multi-component plasma Molecular Dynamics simulation.

Calisti A.[1], Ferri S.[1], Talin B.[1]

[1]CNRS, Aix Marseille Univ, PIIM, Marseille F-13397, France

For various purposes, it is necessary to simulate virtual plasma composed of electrons and ions in different ionization states. Depending on the plasma conditions, it is required to account, in the simulations, for bound states as well as quantum mechanical processes to create and destroy them. This permits to avoid non-physical Coulomb collapse and to extend the applicability of classical MD simulations, which are ideally suited for fully-ionized, non-degenerate plasma, to a widest range of plasma conditions.

For this purpose, we have chosen to simulate the ions and electrons as interacting classical particles and to incorporate some quantum information through a regularized potential allowing to model collisional ionization and recombination processes. The BinGo-TCP code has been designed to deal with neutral mixtures composed of ions of the same atom with different charge states and electrons [1, 2]. Within the limits of classical mechanics, all charge-charge interactions are accounted for in the particle motion.

Characterizing properly, the local electric fields produced by the electrons and ions of the plasma, is very important for spectroscopic diagnostics as they interact with the emitters and modify the radiated spectra. These fields, which derived from the force calculations on individual charges, can be measured by accounting for all the interactions between charges. The TCP simulation is well designed to obtain time sequences of electric field. These can be used in the resolution of the Schrödinger equation describing the time evolution of the emitter wave functions in the time-dependent field, or to infer microfield statistical properties [3].

The discussion here, will be based on a statistical analysis of the microfields at charged points in terms of field distribution and field correlation functions, characterizing the contributions of ions or electrons or both (total).

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Wave packet molecular dynamics study of the plasma phase transition in warm dense hydrogen

Fedorov I. D.[1,2], Orekhov N. D.[1,2], Stegailov V. V.[2,1]

[1]*Moscow Institute of Physics and Technology, RUSSIA*
[2]*Joint Institute for High Temperatures of the Russian Academy of Sciences, RUSSIA*

Despite the fact that hydrogen is the most prevalent element in the universe, its equation of state at high pressures remains poorly understood and raises some fundamental questions. One of such questions is the nature of the plasma phase transition (PPT) [1,2] at pressures above several hundred GPa, at which, perhaps, it passes into a conducting state. Although a large number of experiments dedicated to this problem have been carried out, there is still no consensus on the PPT location: results from experiments with static and ultrafast dynamic compression differ for more than 150 GPa at 1500 K [3,4].

Properties of the dense hydrogen are intensively investigated by means of atomistic ab initio techiques. Quantum Monte-Carlo methods have already given a lot of highly accuracte results for dense hydrogen plasma. First-principles molecular dynamics (FPMD) based on finite-temperature density functional theory (DFT) is another widely deployed tool. However both techniques have difficulties when trying to step beyond Born–Oppenheimer approximation. The difficulties of FPMD applications to non-equilibrium conditions have been considered recently [5]. In this work, we use the wave packet molecular dynamics (WPMD) as a tool that more adequately captures non-adiabatic and non-equilibrium aspects of PPT and gives us the possibility to study the possible metastable states that correspond to this phase transition [2].

Dealing with warm dense hydrogen, we expect the proximity of the electron terms, which, firstly, allows us to work with classical molecular dynamics, and secondly, under these conditions, the contribution from the Pauli prohibition is small, and therefore we can approximate it with a certain potential for accelerating the calculations. In this work, we use the WPMD-based potential eFF [6], in which the contribution from the Pauli exclusion approximates the contribution from the Pauli energy making the unfavorable finding of electrons on one level. eFF provides the combination of particle dynamics for ions with wave packet dynamics for electrons representing them as floating Gaussians. Unlike the more complex antisymmetrized approaches, interactions between electrons in the eFF are restricted to pairwise components only and the total energy of the system is evaluated as in the classical force field methods.

Computations with eFF are carried out at temperatures 1000-15000 K and pressures 80-300 GPa for densities from 0.3 to 1.5 g/cm^3. The analysis of the ionization and dissociation processes in the vicinity of PPT reveals significant influence of the heating rates on the composition hydrogen plasma and gives us a way to describe its metastable states.

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Account for bound states in atomistic plasma model using split-WPMD method

Ilya Valuev[1]

[1]*Joint Institute for High Temperatures of RAS, Russia*

The method of Wave Packet Molecular Dynamics (WPMD) [1-6] is an approximate quantum method for simulation of nonideal plasmas and warm dense matter. In WPMD, antisymmetrized Gaussian wave packets are used to represent electrons and point-like particles represent the ions. The quantum model corresponds therefore to a single-determinant (Hartree-Fock) approximation. In this model both thermodynamic properties such as equation of state for plasma and dynamic quantities may be calculated.

As shown by previous research [3] the original WPMD model, where each electron is represented by a single Gaussian, may largely underestimate the role of bound states and therefore the plasma ionization degree.

In the present work we propose a model based on Split-WPMD approach [3,4]. In the current implementation each electron is represented by two Gaussians, one of which remains attached to one of the ions and the other is free to move. The balance between two parts is controlled by a coefficient, which is treated as a new dynamic variable in the variational approach. Note that after anti-symmetrization electrons may be regarded as equivalent, and the identity connection between the electron density attached to a particular ion and its free counterpart is lost.

Although the new model appears to be more computationally demanding since singularities may appear in the system Norm matrix and require special treatment, it helps to obtain more realistic ionization degrees, especially for lower plasma density.

Using a hydrogen plasma as an example we demonstrate that the new model is capable of describing the whole range of bound states that may appear in hydrogen starting from the molecular gas at low temperatures and densities to the partially ionized plasma whith substantial presence of neutral atoms and molecular ions.

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Crystallization of a quantum plasma at finite temperature.

E.Jaupart[1] and G. Chabrier [1,2]

[1] *CRAL- ENS de Lyon, Lyon, France*
[2]*University of Exeter, Exeter, United Kingdom*

We have conducted Path Integral simulations of a fluid and a crystal of charged particles at finite temperature. Path integration is carried out via Molecular Dynamics while using a semi-classical pair potential derived from the Coulomb potential which takes into account quantum diffraction effects at small distance.

The melting curve is obtained with the so called dynamical melting criterion. This simply brackets the phase transition by examining the stable phase towards which relaxes one simulation. To determine the stable phase, we examine the structure factor and the empirical Lindeman Criterion (Chabrier 1993 [1]).

We verify the importance of finite size effects by running simulations with growing values of the number of polymers P made in the discretization of the Path Integrals. We compare our melting curve with the one obtained analytically (Chabrier 1993 [1]) and the one obtained numerically with P = 54 (Jones & Ceperley 1996 [2]).

Finally, we briefly address the problem of quantum statistics.

Besides the fundamental problem of crystallization of the quantum One Component Plasma (OCP) this problem bears consequences for the thermal evolution of compact astrophysical bodies such as massive white dwarfs and neutrons stars.

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Ultrafast dynamics of complex atoms induced by coherent laser

Yongqiang Li[1], Xiaowei Wang[1] and Jiayu Dai[1]

[1]Department of Physics, National University of Defense Technology, Changsha 410073, Hunan P.R. China

With the development of highly bright coherent X-ray lasers and attosecond extreme-ultraviolet pulses, the strong field physics of light-matter interactions has expanded from the long-wavelength regime into the short-wavelength regime. Here, one experimentally provides the possibility for investigating the coherent dynamics of X-ray-matter systems (also attosecond extreme-ultraviolet pulse induced systems). In contrast to traditional studies, these non-equilibrium systems normally relax in a vast number of decay channels, and the corresponding dominant physical mechanism can be treated as the interplay between coherence and dissipation. Unfortunately, in spite of recent experimental progresses, simulations for these open systems are so far completely lacking, since a large-scale simulation is inevitable for the intense X-ray-matter systems.

Both coherent pumping and energy relaxation play important roles in understanding physical processes of ultra-intense coherent light-matter interactions. Here, using a large-scale quantum master equation approach [1], we describe dynamical processes of practical open quantum systems driven by both coherent and stochastic interactions. As examples, two typical cases of light-matter interactions are studied. First, we investigate coherent dynamics of inner-shell electrons of a neon gas irradiated by a high intensity X-ray laser along with vast number of decaying channels. In these single-photon dominated processes, we find that, due to coherence-induced Rabi oscillations and power broadening effects, the photon absorptions of a neon gas can be suppressed resulting in differences in ionization processes and final ion-stage distributions. Second, we take helium as an example of multiphoton and multichannel interference dominated electron dynamics, by investigating the transient absorption of an isolated attosecond pulse in the presence of a femtosecond infrared laser pulse. In the last part, we demonstrate a new scheme for the investigation of hole dynamics of complex atoms based on two-color ultrashort X-ray pulses.

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Structural properties of strongly coupled ions in quantum plasmas

Zh.A. Moldabekov[1,2], S. Groth[1], T. Dornheim[1], M. Bonitz[1], T.S. Ramazanov[2]

[1] *Institut für Theoretische Physik & Astrophysik, Christian-Albrechts-Universität, Kiel, Germany*
[2] *Institute of Experimental and Thepretical Physics, Al Farabi Kazakh National University, Almaty, Kazakhstan*

Despite recent advances in modeling and computer simulations, a fully self-consistent treatment of highly nonequilibrium electron-ion plasmas has not been possible so far due to the requirement of the simultaneous account of electronic quantum effects together with the strong ionic correlations. The main problem here is the vastly different time scales of electrons and ions resulting from their different masses. A possible solution of this dilemma is a multi-scale approach based on a screened ion potential with a linear response treatment of the electrons [1]. Recently, going beyond the random phase approximation [2], we have performed an analysis of the screened ion potential in the case of non-ideal quantum electrons by making use of local field corrections which are determined on the basis of the Singwi–Tosi–Land–Sjölander approximation (STLS) [3] and Quantum Monte Carlo data [4]. From the analysis of the structural properties of strongly coupled ions on the basis of different screened ion potentials [5, 6], the region of densities and temperatures where the STLS description of screening by partially (or totally) degenerate electrons can be used for the calculation of the structural properties of ions were determined. It was found that correlations (non-ideality) of the electrons result in a larger isothermal compressibility of the ions due to the stronger screening of the ion charge. Additionally, calculations using different screened potentials clearly show that strongly coupled ions can be very sensitive to the shape of the pair interaction potential and, therefore, to the approximation used for the description of screening by electrons.

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Electron Localization properties across the liquid-liquid phase transition in dense hydrogen.

Carlo Pierleoni[1,2], D. M. Ceperley[3], Markus Holzmann[4,5]

[1] *Department of Physical and Chemical Sciences, University of L'Aquila, Italy*
[2] *Maison de la Simulation, CEA, CNRS, Univ. Paris-Sud, UVSQ, Université Paris-Saclay, 91191 Gif-sur-Yvette, France*
[3] *Department of Physics, University of Illinois Urbana-Champaign, Illinois, USA*
[4] *LPMMC, UMR 5493 of CNRS, Université Grenoble Alpes, France*
[5] *Institut Laue-Langevin, BP 156, F-38042 Grenoble Cedex 9, France*

We analyze the electronic properties, as characterized by the off-diagonal single electron density matrix and the electron momentum distribution, of high pressure hydrogen across the liquid-liquid phase transition region based on previous Coupled Electron-Ion Monte Carlo calculations [1].

Below the critical temperature the abrupt changes of these distributions indicate a metal to insulator transition occurring together with the structural transition from the atomic to molecular fluid. At higher nuclear temperature above the critical point of the transition, both the change of electronic correlations as well as the change in molecular character of the fluid are continuous. Inspection of electron-proton and electron-electron pair correlation functions provide complementary information of the transition [2,3].

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Equation of state of styrene at high pressures and temperatures

Rykounov A.A.[1], Vorobyova M.A.[1]

[1]Federal State Unitary Enterprise "Russian Federal Nuclear Center – Academician E.I. Zababakhin All-Russian Research Institute of Technical Physics" (FSUE "RFNC-VNIITF"), Russian Federation

Polystyrene is widely used not only in industry and in everyday life, but also in experimental physics where it is utilized, for example, as the ablator material in inertial confinement targets. The optimization of target parameters requires knowledge of polystyrene properties under shock loading at relatively high pressures (from a few gigapascals to a few megabars). For collecting information on its thermodynamic characteristics and microstructure under extreme conditions, we simultaneously use methods of quantum (QMD) and classical (CMD) molecular dynamics. With such a combination it is possible, on the one hand, to reliably describe all the types of interatomic interactions including those that are quantum in nature, and on the other hand, to track out the evolution of rather large (10^5 – 10^6 atoms) systems on time scales of about 1 ns unachievable for QMD. The equation of state we propose agrees well with available experimental data on the response to shock of both styrene and polystyrene, and our microstructure analysis disputes Ree's hypothesis [1] that shocked hydrocarbons form carbon clusters as nanodiamonds, at least for time scales typical of CMD.

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Thermodynamic properties of tantalum under non-equilibrum heating from first-principles calculations

N. A. Smirnov
Russian Federal Nuclear Center - Institute of Technical Physics, Snezhinsk, Russia

We present research of the relative structural phase stability and lattice dynamics of *bcc* and *fcc* tantalum in the case when electrons are heated up to several electron-volts, while the lattice remains cold. These conditions can appear when the target is irradiated by ultrashort laser pulses. For our investigation we used the all-electron full-potential linear-muffin-tin-orbital method (FP-LMTO). Our calculations show that the *fcc* structure of tantalum becomes thermodynamically more favorable than the *bcc* structure at electron temperatures T_e above 1.5 eV. The *bcc* phase becomes dynamically unstable at T_e > 2 eV. At the same time, *fcc* tantalum is dynamically stable at electron temperatures above 1 eV. In this work we study possibility of the *bcc*→*fcc* structural transition to occur in tantalum target under non-equilibrium heating. Also we consider the possibility of the ultrafast nonthermal melting under these conditions.

Dynamic structure factor using electron foruce field in lithium

Tianyu Gao[1], Xiaowei Wang[1], Jiayu Dai[1], Yongjun Choi[2], Michael Murillo[2]

[1]Department of Physics, National University of Defense Technology, Changsha 410073, Hunan P.R. China
[2]Department of Computational Mathematics, Science and Engineering, Michigan State University East Lansing, Michigan, 48823, USA

Accurate x-ray scattering techniques to measure the physical properties of dense plasmas have been developed for applications in high energy density physics. We notice that structure factors determine the physical properties of matter. We prepare to present molecular dynamics simulations based on electron force field (eFF) that determine self-consistently the dynamic ion structure factor and dynamic electronic structure factor in lithium, Our comprehensive data set allows for the calculation of the dispersion relation for collective excitations, and the calculation of the sound velocity. Due to the use of Gaussian wave function in electron force field method, it can improve the traditional electronic structure factor calculation method without the Chihara approximation. The results will be compared with available experimental x-ray and DFT results. We will check for both the liquid metal and warm dense matter domain.

Action of ultrashort laser pulse on tantalum: physical model of tantalum, simulations, and experiments

S.I. Ashitkov[1,2], P.S. Komarov[1], E.V. Struleva[1], M.B. Agranat[1,2], N.A. Inogamov[2,3], V.V. Zhakhovsky[3,2], V.A. Khokhlov[2], Y.V. Petrov[2,4]

[1]Joint Institute for High Temperatures of the Russian Academy of Sciences, 125412 Moscow, Russian Federation
[2]Landau Institute for Theoretical Physics of the Russian Academy of Sciences, 142432 Chernogolovka, Moscow region, Russian Federation
[3]Dukhov Research Institute of Automatics (VNIIA), 127055 Moscow, Russian Federation
[4]Moscow Institute of Physics and Technology, 141700 Dolgoprudny, Moscow region, Russian Federation

Ablation of refractory metals with ultrashort laser pulses remains little-studied as opposed to other metals with a relatively low melting temperature like aluminum and gold. In this paper ablation of tantalum by femtosecond laser pulses is investigated. The results of hydrodynamic simulation of target evolution are compared to experimental data obtained by a time-resolved interferometry method. The aspects of ablation dynamics induced by electronic pressure and acoustic tension at one- and two-temperature stages respectively are investigated theoretically and experimentally. The data on strength of tantalum liquid phase as function of temperature at the stretching rate of about 10^9 s^{-1} are presented.
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For the application of vacuum-arc units in nanoengineering

Zhukeshov A.M.[1,2], Gabdullina A.T.[1,2], Amrenova A.U.[1,2], Mukhamedryskyzy M.[1,2], Fermakhan K.[1,2], Balmanova N.T.[1], Iliyasov R.K.[1], Maksut D.M.[1], Mansur N.Sh.[1]

[1]*Al-Farabi Kazakh National University, KAZAKHSTAN*
[2]*National nanotechnology laboratory of open type, KAZAKHSTAN*

One of the priority areas of the research is the study and production of nanostructured materials. The priority of this research consists of the prospects and opportunities for the development of this technology [1,2].
Vacuum arc spraying refers to a group of methods for obtaining coatings (including thin films) in vacuum, in which the coating is obtained by direct condensation of vapor of the deposited material and the chemical reaction on the surface of the substrate is activated by heating, or by ionization and dissociation of arc gas [3,4]. In this case, the target from the sputtered material is in a strongly-ionized plasma under a negative potential and plays a role of a cathode, i.e. the electric current creating the arc is fed into the circuit containing the cathode (negative potential) and the body of the vacuum chamber (positive potential) [5].
The paper proposes to use the installation of the vacuum-arc accelerator (VDU-1) for research to obtain nanostructured materials. The unit VDU-1 was developed in the pulsed plasma accelerator laboratory of Al-Farabi Kazakh National University [6,7]. At the moment, works on the modernization of the electrode system have been carried out. To solve this problem, the results of work on optimizing the processing regimes of the materials under study are presented. Calorimeters of various shapes were used to effectively determine the energy parameters of the plasma generated at the accelerator VDU-1. In addition, implemented works on obtaining nanostructured materials at VDU-1. In particular, preliminary data on the investigation of nanofilms and nanopowders are presented, for analysis of which the equipment of Nanotechnology laboratory of open type was used.
The research in this area can be claimed in various branches of science and technology since they can give an economic effect from the use of final products.

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The calculations of thermophysical properties of Pb plasma

Apfelbaum E. M.[1]

[1]*Joint Institute for High Temperatures of RAS, Izhorslaya 13 bldg. 2, Moscow 125412 RUSSIA*

The thermophysical properties of metals have been studied for more than a century in different areas of phase diagram. Among these properties we will consider the equations of states and electronic transport coefficients (electrical conductivity, thermal conductivity and thermal power). The region of relatively high temperatures - approximately more than 5kK, where the plasma of metals is located - presents especial challenge both for measurements and theory [1]. It is the problem itself to penetrate into this area, without any other measurements. For instance, it is almost impossible to measure directly the temperature in corresponding experiments [2]. Nevertheless, during last two decades new measurements and calculations have appeared [3]. These studies have allowed one to shed light on the thermophysical properties of many metals in plasma state. However, for some metals there is still the shortage of data. For instance, for Pb there are measurements and calculations in plasma at relatively high temperatures and densities, for instance in the states of compressed warm dense matter [4]. But the data at expansion rarely reach even the critical density [5]. So present study is aimed to fill this gap.

Earlier we have developed a model for calculations of the considered thermophysical properties based on the chemical approach. Namely a substance is considered as a mixture of electrons positive ions, atoms. The free energy of this mixture can be minimized with respect to the particle densities of separate components. It allows one to find the ionic composition and thermodynamics values as the pressure, internal energy etc. Then the ionic composition is used to calculate the electronic transport coefficients within the relaxation time approximation. The chemical model has also some approximations for the free energy. They limits the considered approach by the density from above. Nevertheless our model was successfully applied to the plasma of gases, metals and semiconductors (see [6,7] and references therein). In present investigation we have applied our model to Pb plasma. We have calculated the pressure, internal energy, conductivity, thermal conductivity, thermal power at the densities less than 1 g/cm^3 and the temperatures 10 - 100 kK.

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Structural and thermodynamic properties of dense non-isothermal plasma.

T.N. Ismagambetova[1], M.T. Gabdullin[1,2], T.S. Ramazanov[1]

[1]*al-Farabi Kazakh National University, Institute of Experimental and Theoretical Physics (IETP), al-Farabi str., 71, Almaty, 050040, KAZAKHSTAN*
[2]*Kazakh-British Technical University, Tole bi str., 59, Almaty, 050000, KAZAKHSTAN*

In this work, dense non-isothermal plasma was considered. Dense plasma presents a great interest in both theoretical and practical areas of research and is actively studied in laboratory conditions (thermonuclear reactors, gas discharges, etc).
In dense plasmas interparticle interactions play an important role, therefore, the models of interaction between particles have been used to study properties of such plasma. Different potentials [1-2], considering variety of effects such as the screening effects at large distances, the quantum-mechanical effects at small distances like diffraction and symmetry, have been used. The symmetry effect appears only in electron-electron interactions due to Pauli exclusion principle, when influence of different directions of spin of electrons is accounted for. The effects in non-isothermal plasma can also be significantly influenced by the difference between temperatures of electrons and ions [3].
Pair correlation functions obtained on the basis of these interaction potentials were compared with the results of classical mapping and computer simulations [4]. Thermodynamic properties were calculated using pair correlation functions.

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Influence of electron shell effects on compressibility of substances in strong shock waves

Kadatskiy Maxim[1,2], Khishchenko Konstantin[1,2]

[1]*Joint Institute for High Temperatures RAS, RUSSIA*
[2]*Moscow Institute of Physics and Technology, RUSSIA*

The maximum pressures and temperatures in substances are achieved in dynamic experiments via relative compressibility methods [1]. Obtaining information on thermodynamic properties of a substance under study by such methods requires knowledge of the equation of state for another substance, which is taken as a reference material.
Quantum-statistical models [2] are successfully used to construct equations of state in a wide range of temperatures and densities. The influence of the discreteness of the spectrum of bound states leads to oscillatory behavior of thermodynamic functions at sufficiently high temperatures (i.e. electron shell effects). But, at the present time, available experimental data for this region of parameters are insufficiently accurate, contradict one another or have been obtained by relative methods, which make it impossible to measure unambiguously the magnitude of the shell effects.
In the present work, we construct equations of state for Al, Cu, Mo, Fe, Pb and SiO_2, which are widely used as standards in the framework of the impedance-matching technique. The calculated equations of state are used to derive the Hugoniots, double shock adiabats and isentropes of unloading, which are required to yield relative dependencies of shock wave velocities. We estimate the magnitude of shell effects by consideration of the difference between results of the quasi-classical (the Thomas–Fermi model with modifications) and quantum-mechanical (the Hartree–Fock–Slater model) calculations with experimental data for different pairs of the investigated substances.
The work is supported by the Russian Science Foundation, grant No. 14-50-00124.

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Equation of state for zinc at high energy densities

Konstantin V. Khishchenko

Joint Institute for High Temperatures RAS, Izhorskaya 13 Bldg 2, Moscow 125412, RUSSIA

Thermodynamic model of equation of state and phase transitions of zinc is necessary for numerical simulations of hydrodynamic processes in this material under intense pulsed influences [1]. In the present work, a semiempirical approach [2] is used for constructing the thermodynamic potential Helmholtz free energy for zinc with taking into account melting, evaporation and ionization effects. The multiphase equation of state is built, and calculations of parameters of the phase diagram in a wide range of densities and temperatures are carried out. A comparison of calculated results with available data from dynamic experiments with Zn in shock and release waves is made.
The work is supported by the Russian Science Foundation, grant No. 14-50-00124.

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DFT-WPMD method for nonideal plasma and warm dense matter simulations.

Lavrinenko Ya.S.[1,2], Morozov I.V.[1,2], Valuev I.A.[1]
[1]*Joint Institute for High Temperatures of the Russian Academy of Sciences, RUSSIA*
[2]*Moscow Institute of Physics and Technology (State University), RUSSIA*

A combination of Density Functional [1] and Wave Packet Molecular Dynamics (WPMD) [2-5] methods is proposed to simulate the thermodynamics and the electronic dynamical properties of non-ideal plasmas and warm dense matter. In this approach we use the non-antisymmetrized single Gaussian wave packets to represent electrons and point-like particles for ions. The kinetic and electrostatic energy contributions for electrons are calculated within the WPMD model, whereas the exchange-correlation energy and its derivatives with respect to the dynamic variables is evaluated on a space mesh. Constraining boundary conditions with a harmonic wall potential are used for wave packets to prevent wavepacket spreading [6].

Although more computationally demanding than the original WPMD method, the proposed technique allows one to account for both exchange and correlation effects within the non-adiabatic approach. The use of GPU acceleration for computing the exchange-correlation energy contribution turns to be quite effective and compensates the extra computational costs.

In this work we benchmark the DFT-WPMD with the basic local spin density approximation with (LSDA) exchange-correlation functional against test systems (homogenous electron gas, atomic and molecular hydrogen) and the nonideal hydrogen plasma in the temperature range of $T = 2 \times 10^4$–5×10^5 K and the nonideality parameter values $\Gamma = 0.01$–6. The results are compared with the classical molecular dynamics, the original wave packet molecular dynamics (WPMD) including the version with antisymmetrized wave packets [2] and the Path Integral Monte Carlo (PIMC) [7] methods.

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Path Integral Monte Carlo and Density Functional Molecular Dynamics Simulations of Warm Dense Plastic, Oxygen, Sodium, and Aluminum

F. Soubiran[1,2], K. P. Driver[2,3], S. Zhang[2,3], B. Militzer[2,4]

[1] *LGLTPE - ENS de Lyon, Lyon, FRANCE*

[2] *Earth and planetary science department, University of California, Berkeley, USA*

[3] *Lawrence Livermore National Laboratory, Livermore, USA*

[4] *Astronomy department, University of California, Berkeley, USA*

Theoretical studies of warm dense matter and plasmas are a key to improving our knowledge of astrophysical objects - such as stars, white dwarfs and planets - shock physics and new plasma energy technologies - such as inertial confinement fusion. Recent developments in path integral Monte Carlo (PIMC) allowed to study heavier elements and to reach lower temperatures by improving the Fermion nodal structure. Combined with density functional theory molecular dynamics (DFT-MD) it is now possible to derive accurate equations of state and electronic structure properties for a variety of materials over a wide range of pressure-temperature conditions. Here we report our results for a set of CH-plastic materials, oxygen, sodium, and aluminum. We derive the equation of state, the pair-correlation function, the electronic density of states and the shock Hugoniot curves. We analyze the ionization of L and K shell electrons as well as relativistic and radiation effects. We conclude by discussing common trends and differences between the materials under consideration.

Equation of state studies of High Energy Density Matter using intense ion beams at the FAIR facility at Darmstadt

N.A. Tahir[1], P. Neumayer[1], I.V. Lomonosov[2], A. Shutov[2], A.R. Piriz[3], V. Bagnoud[1] and C. Deutsch[4]

[1]GSI Darmstadt, Germany
[2]IPCP Chernogolovka, Russia
[3]UCLM, Ciudad Real, Spain
[4]LPGP, University of Paris-Sud, Orsay, France

High Energy Density (HED) physics is important as it involves numerous branches of basic and applied physics including astrophysics, planetary physics, inertial fusion, strongly coupled plasmas and many others. Experimental studies of the Equation of State (EOS) and transport properties of HED matter is an active research area for the past many decades. Traditional method of generating HED matter in the laboratory mainly involves shock compression of matter. With the development of highly energetic, strongly bunched, well focused intense ion beams, a new method has been proposed that induces HED states in matter by uniform and isochoric heating of solid targets.

A powerful heavy ion synchrotron, SIS100 is being constructed at the Facility for Antiprotons and Ion Research [FAIR] at Darmstadt, which will deliver intense ion beams of all stable ion species from protons up to uranium. For the HED physics studies, uranium beam is most desirable as it deposits the highest specific energy. The design beam parameters include an intensity of 5×10^{11} uranium ions per bunch with bunch length of 70 – 100 ns. The transverse intensity distribution in the focal spot is considered to be Gaussian with full width at half maximum (FWHM) of 1 – 2 mm. It is to be noted that during the early stages of operation, the beam intensity will be lower (10^{11} ions per bunch).

To assess the potential of the FAIR facility to generate HED matter in the laboratory, we have carried out extensive simulation studies of beam-matter heating employing a 2D hydrodynamic code BIG2 using the above parameter range. These simulations have shown that the FAIR uranium beam will deposit enough specific power in the target to generate all interesting HED states including that of an expanded hot liquid, two-phase liquid-gas state, gaseous state, critical parameters and strongly coupled plasma phase. Several metallic targets have been considered. An experimental scheme named HIHEX (Heavy Ion Heating and Expansion), has been proposed to measure the EOS properties of HED matter using this technique. Determination of the EOS requires simultaneous measurement of density, temperature and pressure. In the HIHEX experiments, temperature will be measured by using an optical pyrometer, the pressure will be measured using laser interferometry while the density will be measured using the x-ray shadowgraphic technique.

Thermodynamic properties of C-N-O-H mixture in the region of non-ideal plasma

A.A. Rykounov[1], M.A. Vorobyeva[1]

[1]Russian Federal Nuclear Center – All-Russian Research Institute of Technical Physics, Snezhinsk, Russia (arykounov@gmail.com)

The atmosphere of giant planets in the Solar System, such as Uranus and Neptune, consists of mixed water, ammonia, and methane heated to the state of warm dense matter. All these compounds have rather complicated phase diagrams which include some exotic structures, e.g., super-ionic water. A physically consistent description of all interactions in such mixtures can only be attained from first principles. The non-empirical methods, such as quantum molecular dynamics (QMD), are however strongly limited both in the dimensions of systems which can be modeled, and in the times during which their evolution can be tracked. We try to tackle these problems by modifying the classical reaction potential ReaxFF [1] on the basis of the pair correlations functions obtained in QMD calculations. Here we investigate how the calculated thermodynamic properties of mixed carbon, nitrogen, oxygen and hydrogen depend on ReaxFF parameters for systems of several tens of thousands atoms, and do comparisons with similar results obtained from first principles for much smaller systems.

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Absorption and fluorescence spectroscopy of a nanodusty plasma

E. von Wahl[1], S. Iséni[1], T. Lecas[1], T. Gibert[1], S. Tsikata[2], S. Mazouffre[2], M. Mikikian[1]

[1] *GREMI, UMR7344, CNRS/Université d'Orléans, F-45067 Orléans, FRANCE*
[2] *ICARE, UPR3021, CNRS, F-45071 Orléans, FRANCE*

Nanoparticles can be easily produced in typical low-pressure plasmas, either by injecting reactive gases or by sputtering materials deposited on the electrodes. In these cases, a dense nanoparticle cloud is obtained and fills most of the plasma volume. As nanoparticles attach plasma free electrons, a huge nanoparticle density induces a strong disturbance of the plasma properties and stability. It can give rise to a wide variety of low-frequency instabilities and to the appearance of a void region, usually located in the plasma center (Fig. 1), and characterized by an enhanced light emission [1].

In this contribution, laser absorption and laser induced fluorescence are used to evidence the effects of nanoparticle growth on argon metastable atoms. These non-intrusive laser techniques have recently shown their ability to reveal the strong plasma modification as nanoparticles are grown thanks to acetylene addition [2,3]. In the present work, nanoparticles are grown from the sputtering of a carbonaceous layer deposited on the electrodes. The obtained dense nanoparticle cloud can be easily observed with laser light scattering. Absorption and fluorescence profiles are analyzed with a particular attention on spatially dependent effects related to void formation and nanoparticle cloud instabilities.

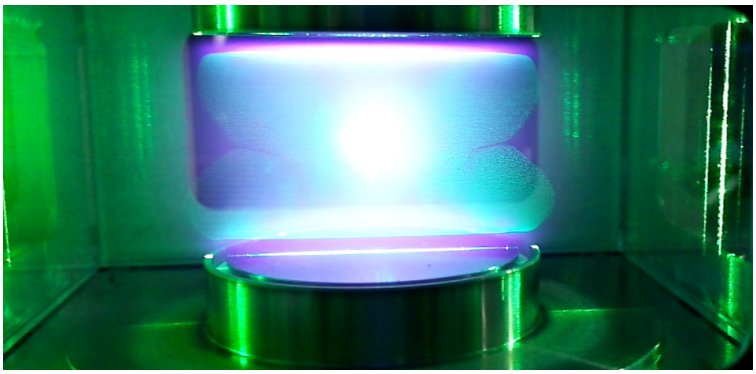

Fig. 1. Nanoparticle cloud illuminated by a green laser and trapped in the plasma volume. The central void is evidenced as a region of enhanced emission

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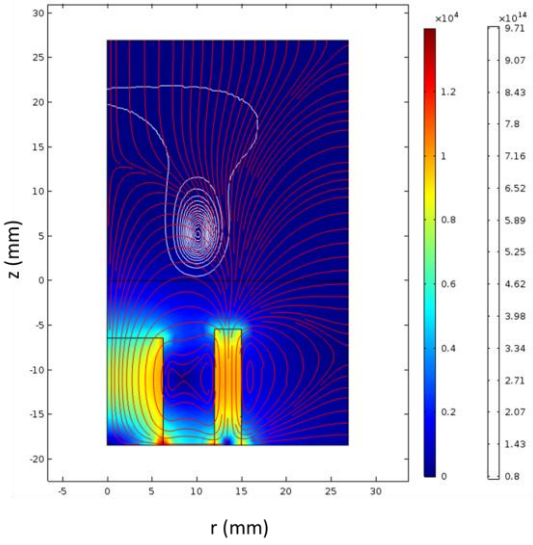
Simulation of a magnetron discharge using CFD.

Sotheara CHUON[1], Jean-Marc BAUCHIRE[1], Pascal BRAULT[1], Erik C. NEYTS[2]

[1] *GREMI UMR7344 CNRS, Orléans, 45067, France*
[2] *PLASMANT, Antwerp, 2610, Belgium*

Nowadays, sputtering deposition is employed for coating synthesis in several domains (i.e. mechanic, optic, electronic…) [1]. To better understand discharge phenomena, numerical simulations associated with experimental results appear as a reliable tool. Different models with analytic, continuum or fluid, particle and hybrid approach can be used [2-4]. Among those, Particle-In-Cell/Monte Carlo Collision (PIC-MCC) is the most common despite a large computing time.
In this work, a Computational Fluid Dynamics (CFD) study using COMSOL Multiphysics®, based on the theoretical model from Costin *et al* [5], is performed. A DC magnetron discharge is simulated in a region close to the cylindrical symmetric target. This model allows the description of the magnetron discharge parameters as the magnetic field, the electric potential, the electrons and ions densities and mean energy. The transport of the electrons and the positive ions is described by the first three moments of the Boltzmann equation: continuity, momentum transfer and mean energy transfer (only for electrons), coupled with the Poisson equation. The coupling with the magnetic field requires some assumptions: classical drift-diffusion expression are used for flux and an effective electric field is considered for ions.
The results obtained will then be coupled, in further work, with Molecular Dynamic (MD) simulations [6-7] applied to the target and the deposition process in order to build a multi-scale approach of the magnetron sputtering process.



Representation of the calculated magnetic flux density (Gauss) and electron density levels in white (m^{-3})

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Band Occupation and Optical Response of Gold far from Equilibrium

P.D. Ndione[1], S.T. Weber[1], B. Rethfeld[1], D.O. Gericke[2]

[1] *Fachbereich Physik, Technische Universität Kaiserslautern, Germany*
[2] *CFSA, Department of Physics, University of Warwick, UK*

The excitation of metals with short-pulse lasers is an often applied method to create warm dense matter states. Here, the large energy input drives the electronic system far out of equilibrium. The subsequent relaxation processes reveal many properties of the system but also strongly influence the outcome of any measurement within the relaxation time. In particular, the optical response depends strongly on the occupation of electronic states within the bands, the number of electrons per band as well as the response of the ionic lattice/ion fluid.

Here, we investigate the behaviour of gold after excitation with very short pulses of visible and VUV light that promote additional electrons into the sp-band. Within the first few 100 femtoseconds, we can assume a stable lattice and thus keep the known band structure in our calculations. First we demonstrate that the number of electrons per band is sufficient to describe probing in the optical limit (k->0). Then we present a system of rate equations that describes this band occupation. For excitations with optical lasers, only d-electrons can be promoted into the sp-band and a two-band model is sufficient. With VUV light like from the FLASH laser at DESY, f-electrons can also be excited and we need a three-band model to describe the band occupation. We show similarities and differences of the two excitation methods. Based on these predictions for the band occupation, we are able to calculate the optical properties, like the reflectivity, of the probe and make predictions of their expected behaviour for time-resolved measurements.

Electrical conductivity of the dense nonideal plasma on the basis of the effective potential

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

[1]IETP, Department of Physics, al-Farabi KazNU, al-Farabi 71, 050040 Almaty, Kazakhstan
[2]Institute of Physics, University of Rostock, A.-Einstein-Str. 23-24, 18059 Rostock, Germany

During the last few years many papers about the transport properties of dense plasmas have been published. The electrical conductivity in fully and partially ionized hydrogen plasma is well investigated [1-3]. Various experiments have been performed in order to measure the electrical conductivity of helium [4], neon [5], argon [4–5], krypton [6], and xenon [4-5]. In this work we consider the electrical conductivity of partially ionized plasmas, which is determined by the scattering of free electrons on electrons, ions and atoms. Therefore, we have to take into account formation, decay and excitation of bound states in two particle collisions. The conductivity have been investigated on the basis of the effective potential approach [7]. The quantum mechanical method of phase functions in connection with the Born approximation has been used for our calculations. The results are compared with data of other theoretical and experimental works.

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First Born approximation in plasma transport properties description

V.S. Karakhtanov

Institute of Problems of Chemical Physics RAS, Chernogolovka, RUSSIA

The quantum statistical approach to the description of plasma transport properties is analyzed. The consideration basis is the linear response theory in the formulation of Zubarev, the Lenard-Balescu-type collision integrals with dynamical screening of Coulomb interaction.
It is pointed out that in the perturbation theory, started from the Hamiltonian of non-interacting particles, approximations beyond the first Born one are not self-consistent. This leads to the suggestion of the better suitability of the chemical model of plasma, where atoms and molecules with previously determined concentrations are included in Hamiltonian on equal terms with electrons and ions from the very beginning.
Conditions for restrictions with the first Born approximation are formulated.

Transport Properties of Asymmetric Mixtures

C. Ticknor[1], A.J. White[1], E.R. Meyer[1], O. Certik[1], J.D. Kress[1], L.A. Collins[1], J. Clerouin[2], Ph. Arnault[2], N. Desbiens[2]
[1]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
[2] CEA, DAM, DIF, 91297, Arpajon, FRANCE

ABSTRACT

We have explored a variety of warm dense matter (WDM) and hot plasma systems with a quantum molecular dynamics (QMD) approach. In the QMD, we solve the many-body Schrodinger equation for a large, representative sample of atoms, periodically replicated through space to effect the characteristics of a fluid, which may include a mix of atoms, molecules, ions, and free electrons. For the electrons, we employ density-functional theory (DFT) in two guises: an orbital-based in the Kohn-Sham (KS) form and an orbital-free (OF), usually in a Thomas-Fermi-Dirac approximation. This dual capability permits thorough coverage of these extreme conditions and provides a set of consistent static, dynamic, and optical properties such as equation of state (EOS), mass transport (viscosity/diffusion), opacity, and conductivity (thermal/electrical).

This versatility has permitted applications to a diverse range of environments including planetary interiors of ice-giant solar and exosolar planets, ICF capsules, and material interfaces, which span densities from solid to hundreds of times compressed and temperatures from a few to 1000 eV. A few examples serve to illustrate this breadth. First, the ice-giant planetary interiors comprise a complex fluid mixture of ammonia, methane, and water that can support very complex chemical reactions yielding a variety of interesting structures such as superionic states and large carbon clusters [1]. Second, simulations in the ICF regime have examined deuterium, polystyrene (CH), silicon [2], and beryllium as well as their mixtures; the resulting properties have been introduced “in-line“ within hydrodynamics programs. The third application involves highly asymmetric mixtures [3] such as H paired with several heavy components ranging from Li to Ag as well as ternary systems such as H-C-Ag and Li-D-U. We have found that certain properties, most notably viscosity, show a strong sensitive to small amounts of the heavy species. Such cases require large-scale simulations and large computational investments.

We present mass transport coefficients for a variety of binary and ternary mixtures from weakly (D-Li-C) to highly [H-C-Ag] asymmetric in the mass concentrations over a broad range of temperatures and densities from QMD simulations in both the OF and KS formulations. The results are compared with various approximations such as the Darken, with classical MD simulations using model potentials such as the Yukawa, and with integrated models such as pseudo-ion in jellium.

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Influence of a charge-gradient force on dust acoustic waves.

Alexey G. Khrapak[1], Sergey A. Khrapak[1, 2]

[1]Joint Institute for High Temperatures, Russian Academy of Sciences, Moscow, RUSSIA
[2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Weßling, Germany

In complex plasmas charged dust particles not only change the electron–ion composition and thus affect conventional wave modes (e.g., ion–acoustic waves), but also introduce new low-frequency modes associated with the microparticle motion, alter dissipation rates, give rise to instabilities, etc. Moreover, the particle charges vary in time and space, which results in important qualitative differences between complex plasmas and usual multicomponent plasmas. The focus of this work is on the influence of the plasma background and grain charge variability on linear waves in weakly coupled unmagnetized complex plasmas. In the long-wavelength limit these waves exhibit acoustic-like dispersion and are called "dust acoustic waves" (DAWs). The dispersion relation of DAWs for ideal isotropic complex plasmas was originally derived by Rao, Shukla, and Yu [1]. In complex plasma, different forces affect particle dynamics. One of these forces is the so-called "polarization" force, which was introduced by Hamaguchi and Farouki [2] and comes from the nonuniformity of the plasma background. The grain charge variability may result in the appearance of an additional component of this polarization force. Actually, the energy of an individual test charge Q immersed in an ideal plasma is $U = -Q^2/2\lambda_D$. The total force acting on a small charged grain in a nonuniform plasma with external electric field $\mathbf{E}$ is $\mathbf{F} = Q\mathbf{E} - \boldsymbol{\nabla}U$. The "gradient" force can be written as

$$F_g = -\boldsymbol{\nabla}U = F_{pol} + F_Q = -\frac{Q^2}{2}\frac{\nabla\lambda_D}{\lambda_D^2} + \frac{Q\boldsymbol{\nabla}Q}{\lambda_D}.$$

F_{pol} corresponds to the conventional polarization force [2], influence of which on the dust acoustic waves was investigated earlier [3]. To determine the dispersion relation of the longitudinal DAWs, the system of forth differential equations (continuity, momentum, charging, and Boltzmann equations) has been solved. After linearization, we have obtained the long-wavelength dispersion relation of low-frequency DAWs of the form

$$\omega^2\left(1 + \frac{n_{d0}}{n_{i0}}\frac{J_0}{\Omega_{ch}}\right) = \omega_d^2\lambda_D^2k^2\left(1 + \mathcal{R}_{pol} + \mathcal{R}_Q\right),\ \ \mathcal{R}_{pol} = \frac{Qe}{4\lambda_D T_i},\ \ \mathcal{R}_Q = \frac{J_0e^2}{\lambda_D\Omega_{ch}T_i},$$

where J_0 is the flux of electrons/ions that the particle collects, Ω_{ch} is the charging frequency, and other parameters are conventional. The effect of the charge-gradient force is expressed by the term $\mathcal{R}_Q$. This term is positive (unlike $\mathcal{R}_{pol}$) and thus, it reduces the effect associated with the polarization force. For typical gas discharge conditions the relation between Ω_{ch} and J_0 (within the collisionless OML theory and under the assumption $T_e \gg T_i$) is

$$\Omega_{ch} \cong J_0\frac{1+z}{z}\frac{e^2}{aT_e}, \quad z = \frac{|Q|e}{aT_e}.$$

The relative importance of polarization and charge gradient force is $\left|\mathcal{R}_{pol}/\mathcal{R}_Q\right| \cong (1+z)/4$. As typical values of z according to the OML are $\cong (2 \div 4)$, these two components of the gradient force are of comparable magnitude and needs to be taken into account simultaneously.

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Coulomb crystals with polarized electron background

Kozhberov A. A.[1]

[1]*Ioffe Institute, Saint Petersburg, RUSSIA*

The model of a Coulomb crystal: point like atomic nuclei and electrons background is used in astrophysics in theory of neutron stars and white dwarfs. Polarizability of electrons in a Coulomb crystal is usually described by the Thomas-Fermi formalism (ex., [1]). It is shown that in this approach the model of a Coulomb crystal is similar to the strongly-coupled Yukawa system which was described in [2]. The only difference is that in astrophysical applications electrons are thought to be degenerated while in Hamaguchi and Farouki model — nondegenerated (this only leads to $\kappa^2 \equiv 4\pi e^2 \partial n_e / \partial \mu_e$ changes while equations for electrostatic and total free energies as function of κ and Γ stay the same). Hence, far from the melting point structural transition between bcc and fcc Yukawa lattices could be described analytically by the simple harmonic approximation. Importance of corrections $\propto \kappa^4$ to the Yukawa potential in this approach is discussed. In particular, it is shown that these corrections could noticeably change the structural diagram of Yukawa systems and transition between fcc and hcp lattices could appears. Analytical equations also allows to consider low temperature effects (results received in [2] are valid at $T \gg T_p$, where T_p is plasma temperature) and influence of the magnetic field.

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Electron-ion relaxation in Al nanoparticles: non-adiabatic wave packet molecular dynamics

Orekhov N. D.[1], Chernyshov A.I. [2,1], Stegailov V. V.[2,1]

[1]*Moscow Institute of Physics and Technology, RUSSIA*
[2]*Joint Institute for High Temperatures of the Russian Academy of Sciences, RUSSIA*

Fast progress in nanoplasmonics determined strict requirements for the synthesis of nanoparticles with specified geometrical properties. Reshaping under femtosecond laser pulses has become a promising technique for such task [1]. Ultrashort laser impulses of high intensity excite electron subsystem which then transfers energy to ions via electron-ion relaxation and transforms the nanoparticle into so-called warm-dense matter state (WDM). WDM remains the subject of great scientific interest from both experimental and theoretical point of view.

Here by means of eFF potential [2,3] we apply non-adiabatic wave packet molecular dynamics (WPMD) approach to calculate the structural evolution of fs-laser irradiated aluminum nanoparticles during the first picoseconds after irradiation. The eFF potential provides the combination of particle dynamics for ions with wave packet dynamics representing electrons as floating Gaussians. Unlike the more complex antisymmetrized approximation [4], interactions between electrons in the eFF model are restricted to pairwise components only and the total energy of the system is evaluated as in classical force field methods. eFF does not utilize Born-Oppenheimer approximation allowing us to model structural properties and non-adiabatic electron dynamics, such as electron-ion relaxation, within a single framework. Our results demonstrate a significant influence of the electronic pressure [5] on the processes of thermalization, melting and acoustic vibrations launching in metal nanoparticles under fs-laser irradiation.

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Surface modification of MF-R particles in a stratified glow discharge in neon

Karasev V.Yu., Dzlieva E.S., Pavlov S.I., Gorbenko A.P., Polischuk V.A.

Saint Petersburg State University, 199034, Universitetskaya nab., 7/9, St. Petersburg, e-mail: v.karasev@spbu.ru, RUSSIA

Complex plasma as in radio frequency discharge, as in stratified glow discharge is an extremely interesting object of experimental and theoretical studying. Surface modification of polymer microparticles (spherical particles with diameters in the micrometer range) in dusty plasma is now becoming an important area of these researches also new applications of plasma-processed dust particles are emerging [1,2].

Changing in surface structure of MF-R spherical particles (11.6 ± 0.4 μm in diameter with a density of 1.5 g/cm^3) in the positive column of a direct current gas discharge (Ne, p=25 ±5 Pa, i = 2.1 ± 0.2 mA) in a cylindrical glass tube has been studied experimentally. Also the change of the microparticles diameter (before their complete degradation) depending on the residence time of particles in the dusty plasma was established. Melamine formaldehyde microparticles were injected into a vertically disposed discharge tube fell into the traps, localized in the region of the striations [3,4]. The particles in the traps were exposed to dusty plasma for a predetermined time. An analysis of the modification of microspheres was carried out using the Merlin Zeiss scanning electron microscope. When processing the 2D imaging with nanometer resolution, we used the Smart Tiff (ZEISS) and the Gwyddion (software for analyzing the height fields and images). Experiments show that surface of polymer particles were heated to a melting point (350°C) which is much higher than the neon plasma temperature. The flow of ions bombarding the particles warmed their surface and affected its texture. After 40 min of plasma exposure, the particles completely degenerated by losing their spherical shape and about half of their mass.

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Nonlinear vertical oscillations of a single dust particle in a stratified glow discharge.

Alexandra Kartasheva[1], Yuri Golubovskii, Victor Karasev.

[1]*Saint Petersburg State University (SPBU), Saint-Petersburg , RUSSIA*

The nonlinear forced oscillations of a single dust particle trapped in a standing striation are investigated. The method of the discharge current modulation [1] is used to obtain the multi-resonance curves at pressures p=0.06 and p=0.16 torr. The frequency responses are investigated depending on value of the modulation depth. In this paper the parametric instabilities, which were previously observed under the conditions of rf discharge in papers [2,3], are investigated under in dc plasma. The amplitude-dependent frequency shift of resonance peaks, which is associated with values of the amplitude of the driving force, is experimentally obtained. The detailed measurements of the amplitude-frequency characteristic near resonances at the fundamental and doubled frequencies make it possible to detect the vibrational hysteresis.
The theory of the anharmonic oscillator provides a good quantitative description of the experimental data. The value of the eigenfrequency is determined and the obtained value is compared with the value experimentally obtained in the similar conditions of the dc glow discharge in [4]. The values of the thresholds of excitation of parametric instabilities, the anharmonic coefficients and the critical values of the oscillation amplitude for the hysteresis were calculated.

Acknowledgements
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The vibrational properties of the dust trap created in standing striation

Alexandra Kartasheva[1], Yuri Golubovskii, Victor Karasev.

[1]*Saint Petersburg State University (SPBU), Saint-Petersburg , RUSSIA*

Complex (dusty) plasmas have recently attracted the attention of researchers as systems available for observation at the kinetic level and have been studied in many aspects, such as phase transitions, waves, response to different external influences, and instabilities [1]. The investigation of free and forced oscillations of dust particles is important for understanding the dynamics of dusty plasma. For example, the investigation of the oscillatory motion of the dust particles can be used to study the phenomena of energy transfer between degrees of freedom in a plasma-dust system. In addition, the experimental investigations of the dust particle oscillations make it possible to determine the charge of a dust particle [3] and to measure the spatial distribution of the electric field [4].
In this paper, the method of the discharge current modulation [5], was used to investigate the vibrational properties of the dust trap in a stratum. Amplitude-frequency characteristics depending on pressure are measured. The resonance frequency, the logarithmic decrement and the amplitude of resonance peak are determined. In order to obtain the value of eigenfrequency the measurement of the phase shift of the forced dust particle oscillations and the investigation of the velocity resonance are carried out. The calculation of the dust particle charge with the help of eigenfrequency is made.
The quantitative description of the resonance behaviour of the dust particle based on the theory of the forced harmonic oscillator was made. The Q-factor of dusty plasma system is measured for the first time and the obtained value is compared with Q-factors of dusty plasma oscillatory systems previously investigated in rf plasma.

Acknowledgements
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Transport coefficients of Dense Helium Plasmas

S.K. Kodanova, T.S. Ramazanov, M.K. Issanova and Zh.A. Moldabekov

IETP, Al-Farabi Kazakh National University, Almaty, KAZAKHSTAN

The study of a dense plasma with helium ions and atoms is a great importance for the inertial confinement fusion (ICF) and astrophysics [1–2]. Experimental investigations of helium under extreme conditions include shock compression [3–4] and laser heating [5].

Accurate values of the transport coefficients of high temperature dense plasmas are necessary input data for the reliable numerical simulation of thermal plasmas. Therefore, in this work we present the results of calculations of the viscosity, diffusion, thermal conductivity, and electrical conductivity of helium plasma at high temperatures. Transport properties are studied on the basis of screened pair interaction potentials using the Coulomb logarithm [6-7]. In the case of a singly-ionized helium, the pair interaction potential between an atom and a proton during the elastic collision is considered as a sum of attractive and repulsive terms [8-9]. The former is the result of the polarization and the latter is due to a Coulomb repulsion of nucleus. A screening by free electrons is taken into account using the quantum polarization function in the random phase approximation. Further, this pair potential was used for the calculation of the Coulomb logarithm. To show the correctness of the model, its results are compared with the results of QMD and OFMD simulations.

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The effect of pulsed RF discharge on complex plasma parameters

S.K. Kodanova[1], A.U. Utegenov[1], N.Kh. Bastykova[1], J. Lin[2], K. Takahashi[2], M.K. Dosbolayev[1], T.S. Ramazanov[1]

[1]IETP, Al-Farabi Kazakh National University, Almaty, KAZAKHSTAN

[2]Kyoto Institute of Technology, Kyoto, JAPAN

In this work experimental and simulation results of investigation of complex plasma parameters in continuous and pulsed RF discharge are presented. Pulsed discharges have a wide range of advantages, for instance, they affect the orbit of etching ions, reduce the damage of substrates, reduce the heating quantity of substrates, and save the source energy. Such RF discharges were used to deposit super hydrophobic coatings, which attracted the interest of many researchers and applicators [1-3].

In the experimental part of this work plasma parameters, such as axial distributions of electron temperature and ion density of plasma of the continuous and pulsed RF discharge were studied by probe diagnostics at different modulation frequencies and duty cycles. It was revealed that a decrease in the modulation frequency with 50% duty cycle of RF signal leads to the reduction of the electron temperature. The influence of the modulation frequency on the ion density is observed only at comparatively large values of pressure.

In the simulation part the continuous and pulsed RF discharge is described by the Particle-in-Cell simulation incorporating Monte Carlo treatment of collision processes (PIC/MCC) [4-5]. The pulsed RF discharge was found to result in a decreased electron temperature and plasma density. This is because, during one pulse period, the time of the pulsed RF discharge is shorter than the time of the continuous discharge, thus the plasma in the pulsed discharge obtains far less energy from the electric field.

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Nanoparticle formation from thin film sputtering: A complex dust cloud structure

E. von Wahl, T. Lecas, M. Mikikian

GREMI, UMR7344, CNRS/Université d'Orléans, F-45067 Orléans, FRANCE

Dense clouds of nanoparticles can be formed in typical capacitively-coupled radio-frequency discharges operating at low pressure, by sputtering thin films deposited on the electrodes. As the nanoparticle size, and thus mass, are small, gravity is not the dominant force and they can easily occupy most of the plasma volume except the sheathes (where the local electric field repels them) and the void, a dust-free region where the outwards ion flux pushes them away.

The void is a very intriguing structure at the origin of many complex phenomena. For example, it is a region where many instabilities are observed and where new generations of nanoparticles can grow following a cyclic process [1-5]. The void can grow in size evacuating all nanoparticles from the discharge before a new generation appears, or successive generations can rapidly succeed each other inside the void and coexist as shown in Fig. 1a. In this last case, clear empty spaces separate the different generations.

Most of the experiments reveal the presence of a single central void. Nevertheless, in a new reactor we observed the existence of two symmetric voids [6]. These voids can stay distinct (Fig. 1b) or merge and form a single one. In both situations, new generations of nanoparticles can emerge from these regions where conditions of fresh nanoparticle nucleation are fulfilled.

In this presentation we will show some particularities of the void formation and how successive generations of nanoparticles can emerge from this region.

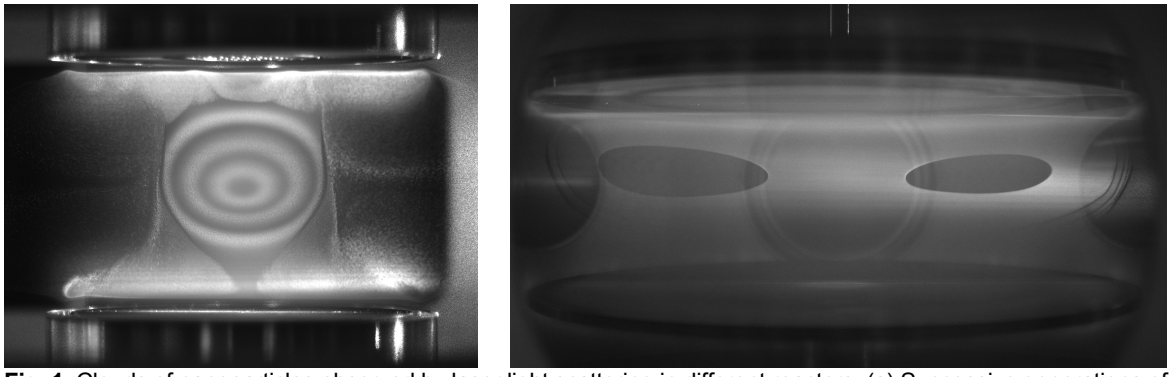

Fig. 1. Clouds of nanoparticles observed by laser light scattering in different reactors. (a) Successive generations of nanoparticles that rapidly succeed each other inside the void. (b) Cloud of nanoparticles with a clear two-void structure

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Thermodynamic approach to dust particles charge in plasmas

F. Kurbanov[1], Ye.S. Mukhametkarimov[1], A.E. Davletov[1]

[1]Al-Farabi Kazakh National University, Science Research Institute of Experimental and Theoretical Physics, Almaty, Kazakhstan

It is rather difficult to work out a unified theoretical approach to determining the charge of dust particles immersed in a plasma. This is explained from the standpoint that the charge of dust particles is governed by the state of ambient buffer plasma, whose parameters can span over a fairly wide range of their variation. For example, in the case of a sufficiently rarefied plasma, the orbital motion limited approximation is known to work well, whereas for a dense plasma one is obliged to apply macroscopic transport equations.
This report deals with an alternative approach based on the chemical model of dusty plasma [1] consisting of electrons, ions and dust particles. In particular, an expression for the free energy of the system is theoretically derived [2] and is then minimized as a function of the plasma constituents number densities, which makes it possible to evaluate the charge of dust particles under the quasi-neutrality condition.
The whole consideration starts from establishing the internal partition function of a dust particle that has absorbed a certain number of electrons. An insight is exploited that a single dust particle is a potential well for electrons, whose depth is determined by the work function of dust material, and after being charged the dust particle creates a macroscopic electric field that possesses a certain positive energy. Such an interpretation allows us to predict the existence of a maximum charge the dust particles can acquire in real experiments and which is determined by the work function of dust material and the dust grain size.
Numerical calculations of the charge of dust particles are performed in quite a broad domain of the plasma density and temperature, and a straightforward comparison is made with the orbital motion limited approximation. It is demonstrated that the proposed calculation scheme predicts larger charge values of dust grains as compared to the orbital motion limited approximation.

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Effect of nonthemal and trapped ions on dust acoustic waves

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Mohamed OUAZENE[1], Rabia AMOUR[2]

[1]Material physics Laboratory, Faculty of Physics, University of Bab-Ezzouar, USTHB, B.P. 32, El Alia, Algiers 16111, Algeria
[2]Theoretical Physics Laboratory, Faculty of Physics, University of Bab-Ezzouar, USTHB, B.P. 32, El Alia, Algiers 16111, Algeria

Abstract: Dusty plasmas are known to support a wide variety of low-frequency wave modes. The most well studied of such modes are the so called dust-acoustic wave (DAW) and dust ion-acoustic wave (DIAW) [1]. The aim of the present communication is to show the existence, formation, and possible realization of large amplitude nonlinear localized dust acoustic waves in dusty plasma with nonthermal trapped ions. These latter are modeled by a combined Cairns- Gurevich distribution function [2]. We show that the spatial patterns of dust acoustic solitary wave are significantly modified by the nonthermal and trapped effects.

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Observation of the dynamics of the dust structure formed in a dust trap in a double electric layer in a magnetic field up to 10000G.

S. I. Pavlov [1], V. Yu. Karasev, E. S. Dzlieva, L.A. Novikov, A.I. Eikhval'd,

[1]Saint Petersburg State University, 199034, Universitetskaya nab., 7/9, St. Petersburg, e-mail: s.i.pavlov@spbu.ru, RUSSIA

A study of dusty plasma in a glow discharge under the influence of a strong magnetic field is carried out. The magnetic field values above 3000 G, at which the magnetization of neon ions is achieved under our conditions, are of interest. For observation, a dust trap which does not change the position when the magnetic field changes was chosen.
There is a potential trap in the area of the change in the cross-section of the current channel formed by placing into the discharge tube a dielectric insert with special form for the stabilizing the discharge. In the literature this area is called a double electric layer or a low-voltage arc. It was found in [1] that in this area the dust trap is able to hold a ring shape structure with a large number of particles.
In this work the investigations of the dynamics of the dust structure, which levitating in a glow discharge in a dust trap in a double electric layer are presented. It has been found that the structure has the shape of a ring with its center coincident with the axis of the hole in the dielectric insert. In the external longitudinal magnetic field the dust particles are rotating. The value of the angular velocity of each particle is depended on the radius at which the particle is located. Earlier the observations of dust structures in this trap were carried out in magnetic fields up to 400 G [2]. In this paper, research in a magnetic field up to 10,000 G is presented. There is a sharp increase in the angular velocity of rotation of the dust structure with increasing magnetic induction. With a magnetic field of 3000 G, the angular velocity reaches 15 rad / s. With further increase of the magnetic field, the angular velocity remains constant.
Finally, we discuss the possible causes of the rotation of the dust particles such as the ion drag force and the effect of dragging by rotating gas owing to Ampere's force [3.4] in a longitudinal magnetic field.

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Dust plasma in the stratified discharge in moderate magnetic field

Pavlov S.I., Karasev V.Yu., Dzlieva E.S., Novikov L.A.

[1]Saint Petersburg State University, 199034, Universitetskaya nab., 7/9, St. Petersburg, e-mail: s.i.pavlov@spbu.ru, RUSSIA

An imposing of magnetic field gives new properties to dusty plasma. The Magnetic field effects on plasma components selectively (depending on the chosen range); it causes anisotropy of dust structure (it reduces cross diffusion and mobility); it creates heterogeneity and instability in the dust trap. A divide of rf discharge on separate vertical "threads" [1,2], an emergence of instability in the glow discharge [3] and also a change of properties of striations and emergence of "magnetic" striations are well known [4].
In our previous research [5] it was obtained for the first time the dusty plasma in the conditions of the glow discharge in magnetic field up to 1 T. In the present thesis we discuss in details the problems of the obtaining of steady dust structures in the trap in standing striation in the glow discharge at a partial magnetizing of the plasma component.
In the experiment the dusty plasma was created in striations in the long discharge tube placed in the magnetic field created by a superconducting magnet. The dynamics of rotation of dust structure at the chosen discharge parameters depending on magnetic induction is measured.
The action of the ion drag force on dust structure and also the action of kinetic and unstable effects of the gas discharge (eddy electric current and convective-current instability) are discussed in details.
The experimental measurements are carried out with the support of RSF grant № 18-12-00009; the calculation of the required parameters corresponding to a partial magnetizing of ions in moderate magnetic field is carried out with the support of the RFBR grant № 18-32-00130.

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The charging of dust particles in ionospheric plasma with non-Maxwellian electrons

K.E. Nurgaliyeva[1], T.S. Ramazanov[1], S.I.Popel [2]

[1]Al-Farabi Kazakh National University, IETP, Almaty, KAZAKHSTAN
[2]Space Research Institute of the RAS, Moscow, RUSSIA

The distribution function of electrons in non-equilibrium dusty ionosphere heated by high power radio waves [1] was investigated in this work. The electron current to the individual dust particle on the basis of kappa-distribution [2,3] was searched. It was shown that the intensity of electrons flux in non-equilibrium case could exceed the electrons current at stationary state for many times. Calculations was made for the ionospheric plasma at the heights of 85 km with temperature 150^0K and concentration of electrons and ions about 10^{10} m^{-3}. The frequency of ions is about 10^5 s^{-1}. The dusty particles assumed of one size are about 10 nm. As far as OML theory couldn't be used for simulation of dust particles charging in this case due to openness character of heating dust layer of mesosphere it was concluded that we need to develop the model of dusty particles charging which takes into account the non-equilibrium processes in considered problem.

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Brownian-like motion of a single dust grain in a radio-frequency plasma discharge – comparison of experiments and simulation

Milenko Rubin-Zuzic[1], Volodymyr Nosenko[1], Sergey Khrapak[1], and Hubertus Thomas[1]

[1]Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Institut für Materialphysik im Weltraum, Gruppe Komplexe Plasmen, Münchener Str. 20, 82234 Weßling, Germany

Bronwnian-like motion of a single dust-grain in a radio frequency plasma has been studied by different research groups. The rise of the particles temperature above “room temperature” is attributed to e.g. random fluctuations of the particle charge and fluctuations of the electrical field. Additional disturbance might occur due to gas density variations, temporal variation of the particles mass and particle interaction with the illuminating laser light. In addition, a non-optimal frame rate of the optical diagnostic system and pixel locking can lead to an incorrect estimation of the particle kinetic temperature.

Our experiments are conducted in a weakly ionized radio-frequency gas discharge at a low neutral gas pressure and power. A single micron sized spherical particle is trapped in a harmonic-like potential trap in the sheath of the lower driven electrode [1]. Its two-dimensional planar motion is recorded with a long-distance microscope and a high-resolution camera. From the measured particle positions we derive the probability density function, the velocity autocorrelation function and the mean squared displacement.

We obtain a particle kinetic temperature above 350 K, a neutral gas damping time of about 0.5 sec and a resonance frequency of 1-2 Hz. Anisotropic oscillation of the particle occurs, leading to angle dependent temperatures along the x and y direction in the plane of the recorded images, which can be explained by the presence of an asymmetric horizontal potential trap.

Experimental observations are compared with our simulations using the Ornstein-Uhlenbeck stochastic process.

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The influence of dust particle geometry on its charge and plasma potential.

G.I. Sukhinin[1], M.V. Salnikov[1], A.V. Fedoseev[1]

[1]*Institute of Thermophysics SB RAS, Lavrentyev Ave. 1, Novosibirsk, 630090, RUSSIA*

The problem of determining the distribution of a potential around a dust particle has been investigated for a long time. Most articles on the topic are devoted exclusively to spherical dust particles [1], relatively few to rod-like particles [2, 3] and none to disk-like particles. In this work, a recently developed [4] self-consistent iterative molecular dynamic method for determining plasma parameters is demonstrated for different dust particle geometries. The charge of a dust particle is calculated from the equality of ion and electron fluxes on its surface. It is shown that in the case of collisionless plasma the charge of dust particles is determined only by their electric capacity, but in the case of a continuous medium (collisions are frequent) these charges differ – the larger the particles, the larger the charges (Fig .1). And yet, particles with different geometries but with the same electric capacity obtain the same charge values.

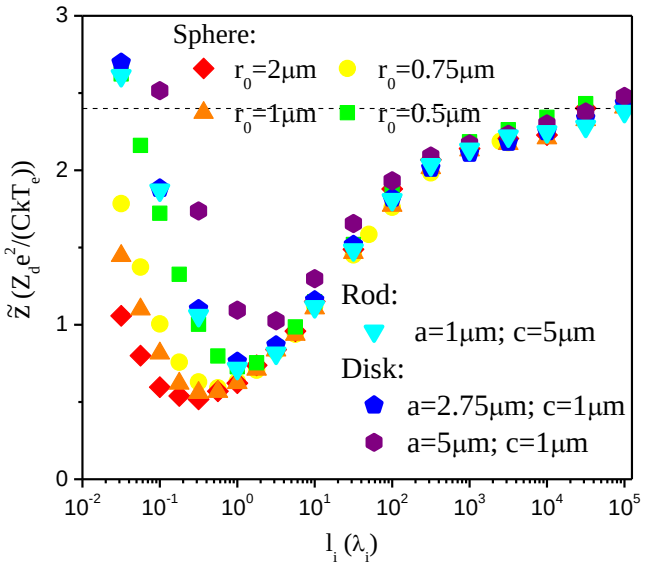

Fig.1. Dependence of a dust particle charge normalized to the capacity on ions mean free path.

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Isothermal compressibility of strongly coupled dust component with varying grain charge

L.T. Yerimbetova[1], A.E. Davletov[1]

[1]Al-Farabi Kazakh National University, Science Research Institute of Experimental and Theoretical Physics, Almaty, Kazakhstan

An effect of dust particle charge variation on wave phenomena in cold and ideal dusty plasmas was intensively investigated, see for instance [1,2], by incorporating the particle charging dynamics. It is argued in the sequel that such a detailed description is essentially unnecessary for dust acoustic waves because the recharging time in ordinary dusty plasmas is estimated to be much less in magnitude than the corresponding inversed frequency of dust acoustic waves, which actually implies that in the course of propagation dust grains are almost instantly recharged. Herein we are primarily interested in the strongly coupled regime in which the dust charge variation for dust acoustic waves must play much more significant role because the thermal pressure is predominated by the mutual interaction of likely charged dust grains. It has to be stressed that dust acoustic waves in strongly coupled dusty plasmas with varying grain charge were also studied in the literature [3,4] but, unfortunately, the isothermal compressibility of the dust component was calculated under the assumption of the constant grain charge. The present consideration is intended to amend this situation.
In order to correctly evaluate the isothermal compressibility of the dust component we propose to use an unconventional parametrization in which the dust particle charge is no longer an independent quantity and is determined by the ambient plasma characteristics as well as by the dust grain size and number density. To this end we start from the examination of the charging process and proceed to the evaluation of the thermodynamic properties of the strongly coupled dust component. The final goal pursued is to demonstrate that the isothermal compressibility accounts for the variation of dust grain charge, which has crucial influence on the dust acoustic waves spectrum in strongly coupled regime.

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The electric field of an electron in a electron-hole plasma with degenerate electrons. Formation of a superconductivity state.

S. P. Sadykova[1], A. A. Rukhadze[2]

[1]*Forschungszentrum Julich (Jlm.), Juelich, GERMANY*
[2]*Prokhorov General Physics Institute, RAS, Vavilov Str. 38., Moscow, 119991, RUSSIA*

We consider the conditions for formation of a superconductivity state either in a semiconductor or in a electron-hole plasma with the degenerate electrons due to the attractive forces between the electrons as a result of the exchange effects through the electron-hole sound wave by analogy to the phonon waves in a solid state. One of the major unsolved problems of the superconductivity theory is determination of the static potential of a point electron. We have determined the view of an interaction potential between two electrons in a degenerate electron-hole plasma (1) with non-degenerate holes. The potential appears to be attractive at distances large than the Debye radius and decreases as $1/r^3$, See Fig.(1). We discuss the conditions at which the bound electron state - Cooper Pair in a such field can be formed. The interaction potential of two electrons α and β in a electron-hole plasma can be described by the following equation [1]:

$$U(r)=\int e^{\imath \vec{k}\vec{r}} U(\vec{k})\, d\vec{k}\,,\ U(k)=\frac{e_\alpha e_\beta}{2\pi^2}\frac{1}{k^2\varepsilon^l(kV_\alpha,k)}, \tag{1}$$

where [2]

$$k^2\varepsilon^l(kV_\alpha,k)=k^2+\frac{3\,\omega_{L-}{}^2}{V_{F-}{}^2}-\frac{\omega_{L+}{}^2}{V_\alpha{}^2}+\imath\beta,\ \beta=3\pi\frac{V_\alpha\omega_{L-}{}^2}{V_{F-}{}^3}, \tag{2}$$

here V_α is the speed of a test electron with the charge e_α producing the potential ϕ_α at a point $r=0$ where the charge e_β is located; V_{F-} - the speed of a weakly damped electron-hole sound wave, $\omega_{L+,L-}$ - the hole and electron Langmuir frequencies.

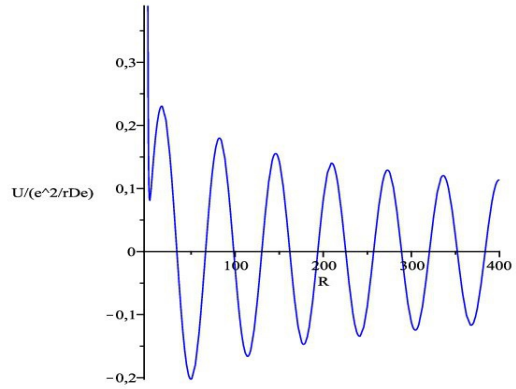

Figure1. The potential (1) where the integration till the $k\le 1/r_{Di}$ was performed, here $R=r/r_{De}$

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The effective potential for the ion-ion interaction of a dense plasma

M.T. Gabdullin[1,2], Zh.Y.Otarbay[1,3], T.S. Ramazanov[1,3], Zh.A.Moldabekov[1,3]

[1]al-Farabi Kazakh National University, Institute of Experimental and Theoretical Physics (IETP), al-Farabi str., 71, Almaty, 050040, KAZAKHSTAN
[2]Kazakh-British Technical University, Tole bi str., 59, Almaty, 050000, KAZAKHSTAN
[3]Institute of applied physics and Information technologies, Shashkina 40, Almaty 050038, KAZAKHSTAN

A dense plasma is a plasma where the average interparticle distance is comparable to the thermal de Broglie wavelength of particles. In this work, a one-component plasma of classical ions with a degenerate electron Fermi gas is considered.. In a dense plasma, the probability of collisions of particles with the maximum approach is high, it becomes important to take into account the wave nature of the colliding particles, which is due to the quantum mechanical effects such as diffraction and symmetry. These effects at small distances can be taken into account in the micro-potential [1].
In order to obtain an analytical expression for the effective potential, the dielectric response function method was used, where the Deutsche potential taking into account the diffraction effect was used as the micro-potential in the first case. In the second case, the local empty core model [2] was used as a micro-potential to obtain the pseudopotential. Influence of core electrons can be considered through effective potential [3] which is modified at small distances and approaches Coulomb potential at large distances [4].

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PARTICIPANT MAILING LIST

Name		Email
Antonova	Tetyana	tetyana.antonova@dlr.de
Apfelbaum	Evgeny	apfel_e@mail.ru
Arnault	Philippe	philippe.arnault@cea.fr
Baggott	Rory	r.baggott@imperial.ac.uk
Bethkenhagen	Mandy	mandy.bethkenhagen@uni-rostock.de
Bonitz	Michael	bonitz@theo-physik.uni-kiel.de
Bornath	Thomas	thomas.bornath@uni-rostock.de
Brault	Pascal	pascal.brault@univ-orleans.fr
Bystryi	Roman	broman.meld@gmail.com
Caillabet	Laurent	laurent.caillabet@cea.fr
Calisti	Annette	annette.calisti@univ-amu.fr
Cangi	Attila	acangi@sandia.gov
Celliers	Peter	celliers1@llnl.gov
Chabrier	Gilles	gilles.chabrier@ens-lyon.fr
Clay	Raymond	rclay@sandia.gov
Clerouin	Jean	jean.clerouin@cea.fr
Dai	Jiayu	jydai@nudt.edu.cn
Debras	Florian	florian_debras@hotmail.com
Desbiens	Nicolas	nicolas.desbiens@cea.fr
Deutsch	Claude	claude.deutsch@u-psud.fr
Dubovtsev	Denis	denis.dubovcev@gmail.com
Dzhumagulova	Karlygash	dzhumagulova.karlygash@gmail.com
Fedorov	Ilya	ilya.d.fedorov@phystech.edu
Fedoseev	Alexander	fedoseev@itp.nsc.ru
Ferri	Sandrine	sandrine.ferri@univ-amu.fr
French	Martin	martin.french@uni-rostock.de
Gabdullin	Maratbek	gabdullin@physics.kz
Gericke	Dirk	D.Gericke@warwick.ac.uk
Gorelov	Vitaly	vitaly.gorelov@cea.fr
Groth	Simon	groth@theo-physik.uni-kiel.de
Inogamov	Nail	nailinogamov@gmail.com
Ismagambetova	Tomiris	ismagambetova@physics.kz
Jaupart	Etienne	etienne.jaupart@ens-lyon.fr
Kadatskiy	Maxim	makkad@yandex.ru
Karakhtanov	Valery	valera@chgnet.ru
Karasev	Viktor	kaviyur@gmail.com

Kartasheva	Alexandra	alexkartasheva@gmail.com
Kazandjian	Luc	luc.kazandjian@cea.fr
Khishchenko	Konstantin	konst@ihed.ras.ru
Khrapak	Sergey	Sergey.Khrapak@dlr.de
Kodanova	Sandugash	kodanova@physics.kz
Koenig	Michel	michel.koenig@polytechnique.edu
Kozhberov	Andrew	kozhberov@gmail.com
Kraeft	Wolf	wolf-dietrich.kraeft@uni-rostock.de
Kraus	Dominik	d.kraus@hzdr.de
Kurbanov	Farkhad	deguar12@gmail.com
Larder	Brett	brett.larder@physics.ox.ac.uk
Lavrinenko	Yaroslav	lavrinenko@phystech.edu
Levashov	Pavel	pasha@ihed.ras.ru
Li	Yongqiang	li_yq@nudt.edu.cn
Mann	Ingrid	ingrid.b.mann@uit.no
Marizy	Adrien	adrien.marizy@cea.fr
Martynova	Inna	martina1204@yandex.ru
Maynard	Gilles	gilles.maynard@u-psud.fr
Mehlhorn	Thomas	tom.mehlhorn@nrl.navy.mil
Mikikian	Maxime	maxime.mikikian@univ-orleans.fr
Mintsev	Victor	minvb@icp.ac.ru
Moldabekov	Zhandos	zhandos@physics.kz
Mukhamedryskyzy	Marzhan	mukhamedryskyzym@gmail.com
Muratov	Mukhit	mukhit.muratov@gmail.com
Nosenko	Volodymyr	V.Nosenko@dlr.de
Orekhov	Nikita	nikita.orekhov@gmail.com
Ouazene	Mohamed	ouaz_moh@yahoo.fr
Pavlov	Sergei	s.i.pavlov@spbu.ru
Pierleoni	Carlo	carlo.pierleoni@cea.fr
Ramazanov	Tlekkabul	ramazan@physics.kz
Ravasio	Alessandra	alessandra.ravasio@polytechnique.fr
Recoules	Vanina	vanina.recoules@cea.fr
Redmer	Ronald	ronald.redmer@uni-rostock.de
Reinholz	Heidi	heidi.reinholz@uni-rostock.de
Roepke	Gerd	gerd.roepke@uni-rostock.de
Rubin-Zuzic	Milenko	milenko.rubin-zuzic@dlr.de
Rykounov	Alexey	arykounov@gmail.com
Sadykova	Saltanat	saltanat.sadykova@googlemail.com
Saitov	Ilnur	saitovilnur@gmail.com
Sartan	Roman	r.sartan@gmail.com

Schöttler	Manuel	manuel.schoettler@uni-rostock.de
Smirnov	Nikolai	deldavis@mail.ru
Son	Eduard	son.eduard@gmail.com
Soubiran	François	francois.soubiran@ens-lyon.org
Stegailov	Vladimir	stegailov@gmail.com
Sukhinin	Gennadiy	sukhinin@itp.nsc.ru
Tahir	Naeem	n.tahir@gsi.de
Tkachenko	Igor M.	imtk@mat.upv.es
Townsend	Joshua	jptowns@sandia.gov
Valuev	Ilya	valuev@physik.hu-berlin.de
Vorberger	Jan	j.vorberger@hzdr.de
Vorobeva	Marina	m.a.vorobyova@mail.ru
Wang	Xiaowei	xiaowei.wang@aliyun.com
White	Alexander	alwhite@lanl.gov
Witte	Bastian B.L.	bastian.witte@uni-rostock.de
Yerimbetova	Lazzat	lyazzat.yerimbet.26@gmail.com
Zastrau	Ulf	ulf.zastrau@xfel.eu

	Sunday 23		Monday 24		Tuesday 25		Wednesday 26		Thursday 27		Friday 28
8:50			Welcome adress								
9:00	9:00										
9:00 9:10 9:20 9:30		I1_01	Chabrier Gilles	I2_01	Ravasio Alessandra	I3_01	Stegailov Vladimir	I4_01	Mann Ingrid	I5_01	Levashov Pavel
9:40 9:50		C1_01	Schoettler Manuel	C2_01	Celliers Peter	C3_01	Vorberger Jan	C4_01	Dzhumagulova Karlygash	C5_01	Tkachenko Igor
10:00 10:10		C1_02	Soubiran Francois	C2_02	Mintsev Victor	C3_02	Larder Brett	C4_02	Khrapak Sergey	C5_02	Tahir Naeem
10:20 10:30		C1_03	Debras Florian	C2_03	Mehlhorn Thomas	C3_03	Townsend Joshua	C4_03	Nosenko Vladimir	C5_03	Bonitz Michael
10:40-11:10			Break		Break		Break		Break		Break
11:10	11:10										
11:10 11:20 11:30		C1_04	*Pierleoni Carlo*	C2_04	*Zastrau Ulf*	I3_02	Groth Simon	I4_02	Inogamov Nail	C5_04	*White Alexander*
11:40 11:50		C1_05	Sartan Roman	C2_05	Karasev Viktor	C3_04	Ramazanov Tlekkabul	C4_04	Antonova Tetyana	C5_05	Cangi Attila
12:00 12:10		C1_06	Clay Raymond	C2_06	Brault Pascal	C3_05	Moldabekov Zhandos	C4_05	Bethkenhagen Mandy	C5_06	Dubovtsev Denis
12:20 12:30		C1_07	Kazandjian Luc								Conference closure
12:40-14:30			Lunch		lunch		Lunchbox		Lunch 12:30-14:30 PC Lunch		
14:30	14:30										
14:30 14:40 14:50 15:00		I1_02	Kraus Dominik	I2_02	Witte Bastian B. L.		Excursion to Mont Saint-Michel or City Tour	I4_03	Dai Jiayu		
15:10 15:20		C1_08	Redmer Ronald	C2_07	Baggott Rory			C4_06	Fedoseev Alexander		
15:30 15:40		C1_09	French Martin	C2_08	Bornath Thomas			C4_07	Muratov Mukhit		
15:50 16:00		C1_10	Saitov Ilnur	C2_09	Gericke Dirk			C4_08	Sukhinin Gennadiy		
16:10 16:20				C2_10	Reinholz Heidi			C4_09	Martynova Inna		
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17:00	17:00										
17:00 17:10		P1	POSTERS Session 1	C2_11	Roepke Gerd			P2	POSTERS Session 2		
17:20 17:30				C2_12	Arnault Philippe						
17:40 17:50				C2_13	Ferri Sandrine						
18:00 18:10	Get together drink						19:00-22:00 Dinner				
18:20											
18:30											