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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (13th Meeting of the A+M Data Centres and ALADDIN Network)

10-11 July 1995, IAEA Headquarters, Vienna

SUMMARY REPORT

Prepared By J. Botero

December, 1995

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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Abstract

The proceedings of the IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange (13th Meeting of A+M Data Centres and ALADDIN Network)", held on July 10-11, 1995, in Vienna is briefly described. The meeting conclusions and recommendations on the priorities in A+M data compilation, evaluation and generation and on the technical aspects of data processing and exchange are also presented.

Reproduced by the **IAEA** in Austria
December, 1995

TABLE OF CONTENTS

1 Introduction

On July 10-11, 1995, the IAEA organized the regular Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Exchange and Processing (13th Meeting of the Atomic and Molecular (A+M) Data Centres and ALADDIN Network)" with the objectives of reviewing the progress in the A+M data related activities in the data centres, the methods and procedures applied in the data processing and exchange, the developings in the ALADDIN system, and to co-ordinate the working plans for the next period. The meeting was attended by 14 participants and one observer from 12 data centres (**see Appendix 1**). The Troitsk Institute of Innovation and Fusion Research was represented for the first time at this series of Advisory Group Meetings.

2 Meeting Proceedings

The Meeting was opened by **Dr. R. K. Janev**, Head of the Atomic and Molecular Data Unit, RIPC. He stressed the necessity of strengthening the communication and collaboration among the data centres and the importance of having ALADDIN as the international format for data exchange.

After adopting the Agenda (**see Appendix 2**), the meeting proceeded in four sessions:

1. Current activities of the A+M data centres,
2. Priorities in A+M, Plasma-Material Interaction and Materials Data Compilation and Evaluation,
3. Data Processing and Exchange,
4. Meeting conclusions and recommendations.

2.1 Session 1: Current Activities of the A+M Data Centres (Chairmen: Drs. Abramov, Wiese, Tawara)

In Session 1, progress reports on the activities of individual data centres during the period September 1993- June 1995 were presented. These reports, which are reproduced in **Appendix 3**, describe the work of the data centres on A+M data compilation, evaluation and generation, the data centres publications during the reporting period, the status of ongoing programmes and the plans for immediate future work in this area. The presentations in this session have demonstrated that the data centre activities closely follow the recommendations of the previous Advisory Group Meeting, both in terms of content and mutual co-operation.

The session started with the presentations of **Dr. W. L. Wiese** (NIST) and **Dr. Tawara** (NIFS), who described the ongoing work on establishing A+M data bases in their respective centres. **Dr. Wiese** reported recent work on compilation and evaluation of data for wavelengths of Kr V-XXXVI; for energy levels of Zn, and Ga; and transition probabilities of the ions of C, N and O. Work in progress in his data centre includes data

compilation and evaluation for the wavelengths of Si I; the energy levels fo Si I and Ar; and the transition probabilities of H, D, He, Li, Be, B and Ne. **Dr. Tawara** from NIFS, Nagoya, reported on the recent A+M data compilation, evaluation and recommendation activities, which include: a new (revised) empirical formula for systematic calculations of sputtering yields from monatomic solids under ion impact; systematic calculations of excitation cross sections of excited helium atoms by electron impact; a semi-empirical formula for multiple ionization of atoms and ions by electron impact; new cross sections, based on the close coupling method, for excitation, ionization and electron transfer in highly charged ions collisions with H; quantum mechanical calculations of heavy particle collisions involving molecules in vibrational excited states relevant to divertor physics; developments of collisional radiative models and development of data management systems.

The session continued with the presentation of **Dr. E. Mansky** from ORNL, CFADC. He reported on the continued bibliographic data compilation; the progress towards establishing on-line access to the bibliographic data base and ALADDIN formatted numerical A+M data bases through the World Wide Web; the implementation of ADAS (a suite of codes and data collection for extracting fundamental and derived atomic data and modelling radiating properties of atoms and ions in plasmas); efforts to provide theoretical cross sections and rate coefficients needed by fusion energy research and further develop theoretical techniques in electron- and heavy-particle-impact collisions (excitation, ionization, dielectronic recombination, charge transfer and elastic scattering). The report of the A+M activities at the Nuclear data center of the Japan Atomic Energy Research Institute was presented by **Dr. T. Shirai**. He reported ongoing work on the analytical fits to recommended cross sections in collisions with H, H_2, He and Li atoms and ions with atoms and molecules; the compilation of measured cross sections for particle rearrangement; calculations of total ionization cross sections of excited hydrogen atoms and hydrogenlike ions by bare ions; and critical evaluation of spectroscopic data of interest to fusion.

New developments on the GAPHYOR data base were reported by **Dr. J.L. Delcroix** (GAPHYOR, Orsey). The data base has been moved to a UNIX workstation, using the ADABAS software. Several new features and descriptors were reported.

The data activity of the A+M data centre at the Kurchatov Institute, Moscow, was presented by **Dr. V. A. Abramov**. The main activities reported were: collection of the A+M bibliography from Russian publications, compilation of cross sections for processes involving Ga, Be, C and B ions, calculations of the radiative cooling rates for Be-seeded plasmas, evaluation of excitation cross sections for different metallic ions, electron impact excitation cross sections of Be ions and hydrogen retention and release in carbon graphite materials. **Dr. Sun Yongsheng** presented the progress report of the A+M data activities at CRAAMD, Beijing. Compilation and ALADDIN formatting of cross sections for electron collisions with hydrogen molecules and molecular ions and for hydrogen atoms and ions were reported.

Dr. W. Eckstein (MIPP, Garching) reported on data production, collection and evaluation at MPIPP. The main area of the data activities at MPIPP are kinetic reflection and sputtering. Both types of data are being generated experimentally and by computer

simulation. Particle and energy reflection coefficients for a large number of projectile-target combinations over a wide rage of energies and angles were reported. Sputtering yield data for a large number of target-projectile combinations for normal and oblique incidence were also reported. A new analytical fit, the revised Bohdansky formula with the Yamamura factor for oblique incidence, was shown to give accurate sputtering yields over a wide range of energies and incident angles. The progress report on the A+M activities at the Chinese Nuclear Data Centre (Beijing) was presented by **Dr. Jinzhang Yao**. This activities include the evaluation and compilation of physical sputtering data of plasma facing materials by light projectiles H^+, D^+, T^+ and He^+; the generation and evaluation of particle reflection coefficients from solid surfaces and the calculation of radiative loss rates for plasma impurities with the modified corona model with metastable state effects. **Dr. E. Menapace** (ENEA NDC Data Unit, Bologna) reported on evaluation of molecular spectroscopic data obtained with algebraic methods; calculations of electron impact excitation cross sections of vibrationally excited molecules; and low energy interactions of protons with metal surfaces using the molecular dynamics approach.

At the end of this session **Dr. J. Botero** (IAEA, A+M Data Unit) presented the report of activities of the IAEA A+M Data Unit. The activities were divided into three areas: data base development, data evaluation and recommendation and co-ordinated research projects. In the first area, the establishment of AMDIS (Atomic and Molecular Data Information System) was reported. AMDIS currently contains an on-line service for ALADDIN, the IAEA Bibliographic Data Base and an electronic bulletin board. The efforts of the IAEA A+M Data Unit on data base development have been concentrated mainly on AMDIS. In the data evaluation and recommendation area, the following reports were presented: Atomic Collision Database for Lithium Beam Interaction with Fusion Plasmas; Particle Interchange Reactions Involving Plasma Impurity Ions and H_2, D_2 and HD; Particle-impact Induced Electron Ejection from Surfaces; Analytical Representation of Electron Impact Excitation Cross Sections of Vibrationally Excited H_2 and D_2 Molecules; Radiative Losses and Electron Cooling Rates of Hydrogen, Helium, Carbon and Oxygen; Material Properties Data Base (in progress); and Plasma-Surface Interaction Induced Erosion Data Base (in progress). Finally a summary of the current and planned co-ordinated research programmes on A+M, PSI and material properties data was presented.

At the end of the session, there was a demonstration of software by **Dr. Godunov** (Troitsk), **Dr. Mansky** (ORNL) and **Dr. Botero** (IAEA) in the NDS reference library (Room A23-40).

2.2 Session 2: Priorities in A+M, PSI and Materials Data Compilation and Evaluation (Chairman: Dr. Shirai)

Session 2 was dedicated to discussing the priorities in A+M, PSI and material properties data compilation and evaluation. The session started with a short presentation by **Dr. R. L. Langley** (IAEA A+M Data Unit), who presented a summary of the priorities of materials data generation and evaluation and the actions being taken by the IAEA A+M

Data Unit in those regards. It included the recommendations of recent IAEA meetings on the co-ordinated research programmes: "Plasma-Interaction Induced Erosion of Fusion Reactor Materials", "Collection and Evaluation of Reference Data on Thermomechanical Properties of Fusion Reactor Plasma Facing Materials" and "Tritium Retention in Fusion Reactor Plasma Facing Components".

Dr. R. K. Janev (IAEA A+M Data Unit) presented a report on the status of A+M data for ITER, (see **Appendix 4**). The priorities on A+M data evaluation have not change much with respect to those presented in 1993. Small shifts and extensions were presented, mainly resulting from the adopted dynamic gas target divertor concept for ITER. The priorities are summarized in Appendix 4.

After some discussion, the advisory group arrived at the conclusions and recommendations presented in Section 3.

2.3 Session 3: Data Processing and Exchange (Chairman: Dr. Delcroix)

This Session was devoted to a discussion on the ALADDIN implementation, developments and future DCN activities. There were open discussions on all points, with contributions from all meeting participants. The ALADDIN data format is recognized as the internationally adopted format for atomic, molecular, particle-surface interaction and material properties data exchange among data centres themselves and among data centres and the fusion community. The on-line services now available at the IAEA, Gaphyor and ORNL were regarded as very important, and it was agreed that efforts of the IAEA A+M Data Unit regarding data base management should be concentrated on this service. The need for enhancing the compilation of data was pointed out by **Dr. R. K. Janev** (IAEA).

The importance of the ALADDIN format for collaboration among different data centers was also stressed. These collaborative projects consist mainly of data processing, data distribution, and the preparation of special-purpose data bases.

It was agreed that all Data Centres would collaborate on a specific project: the stablishment of a collisional and spectroscopic database for Ne having all processes of Ne and its ions with electrons, protons, H, He, He^+ and He^{2+}. All participants agreed to consult with their respective Data Centre to define their contribution to the project.

It was agreed that a quarterly report from all data centres will be circulated by e-mail among all data centres to improve the communication and make collaboration easier.

3 Meeting Conclusion and Recommendations

The presentations and discussions at the Advisory Group meeting regarding the A+M, PSI and material properties data related activities in the A+M Data Centre Network and the IAEA A+M Data Unit, the data processing, management and exchange methodology, the ALADDIN system implementation and development, as well as regarding the priorities

in A+M data compilation and evaluation work, have resulted in the following sets of conclusions and recommendations:

3.1 Conclusions

3.2 Status of Data Compilation and Evaluation Activities

1. The present level of A+M data compilation activity in the areas of spectroscopic and A+M collisional data has to be extended to satisfy the increasing and evolving data needs of ITER. The insufficient manpower and the scarcity of funds may hinder this activity. On the other hand, apart from the members of the A+M Data Centre Network, this activity is being carried out also by individual experts in relation with Agency organized meetings on specific topics, as well as within several ongoing Agency's Co-ordinated Research Programmes.
2. The Advisory Group is of the opinion that the present level of the data evaluation effort in all areas, A+M collisional, PSI and material properties, data, is insufficient to respond to the growing needs of fusion research and reactor design work. The main reason for this is the lack of manpower and consultancy funds in the A+M Data Centre Network for data evaluation purposes. The IAEA experts' meetings, co-ordinated research programmes and individual consultants make a significant contribution to the data evaluation effort, but the size of this effort which is limited by the available Agency's resources, appears to be insufficient to change the situation. A stronger collaboration between the data centres should be beneficial in this respect. Enhancement of the evaluation activity, both in the A+M data centres and through the IAEA, is essential for meeting the A+M and PSI data needs of ITER EDA. Closer collaboration with the fusion community for identification of most urgently required data would also help in minimizing and better focussing the evaluation efforts.
3. The Advisory Group observes an increase of data generation activities in the A+M Data Centre Network. The strengthening of this effort, which strictly follows the demands of fusion researchers for A+M and PSI data, is highly encouraged.
4. The Advisory Group has agreed to start a project to establish a collisional and spectroscopic database for Ne within a time scale of one year.

3.3 Data Processing and Exchange (ALADDIN)

1. The implementation of ALADDIN in the data exchange among the A+M data centres can now be considered as well established. As for data base management, it seems more appropriate that each data centre develops its own system,

depending on the hardware and software available. Compatibility is guaranteed by the fact that all data centres have an interface of their own system to ALADDIN formatted data. A good example is the system established at Troitsk by **Dr. Godunov**.

2. In order to improve the communication and data exchange among data centres, a quarterly report on the data related activities from all data centres will be circulated by e-mail.
3. The Advisory Group concluded that the efforts on data compilation and ALADDIN formatting of data have to be strengthened.

3.4 Priorities in Data Compilation, Evaluation and Generation

The long-term priorities in A+M and PMI data compilation, evaluation and generation, were throughout reviewed during the IAEA Technical Committee Meeting on "A+M Data for Fusion Reactor Technology" held in October 12-16, 1992 in Cadarache, France (see IAEA Report INDC(NDS)-277 and "Atomic and Plasma-Material Interaction Processes in Controlled Thermonuclear Fusion", R . K. Janev and H. W. Drawin, editors, Elsevier Science Publishers B.V., Amsterdam, 1993). Based on this review, the recommendations of the 8th IFRC Subcommittee on A+M Data for Fusion, and on the finding of some recent IAEA experts mmeetings as well as on the discussions of this meeting, the Advisory Group adopted the following priorities in the A+M, PMI and material properties data compilation, evaluation and generation:

1. Atomic and Molecular
   (a) Spectroscopic Data
      i. Transition probabilities for the He-, Li-, Be-, B-like isoelectronic ions.
      ii. Energy levels, wavelengths, transition probabilities for low-q metallic ions, high-Z impurities (Ga, V, Mo, W) and for Kr, Si and Xe.
      iii. Updating and compilation of spectroscopic data bases for Be^{q+} and B^{q+} ions (including publication in the ORNL "Red book" series).
      iv Complete spectroscopic characterization of Ne-, Ar ions.
      v. Spectroscopic characterization of H_2 (H_2^*), H_2^+, H_3^+ and isotopic variants.
      vi. Impurity plasma edge molecules (CO, CO_2 and hydrocarbons).
   (b) Collisional Data for Plasma Edge Studies
   (Includes: neutral particle transport modelling and diagnostics, H-recycling, He-exhaust).
      i. Elastic and momentum transfer ion-neutral and neutral- neutral collisions in the energy range 1eV - 1keV/amu, involving H, H^+, He, He^+, He^{2+}, H_2 and H_2^+.

ii. Ro-vibrational excitation of H_2 and H_2^+ by electron and proton impact in the energy range from threshold to $\sim$ 500 eV.

iii Electronic excitation and ionization of vibrationally excited $H_2^*(v)$ and $H_2^+(v)$ in low-energy collisions with e, H and H^+ (including dissociative processes and information on energy distribution of reaction products).

iv. Inelastic collision processes of He, He^+ and He_2^+ with e, H, H^+, H_2, H_2^+ at low energies, including processes with excited H, He and H_2.

v. Completion of collisional data bases for Be, B and their ions (including collision processes of Be^{q+}, B^{q+} with electrons, and quasi-resonant processes of Be^{q+}, B^{q+} with H, He and H_2).

vi. Further development of the data bases for hydrocarbons (all processes with electrons and protons), H_2O and CO, and Be-, B-oxides and hydrides (including their ions).

vii. Collision processes of high-Z impurities (Ga, V, Mo, W) with e, H^+, H, H_2.

viii. Three-body processes among primary species and impurities

ix. Particle interchange reactions among primary species, C, O, metals and hydrocarbons.

(c) Radiative Plasma Cooling

i. Plasma core region

A. Electron impact processes (excitation, ionization, radiative and dielectronic recombination) of medium- and high-Z impurities (Ti, Ni, Cr, Fe, Mo, W, Ga, V) (Pertinent energy range: from a few keV to 30 keV).

B. Charge exchange collisions of A^{q+} (A as above) with H, H^+ and He_2^+ (Pertinent energy range: from 1 eV (or threshold) to 500 eV).

ii. Plasma edge region

A. Electron impact processes involving low-, medium- and high-Z impurities in low charge states ($q \geq 5$). The most important low-Z impurities are Be and B. (For C and O the data base is in good shape).

B. Collisions of A^{q+} ($q \geq 5$) with H, He, H_2, including state-selective electron capture

C. All processes of Ne, Ar and their ions with e, H, H^+, H_2, H_2^+, He, He^+, He_2^+ (for the proposed radiative cooling scheme of divertors).

2. Plasma-Material Interaction

(a) Physical sputtering: Data needed for: the threshold regime for self-sputtering, for grazing angles vs. surface roughness and surface composition changes, and for self-sputtering of Be and Li.

(b) Chemical Sputtering in carbon-based materials: Data needed for yield dependence on flux, energy of molecules and surface composition.

(c) Radiation enhanced sublimation (for carbon-based materials): Data needed for flux dependence and for the description of the loss of dopant at high temperature.

(d) Thermal evaporation: Assessment of data needed for Be, carbon-based materials and medium- and high-Z materials (Ti, V, Mo, Nb, W)

(e) Disruption erosion: Data for a full collisional-radiative model for the impurity in question (all processes with e^-, H^+, including three-body processes and radiation transport).

(f) Quantum processes on surfaces: molecular (molecular ion) formation and destruction with identification of product charge and quantum state.

(g) Particle sticking.

3. Material Properties

   (a) Data generation

      i. Thermo-mechanical properties of the new carbon fiber composites are needed

      ii Mechanical and post-irradiation thermo-mechanical properties of Be and other plasma-facing components candidates are needed.

      iii. Thermo-mechanical properties of new classes of materials, such as Ti-doped graphite, are needed.

      iv. Data on the effects on the physico-mechanical properties of material after neutron irradiation.

   (b) Data evaluation and compilation is very important for new materials, such as CFC and Ti-doped materials. Existing databases need throughout evaluation.

3.5 Recommended Actions

The Advisory Group recommended the following actions be taken by the IAEA A+M Data Unit:

1. Continue the efforts on the co-ordination of data compilation, evaluation and recommendation by the data centre network along the lines presented in the conclusions of this meeting (see previous section).
2. Strengthen its efforts on the coordination of data generation projects through its Co-ordinated Research Programmes in order to meet the evolving A+M, PSI and material properties data needs of the fusion community, specially of ITER.
3. Continue the maintenance and development of AMDIS.
4. Co-ordinate the circulation (via e-mail) of a quarterly informal report of all members of the DCN among themselves.

Appendix 1

IAEA Advisory Group Meeting on
"Technical Aspects of Atomic and Molecular Data Processing and Exchange
(13th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)"

10-11 July 1995, IAEA Headquarters, Vienna, Austria

LIST OF PARTICIPANTS

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Appendix 2

IAEA Advisory Group Meeting on
"Technical Aspects of Atomic and Molecular Data Processing and Exchange
(13th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)"

10-11 July 1995, IAEA Headquarters, Vienna, Austria

MEETING AGENDA

Monday, July 10 — **Meeting room: A-19-72**

09:30 - 09 45	- Opening (R.K. Janev, Head A+M Data Unit) - Adoption of Agenda
Session 1.	Current Activities of the A+M Data Centres
Chairman:	Abramov
09:45 - 10:45	Reports from Data Centres Wiese (NIST), Tawara (NIFS)
10:45 - 11:00	**Coffee break**
11:00 - 12:00	Reports from Data Centres: Mansky (ORNL), Shirai (JAERI)
12:00 - 14:00	**Lunch**
Session 1.	(Cont'd.)
Chairman:	Wiese
14:00 - 15:30	Reports from Data Centres: Delcroix (GAPHYOR), Abramov (Kurchatov Institute), Sun Yongsheng (IAPCM, Beijing)
15:30 - 16:00	**Coffee break**
16:00 - 17:30	Reports from Data Centres: Eckstein (Max-Planck, Garching), Yao Jinzhang (IAE, Beijing) Menapace (ENEA, Bologna)

Tuesday, July 11

Session 1.	(Cont'd)
Chairman:	Tawara
09:30 - 10:30	Reports from Data Centres Godunov (Troitsk Institute), Botero (IAEA)
10:30 - 11 00	**Coffee break**
Session 2.	Priorities in A+M, PSI and Materials Data Compilation and Evaluation
Chairman:	Shirai
11:00 - 11:30	Priorities in A+M Data Compilation and Evaluation (Janev)
11:30 - 12:00	PSI and Materials Data Base at IAEA (Langley)
12:00 - 12.30	Demonstration of Software (Godunov, Botero) - **Room: A23-40**
12:30 - 14 00	**Lunch**
Session 3.	Data Processing and Exchange
Chairman:	Delcroix
14:00 - 15:30	ALADDIN Implementation and Developments; Possibilities for Technical Improvements: Comments from all Data Centres (all participants)
15:30 - 16:00	**Coffee break**
16 00 - 16 30	Plan of DCN Activities for the Near Future (coordination Janev)
Session 4:	Meeting Conclusions and Recommendations
Chairman:	Botero
16:30 - 17:00	Formulation of Meeting Conclusions and Recommendations
17:00 -	**Adjourn of the Meeting**

Appendix 3

Data Centres Report of Activities

Activities of the Atomic Spectroscopy Data Centers at the
National Institute of Standards and Technology (NIST)

1994/95

W. L. Wiese

	Data Center	Director	Workforce
1.	Atomic Energy Levels and Wavelengths	W. C. Martin	J. Sugar, A. Musgrove
2.	Atomic Transition Probabilities	W. L. Wiese	D. E. Kelleher, J. R. Fuhr
3.	Spectral Line Shapes and Shifts	W. L. Wiese	Occasional contractors, guest scientists

Compilations of Numerical Data

	Recent Work	In Progress
Wavelengths:	Kr V-XXXVI	Si I
Energy Levels:	Zn, Ga	Si I, Ar
Transition Probabilities	All spectra of C, N, O	H, D, He, Li, Be, B, Ne

Database work

1. Annotated Bibliographic databases:

   Transition Probabilities, starting 1980, available on Internet using the WWW*.

   Line Widths and Shifts, starting 1978, available on Internet.

   Energy levels and wavelengths, starting 1985, soon available on WWW.

2. Numerical databases:

General database with wavelengths, energy levels and transition probabilities developed and many data loaded into it available on Internet, using the WWW*.

Also, two user friendly databases have been developed for PC users with DOS operating systems:

1. NIST Spectroscopic Properties of Atoms and Atomic Ions, J. W. Gallagher, Standards Reference Database 38
2. NIST Database for Atomic Spectroscopy, D. E. Kelleher, Standard Reference Database 61.

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*Both of these new WWW databases, "Bibliographic Database on Atomic Transition Probabilities" and "NIST/ADS Atomic Spectroscopic Database" may be found at the URL (uniform resource locator): http://physics.nist.gov - under the section on "Physical Reference Data."

New NIST data publications (1994/1995)

1. Spectral Data for Mn VII through Mn XXV, J. Phys. Chem. Ref. Data 23, 179 (1994).

2. Energy Levels of Zn I through Zn XXX, J. Phys. Chem. Ref. Data 24, in press (1995)
3. Spectral Data for Kr V - XXXVI, J. Phys. Chem. Ref. Data (1995)
4. Energy Levels of Gallium, Ga I through Ga XXXI, J. Phys. Chem. Ref. Data, submitted (1995)
5. Spectral Data for Moderately to Highly Ionized Atomic Ions Relevant to Fusion Research Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Ga, Kr, Mo, J. Phys. Chem. Ref. Data Monograph in preparation (1995).
6. "Atomic Transition Probabilities for Carbon, Nitrogen and Oxygen," J. Phys. Chem. Ref. Data Monograph 7 (in press, 1995)

Atomic and Molecular Data Activities (1994/95) at DPC, NIFS

NIFS Hiro Tawara

1) General activities

a) Plasma-surface interactions :

A new (revised) empirical formula for systematic calculations of sputtering yields from monatomic solids under ion impact in normal incidence has been proposed.

b) Electron collisions :

(1) Systematic calculations of excitation cross sections of excited helium atoms in electron impact : partial-wave method has been used and compared with other calculations.

(2) Semi-empirical formula for multiple ionization of atoms and ions by electron impact and comparison with the compiled data

c) Ion-atom collision data :

(1) New cross sections have been calculated, based on the close-coupling method, for excitation ($H^*(n)$), ionization (H^+) and electron transfer ($A^{(z-1)+}(nl)$) in highly charged ions (He^{2+}, Li^{3+}, Be^{4+}, B^{5+}, C^{6+}, N^{7+}, O^{8+} and Ne^{10+}) + H collisions over 5 - 500 keV/amu.

d) Ion-molecule collision data :

Quantum-mechanical calculations of heavy particle collisions involving molecules in the vibrationally excited states relevant to divertor physics : $He + H_2^+(v) \rightarrow HeH^+(v) + H$, $He + H^+ + H$ at around dissociation threshold region (2.2 - 10 eV) in collinear collisions

e) Developments of collisional radiative models and atomic data need for collisional-radiative models

f) Developments of data management system using workstations

2) International collaboration

We have a number of the (long-term) visitors and collaborators from various countries :

J. Dubau (Maudon, 1994, 1995), U. Safronova (Inst. Optical Spectroscopy, 1994, 1995), L.Presnyakov (Lebedev Physics Inst., 1994), V.P.Shevelko (Lebedev Physics Inst., 1995)

3) NIFS-DATA Report series (over the period of 1994-95)

DATA-21 : J.Dubau and T.Kato, Dielectronic recombination rate coefficients to the excited states of C I from C II (1994)

DATA-22 : T.Kawamura, T.Ono and Y.Yamamura, Simulation calculations of physical sputtering

and reflection coefficients of plasma-irradiated carbon surface (1994)

DATA-23 : Y.Yamamura and H.Tawara, Energy dependence of ion-induced sputtering yields from monatomic solids at normal incidence (1995)
(to be published in At. Data & Nucl.Data Tables)

DATA-24 : T.Kato, U.Safronova, A.Shlyaptseva, M.Cornille and H.Dubau, Comparison of the satellite lines of H-like and He-like spectra (1995)

DATA-25 : H.Tawara, Roles of atomic and molecular collisions in fusion plasma researches (1995)

DATA-26 : N.Toshima and H.Tawara, Excitation, ionization and electron capture cross sections of atomic hydrogen in collisions with multiply charged ions (1995)

DATA-27 : V.P.Shevelko, H.Tawara and E.Salzborn, Multiple-ionization cross sections of atoms and positive ins by electron impact

DATA-28 T.Nishikawa, T.Kawachi, K.Nishihara and T.Fujimoto, Recommended atomic data for collisional-radiative model of Li-like ions and gain calculation for Li-like Al plasma in the recombining phase

DATA-29 : V.P.Shevelko and H.Tawara, Spin-allowed and spin-forbidden transitions in excited He (n, n' = 2, 3, 4) induced by electron impact (1995)

Semiempirical formulae for multiple-ionization cross sections of neutral atoms and positive ions by electron impact

$$\sigma_n(u) = \frac{a(n)\, N^{b(n)}}{(I_n/Ry)^2} \left(\frac{u}{u+1}\right)^c \frac{\ln(u+1)}{u+1} \; [10^{-18}\,cm^2], \quad n \geq 3, \qquad (7)$$

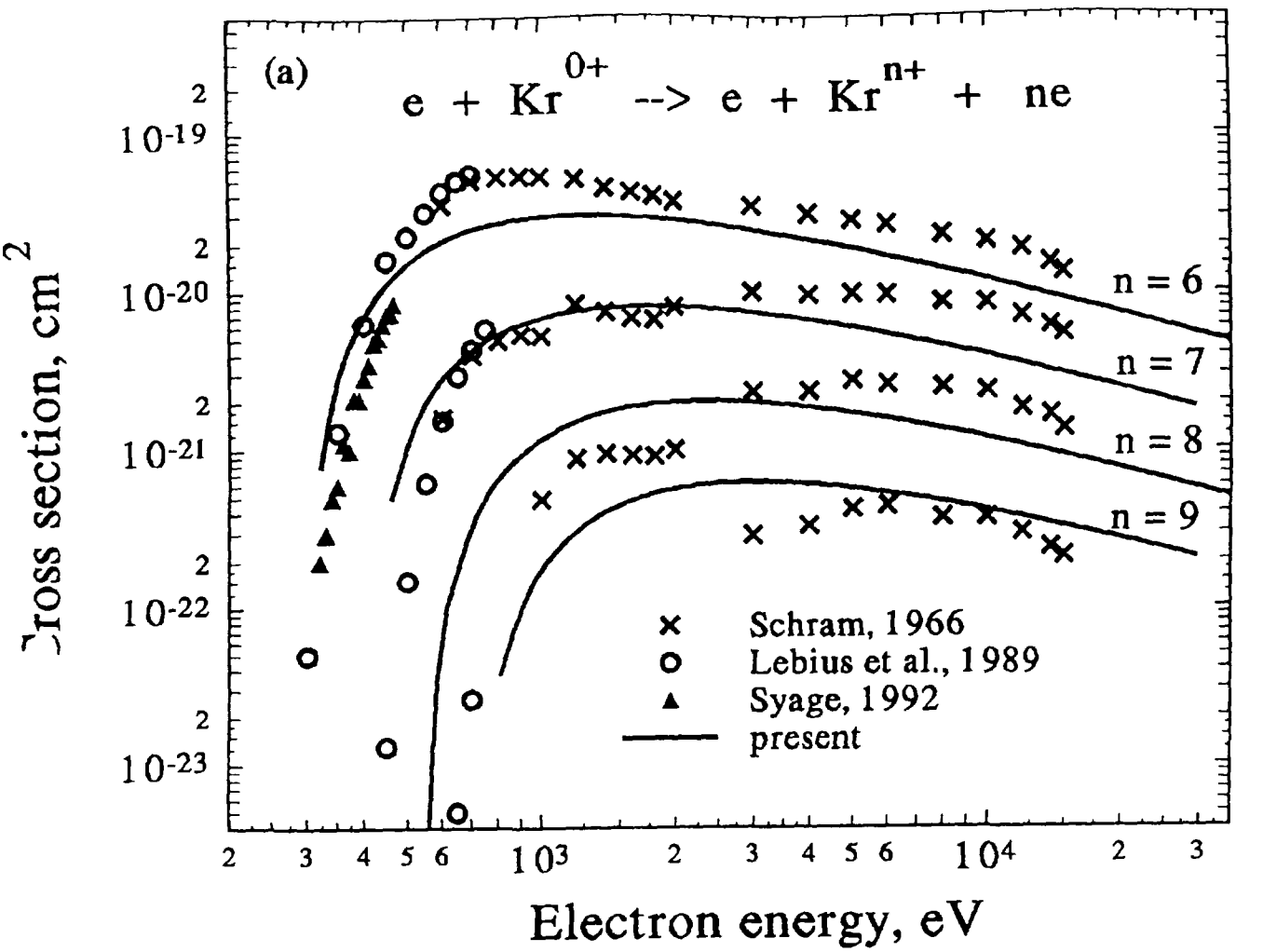
where $c = 1$ for atoms and $c = 0.75$ for ions.

Table 1. Fitting parameters a(n) and b(n) for removal of $3 \leq n \leq 10$ electrons from atoms or ions.

n	a(n)	b(n)
3	6.30	1.20
4	0.50	1.73
5	0.14	1.85
6	0.049	1.96
7	0.021	2.00
8	0.0096	2.00
9	0.0049	2.00
10	0.0027	2.00

asymptotic values:

$$a(n) \approx 1350/n^{5.7}, \quad b(n) = \text{const} = 2, \quad n \geq 10 \qquad (8)$$


(a)
e + Kr^0+ --> e + Kr^n+ + ne
Cross section, cm^2
n = 6
n = 7
n = 8
n = 9
Schram, 1966
Lebius et al., 1989
Syage, 1992
present
Electron energy, eV

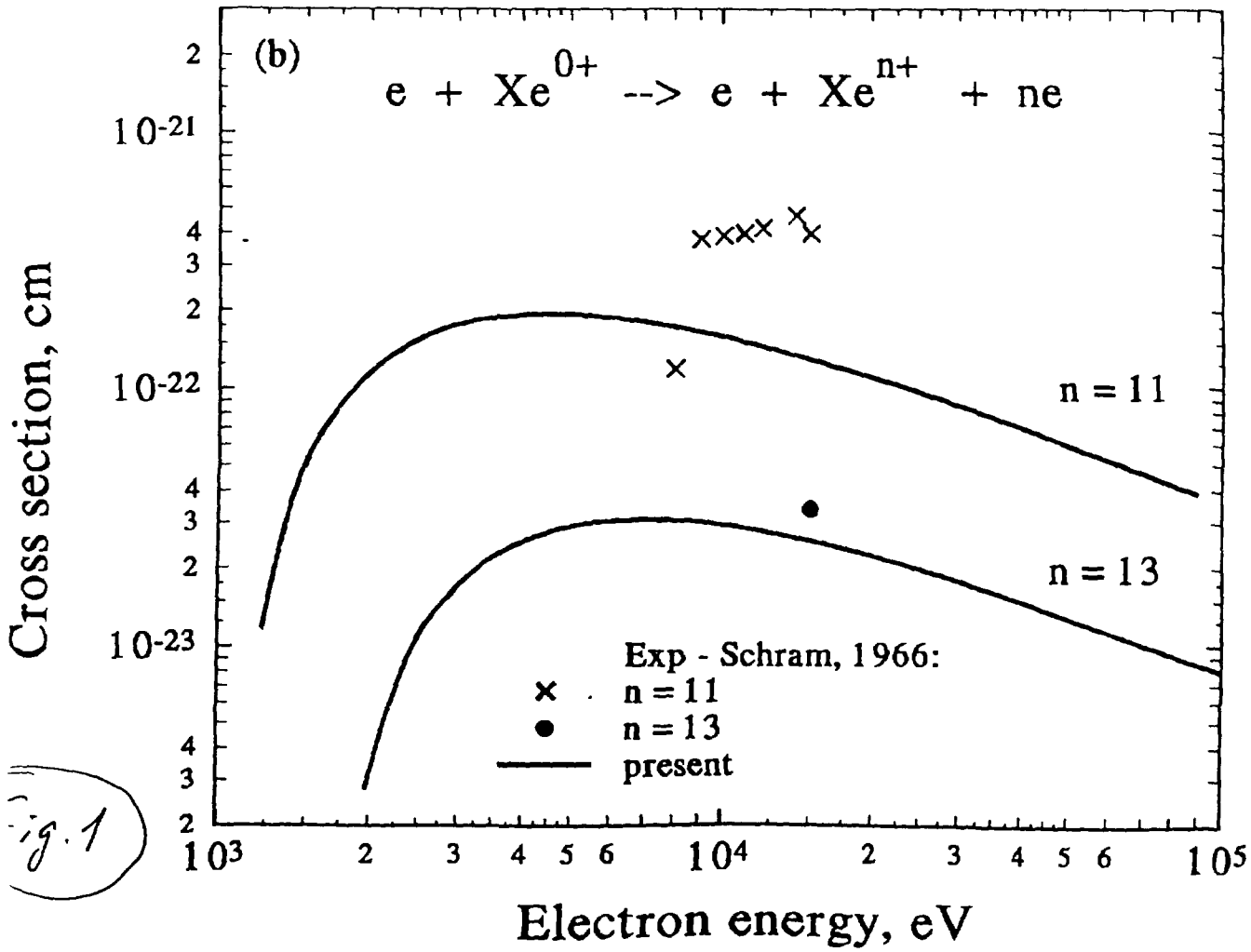
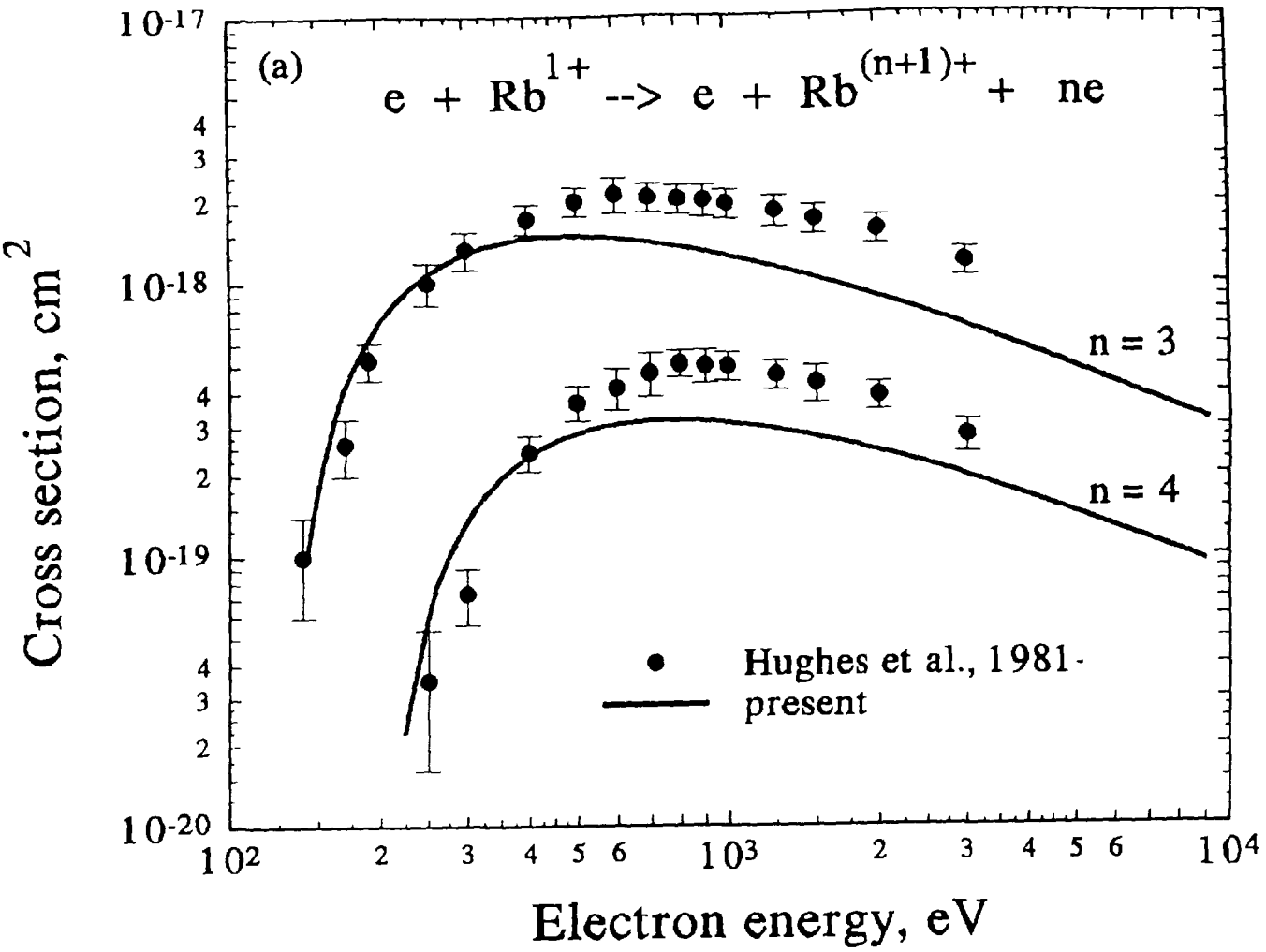

(b)
e + Xe^0+ --> e + Xe^n+ + ne
Cross section, cm
n = 11
n = 13
Exp - Schram, 1966:
n = 11
n = 13
present
Electron energy, eV

Fig. 1


(a)
e + Rb1+ --> e + Rb(n+1)+ + ne
n = 3
n = 4
Hughes et al., 1981
present
Cross section, cm2
Electron energy, eV

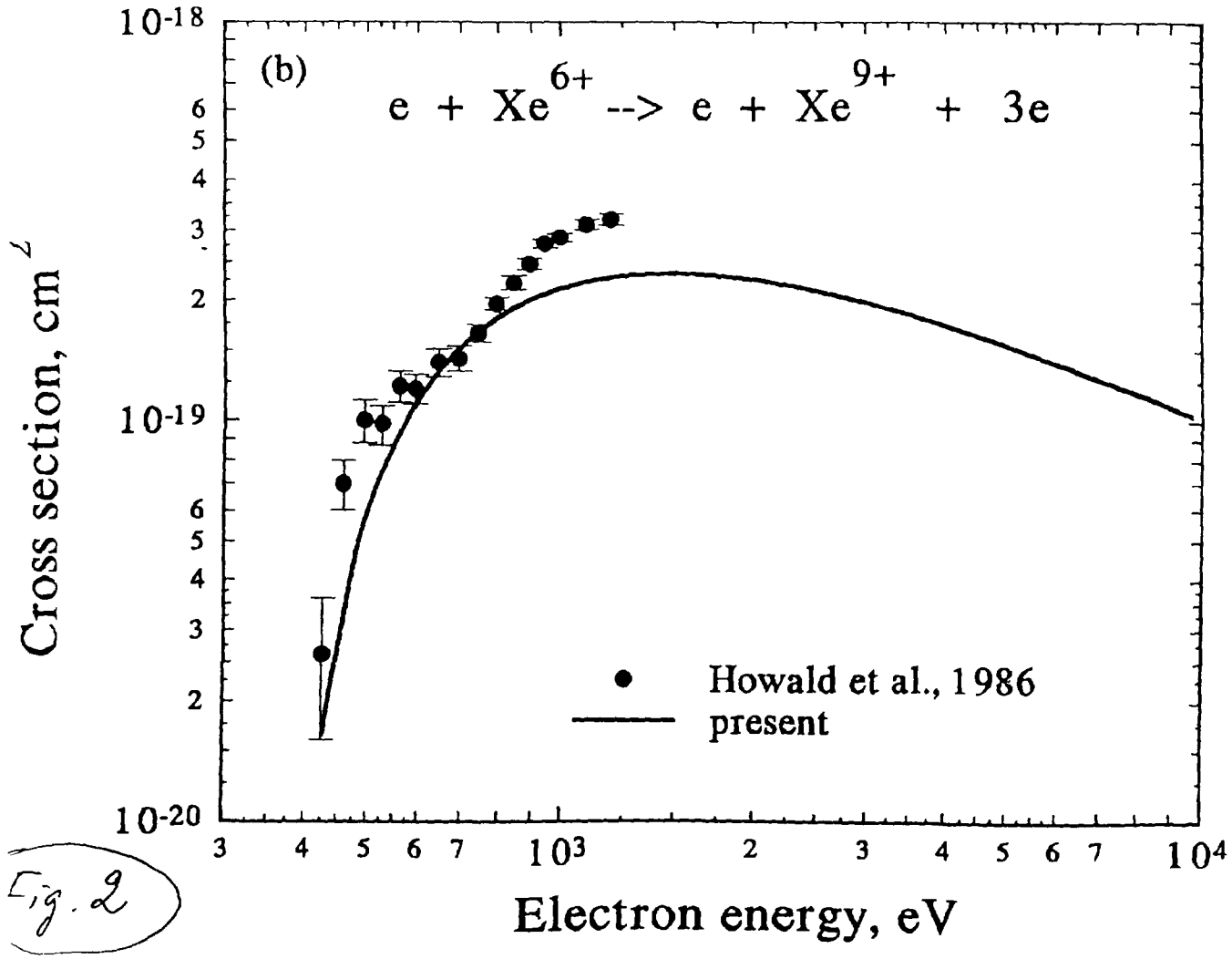

(b)
e + Xe6+ --> e + Xe9+ + 3e
Howald et al., 1986
present
Cross section, cm2
Electron energy, eV

Fig. 2

The Controlled Fusion Atomic Data Center

Mission

To compile, evaluate, recommend, and disseminate atomic and molecular data relevant to fusion energy research and development

Staff:	D.R. Schultz	Consultants:	A.Ya. Faenov†
	M.I. Kirkpatrick*		H.B. Gilbody
	P.S. Krstic		E.W. McDaniel
	E.J. Mansky		T.J. Morgan
			R.A. Phaneuf†
	F.W. Meyer‡		M.S. Pindzola
	C.C. Havener‡		E.W. Thomas

* Retired 8/94

† Contract not renewed

‡ ORNL staff acting as consultants, supported by other activities

ORNL Physics Division

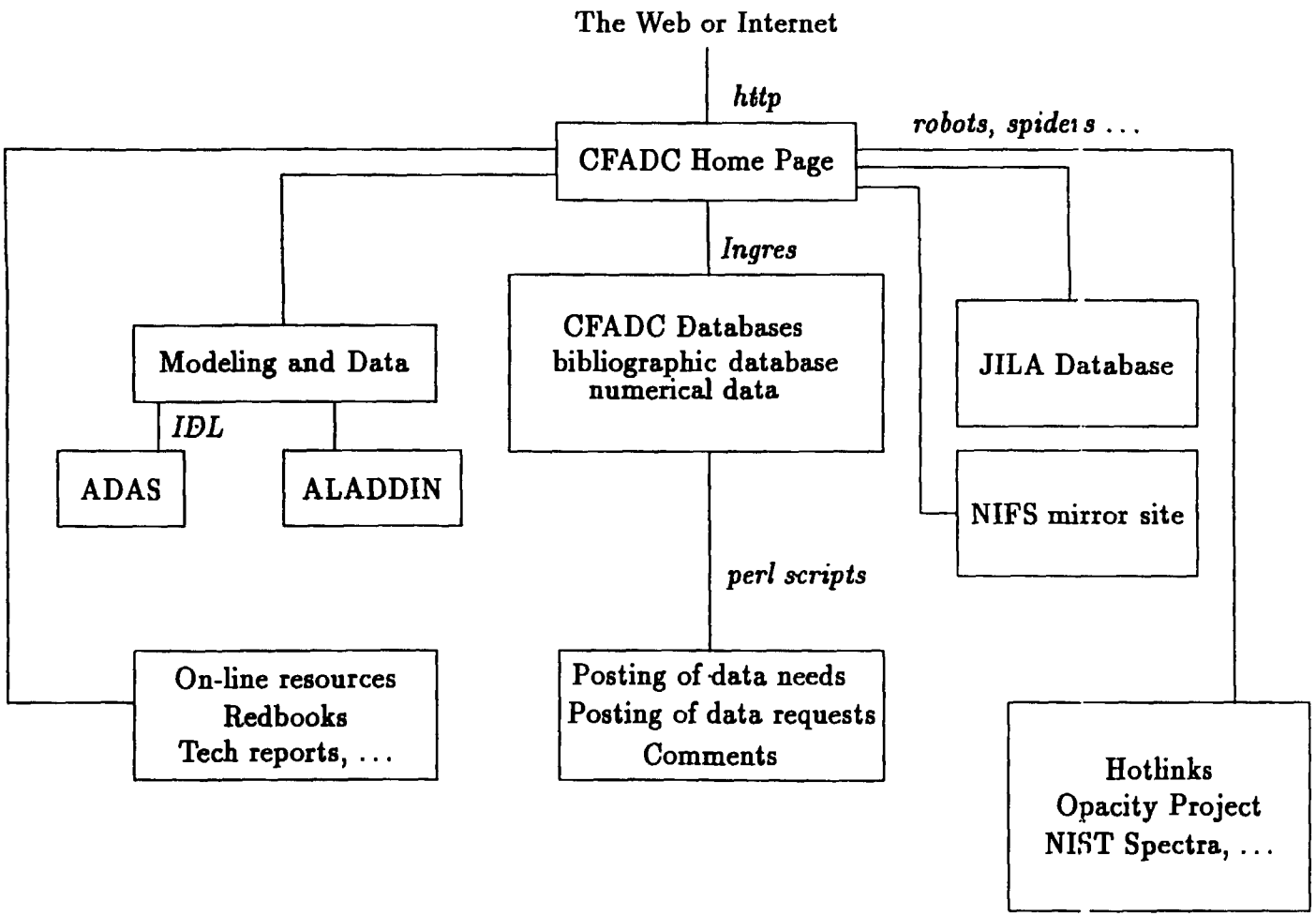
Principal Initiatives

- Develop workstation-based system for placing resources on-line for access by interested users – (*i*) in response to user demand, (*ii*) taking advantage of modern data management tools, and (*iii*) to leverage limited manpower
  - Convert bibliography (PC-based and archival) to INGRES
  - Participate in international network of host sites for the JET/Strathclyde *Atomic Data and Analysis Structure* suite
  - National Institute of Fusion Science (Nagoya) atomic database mirror site
  - Preserve and continue JILA atomic database
  - Provide on-line data reports (e.g. the *Redbooks*)
- Participate in Physics Division efforts to seek funding for atomic and nuclear physics in support of astrophysics – (*i*) the Theory Section and HRIBF are developing emphasis in astrophysics, (*ii*) strong overlap in the atomic data needs in fusion and astrophysics indicates the logic of collecting data of use to both, and (*iii*) broadening of the CFADC funding base could help to ensure the longevity of the data collection, dissemination, and preservation activities

Principal Needs

- In addition to assured continuation of present level of funding, the CFADC requires a modest increase to convert one temporary position into a full time staff position

URL **http://www-cfadc.phy.ornl.gov/** home.html



ORNL Physics Division

ADAS: Atomic Data and Analysis Structure

ADAS is a suite of codes and data collections for extracting fundamental and derived atomic data, and modelling radiating properties of ions and atoms in plasmas

Examples of Key Elements

- **ADAS1**: Fundamental atomic reaction data, electron-impact excitation, ionization, dielectronic recombination, radiative recombination, charge exchange recombination, etc.
- **ADAS2**: Excited populations in a plasma environment, radiation emission, population model
- **ADAS3**: Neutral hydrogen, helium interactions, ion-atom excitation, ionization, charge transfer data, beam stopping
- **ADAS4**: Ground and metastable populations of ions in a plasma, parametric forms for isonuclear data
- **ADAS5**: Supplementary programs, to aid in interpreting plasma parameters
- **ADAS6**: Printing, plotting, and output routines

Fusion Atomic Theory

Mission

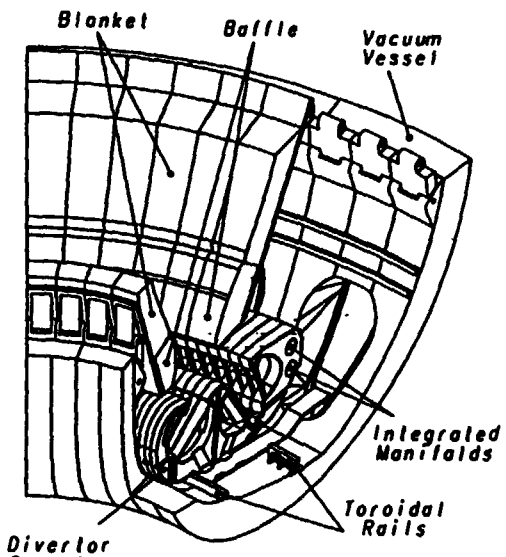
To provide theoretical cross sections and rates needed by fusion energy research for diagnostics and modeling, and further develop theoretical techniques used for this data production

Staff: D.R. Schultz
P.S. Krstic
E.J. Mansky

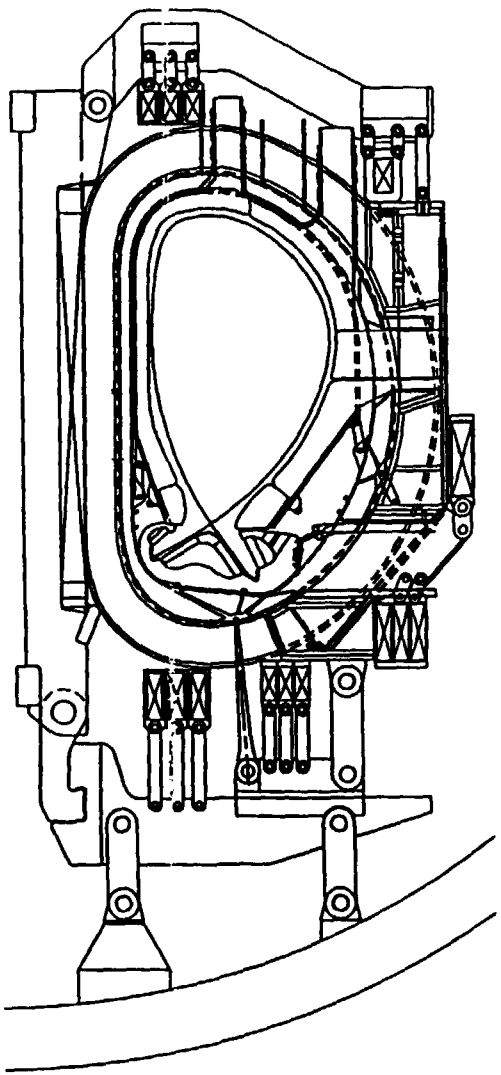
Collaborators: M.S. Pindzola
D.C. Griffin
N.R. Badnell
T.W. Gorczyca
R.E. Olson
C.O. Reinhold

- Electron- and heavy-particle-impact collisions
- Excitation, ionization, dielectronic recombination, charge transfer, elastic scattering
- Emphasis on species and reactions of present interest, currently being driven by modeling needs for ITER Engineering and Design Activities

The International Thermonuclear Experimental Reactor



ITER DIVERTOR ASSEMBLY

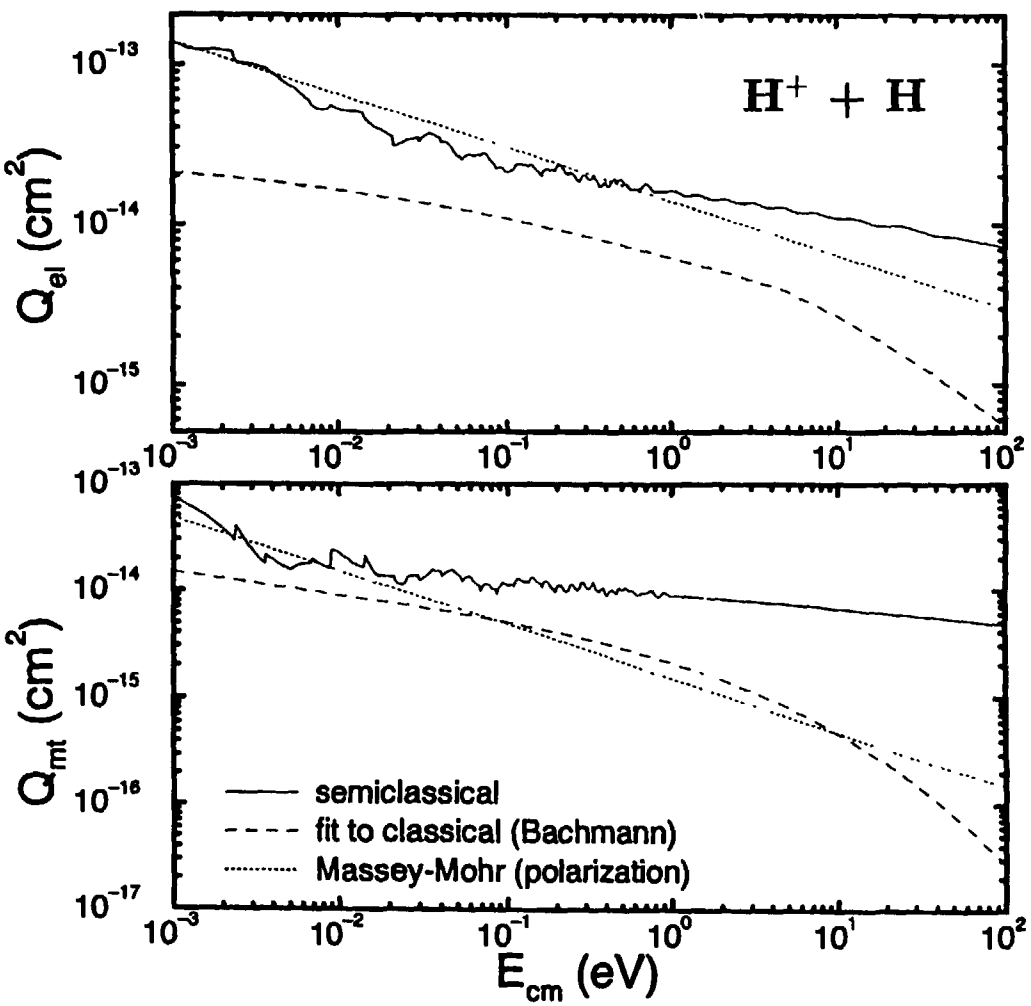


Plasma density (averaged)	10^{20}	m^{-3}	
Ion temperature (averaged)	13	keV	
Fusion power (nominal)	1.5 ± 0.3		GW
Burn time	1000	s	
Major radius	8.1	m	
Minor radius	3.0	m	
Elongation	1.6		
Toroidal magnetic field at 8.1 m	5.7	Tesla	
Plasma current	24	MA	

- Data production for ITER is being driven by
  - the selection of materials for the plasma facing components (Be, B, C, Mo, W, Ti, V, Cr, etc.)
  - atomic and plasma physics governing the insulation of these components from the hot, dense core plasma by the edge plasma
  - the need to cool and neutralize the plasma for helium ash removal, hydrogen recycling, and energy removal in the divertor

- Consequently, we are emphasizing, for example,
  - Low-energy, heavy-particle elastic and related cross section database of total and differential cross sections (energy and momentum transport in edge and divertor)
  - Ionization and state-selective capture cross sections for Be and B ions colliding with H, H_2 and He (candidate low-Z plasma facing components)
  - Reaction database for Ne ions colliding with H, H_2 and He (candidate radiative cooling enhancer in divertor)
  - Development of "Hidden Crossings" technique generalized to multielectron, multicenter systems for low energy ion/atom/molecule collisions

- Improve fits to total elastic, momentum transfer, viscosity, and charge transfer cross sections presently used by modelers (ions, neutrals, and isotopes of H, H_2, and He)
- Provide database or fits to differential elastic scattering cross section



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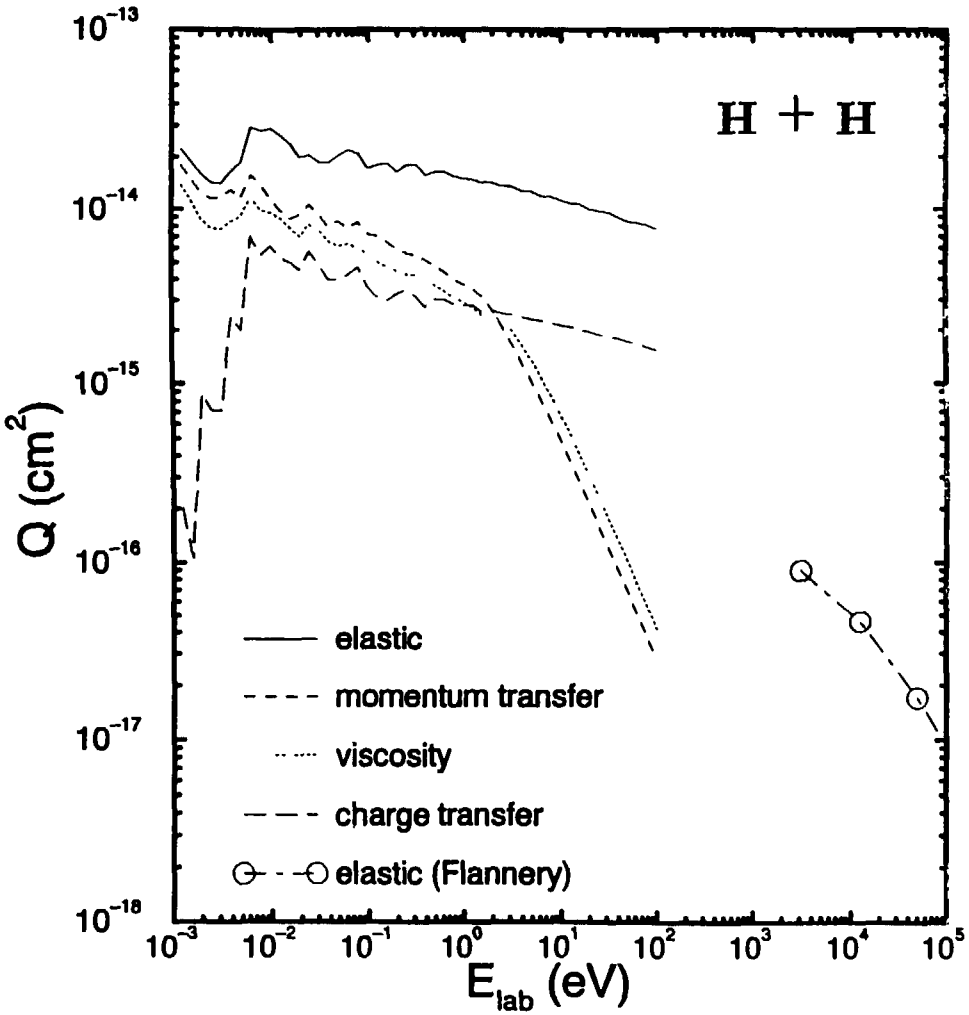

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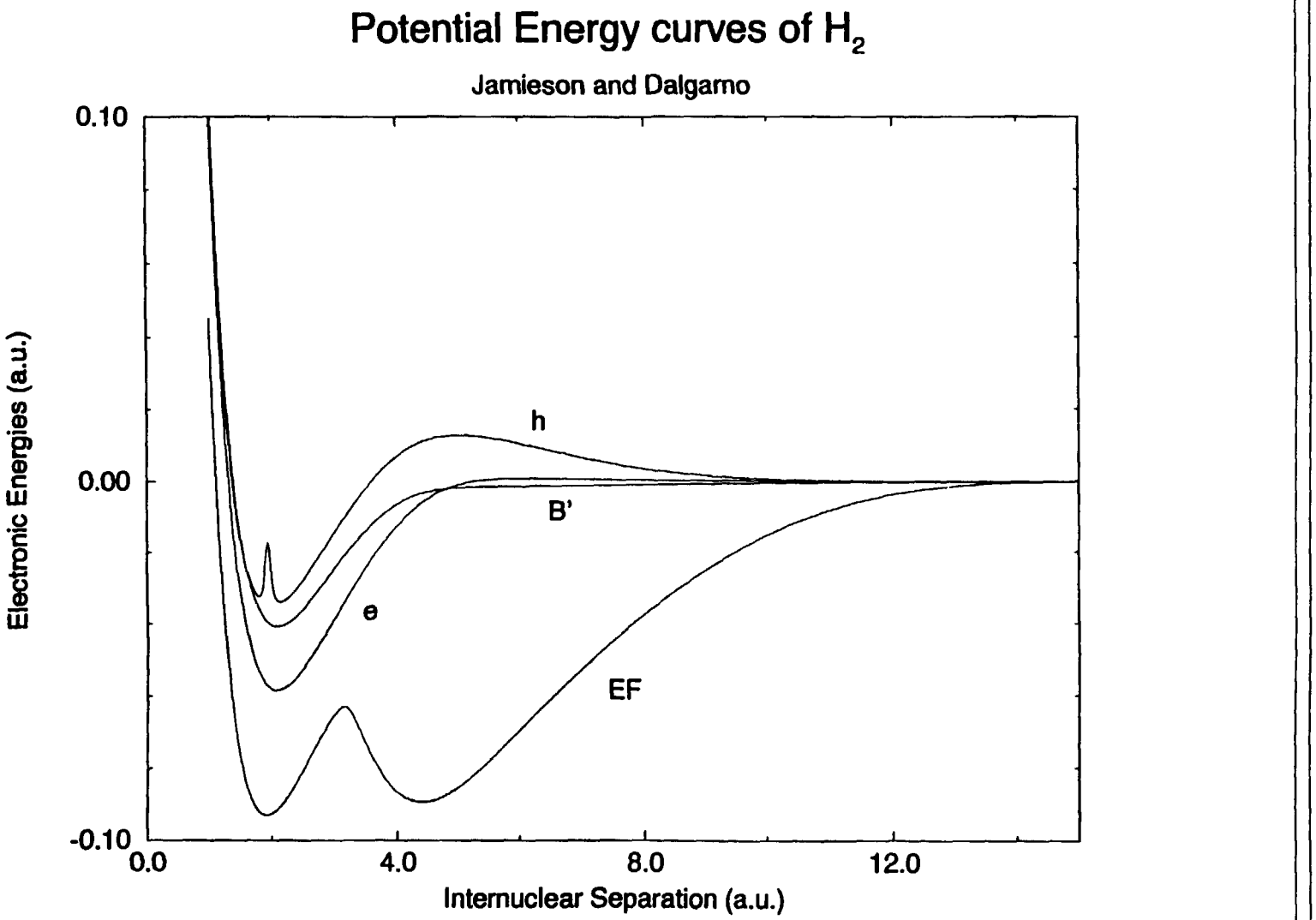
- Two-state model (lowest singlet and triplet states) for H + H elastic scattering is inadequate for impact energies above the first excitation threshold
- Use representation of the potential energy curves for the next excited states within the Σ manifold for H_2 provided by Jamieson and Dalgarno ($B^1\Sigma_u^+, e^3\Sigma_g^+, EF^1\Sigma_g^+, h^3\Sigma_g^+$)
- Adapt existing semiclassical close coupling codes of Flannery and Mansky for calculation of the elastic cross section at intermediate energies

$$
\begin{aligned}
i\frac{\partial a_n(t)}{\partial t} &= \sum_k a_k(t) V_{nk}(\vec{R}(t)) e^{i\epsilon_{nk}t} \\
\frac{\partial q_j}{\partial t} &= \frac{p_j(t)}{\mu} \quad j = 1-3 \\
\frac{\partial p_j}{\partial t} &= -\frac{\partial \mathcal{V}(\vec{R}(t))}{\partial q_j} \quad j = 1-3
\end{aligned}
$$



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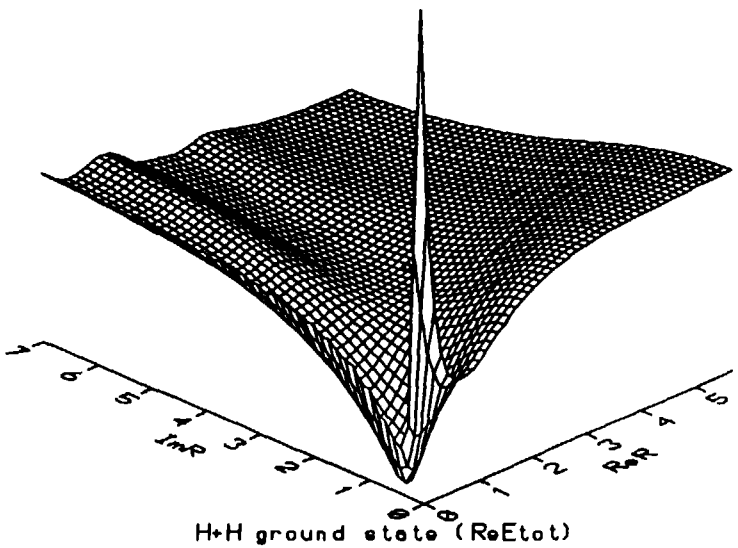
Multicenter, Multielectron Hidden Crossing Method

- The hidden crossing method has been demonstrated to provide reliable excitation, ionization, and charge transfer cross sections in the two-center, one-electron case
- Accuracy competes with close coupling with the same number of states n taken into account, but with n^2 shorter computation time
- Method relies on the analyticity of the adiabatic electronic Hamiltonian as a function of R, enabling the analytic continuation to the plane of complex R
- Transitions are strictly localized around isolated branch-point singularities that connect, often multiply, pairs of Riemann sheets
- Analyticity of the electronic Hamiltonian for multicenter, multielectron systems enable the extension of this method to much more complex collisions
- Generalize unrestricted HF-LCAO method to the plane of complex R (CI needs to be added to consistently treat singly and doubly excited states)
- Preliminary cross sections for single ionization in H + H collisions computed



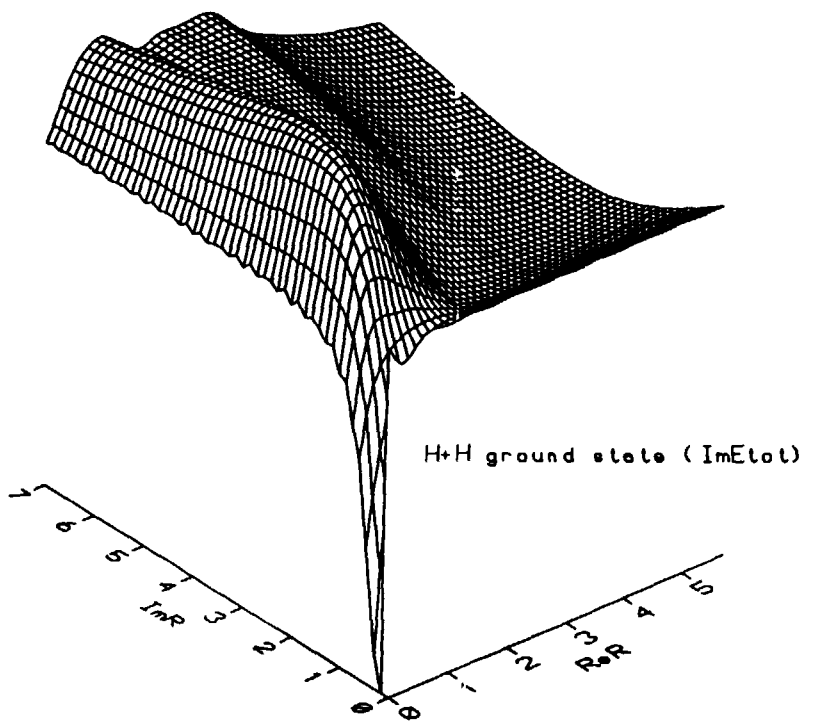


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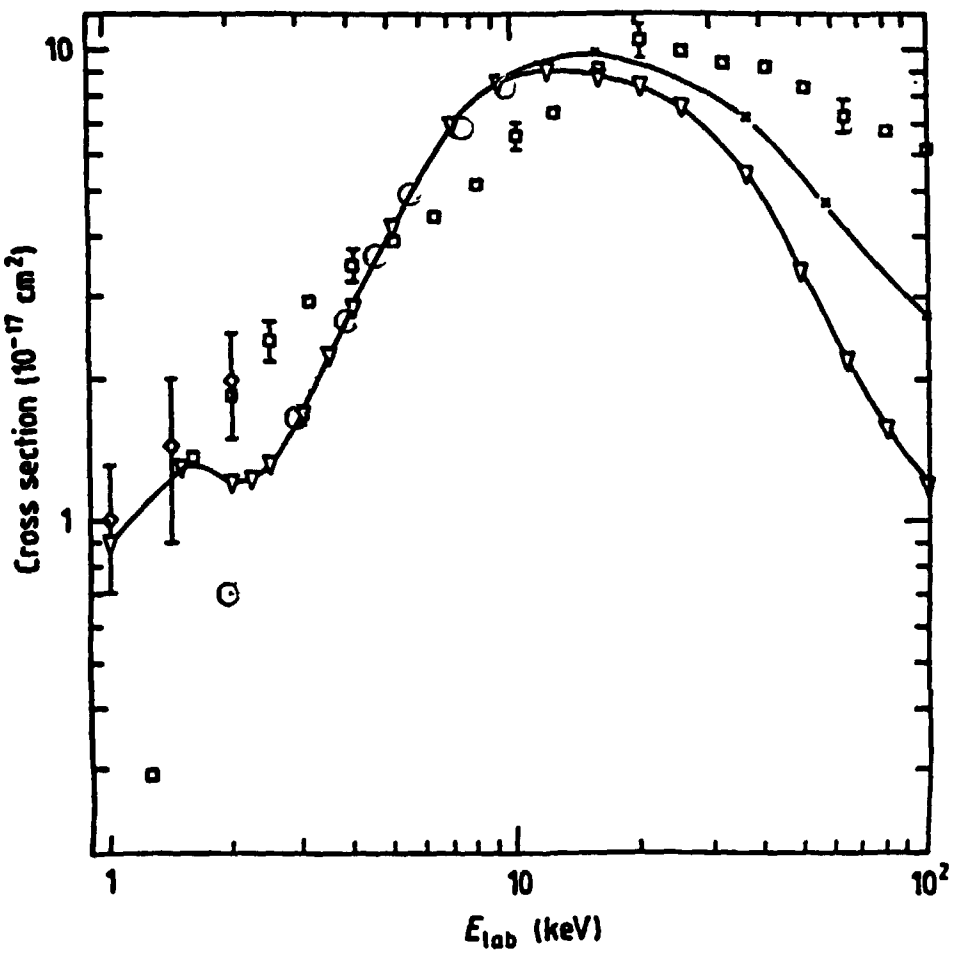
Figure from Shingal, Bransden, and Flowers (1989)

Cross Section for $H + H \rightarrow H(nlm) + H^+ + e^-$



22 state close coupling

○ Hidden crossing model

□ experiment, McClure (1968)

◇ experiment, Gealy and Van Zyl (1987)

ORNL Physics Division

Progress Report on A+M Data Activities at Nuclear Data Center Japan Atomic Energy Research Institute (JAERI) October 1993 - June 1995

Toshizo Shirai

Compilation and evaluation work has been continued to make the 4th edition of Evaluated Atomic and Molecular Data Library (JEAMDL-4) for fusion in collaboration with the JAERI Research Committee on A+M Data and with researchers of ORNL and NIST under the US-Japan fusion cooperation program.

Recent Activities and Work in Progress

A project of analytical fits to the recommended cross sections for collisions of H, H_2, He, and Li atoms and ions with atoms and molecules is now in progress. As the sequel to the previous work on electron capture, the cross sections for excitation and spectral line emission [1], and for ionization, charge-production, electron-loss, and electron detachment [2] were parametrized. These results are available in the ALADDIN format. A similar work is undertaken for dissociation and particle-rearrangement.

Data compilation was made of experimental cross sections for particle-rearrangement in ion-molecule collisions involving hydrogen and helium species [3].

Total cross sections for the ionization of excited hydrogen atoms by bare ions were calculated using the continuum distorted wave-eikonal initial state (CDW-EIS) approximation [4]. It was shown that a combination of the present results with other predictions at low energies provides reliable total cross section in the wide energy range covering the requirement from the fusion community. We also applied the CDW-EIS approximation to the ionization of hydrogenlike ions in collisions with bare ions [5]. Our results showed that the CDW-EIS approximation predicts cross-section values in agreement with the close-coupling calculations for collision processes where the atomic number of the incident ion is smaller than that of the target ion. Calculations have been made for the cross sections for excitation and ionization of excited helium atoms in collisions with H^+, Be^{4+}, and B^{5+} ions using the Born, Glauber, and CDW-EIS approximations.

We are calculating cross sections for some collision processes relevant to gas divertor for ITER. The potential energy surfaces of H_3^+ in the ground and first excited states have been determined by Ichihara, which are used for

calculations of the cross sections for charge transfer and particle-rearrangement in its collision system. In a research contract with Takagi, Kitasato Medical University, calculations within the framework of multi-channel quantum defect theory are being carried out of the cross sections for vibrational transition, dissociative recombination, and dissociative excitation in collisions between electrons and hydrogen molecular ions at energies below 10 eV.

We have undertaken publication of a series of compilations of spectra of highly ionized atoms of particular interest to the fusion energy community. Monographs of Ti, V, Cr [6], Mn[7], Fe, Ni, Co, Cu, Kr, and Mo have been published so far (Kr [8] is in press). These monographs will be put into a book with addition of more recent data for these elements. Compilation has been almost completed for the wavelength data of Ga in all stages of ionization.

References

[1] JAERI-Data/Code 94-005: "Analytic cross sections for collisions of H, H_2, He, and Li atoms and ions with atoms and molecules. II," R. Ito, T. Tabata, T. Shirai, and, R.A. Phaneuf.

[2] JAERI-Data/Code 95-008: "Analytic cross sections for collisions of H, H_2, He, and Li atoms and ions with atoms and molecules. III," R. Ito, T. Tabata, T. Shirai, and, R.A. Phaneuf.

[3] JAERI-Data/Code 94-015: "Cross sections for particle-rearrangement in ion-molecule collisions I. Hydrogen and helium species," A. Ichihara, S. Hayakawa, M. Sataka, and T. Shirai.

[4] Phys. Rev. A 50, 4945 (1994): "Ionization of excited hydrogen atoms by collisions with bare ions," A. Igarashi and T. Shirai.

[5] Phys. Rev. A 51, 4699 (1995): "Ionization of excited hydrogenlike ions by collisions with bare ions," A. Igarashi and T. Shirai.

[6] J. Phys. Chem. Ref. Data 22, 1279 (1993): "Spectral data and Grotrian diagrams for highly ionized chromium, Cr V through Cr XXIV," T. Shirai, Y. Nakai, T. Nakagaki, J. Sugar, and W.L. Wiese.

[7] J. Phys. Chem. Ref. Data 23, 179 (1994): "Spectral data and Grotrian diagrams for highly ionized manganese, Mn VII through Mn XXV," T. Shirai, T. Nakagaki, K. Okazaki, J. Sugar, and W.L. Wiese.

[8] J. Phys. Chem. Ref. Data, in press: "Spectral data and Grotrian diagrams for highly ionized krypton, Kr V through Kr XXXVI," T. Shirai, K. Okazaki, and J. Sugar.

GAPHYOR

(GAz - PHYsique - ORsay)

Système de

DOCUMENTATION AUTOMATIQUE

sur les propriétés des ATOMES

des MOLÉCULES et des GAZ

GAPHYOR DATA CENTRE 1994-1996
Status report and projects

J.L.Delcroix, D.Humbert, C.Leprince

presented at the 13th Atomic and Molecular
Data Centre Network Meeting
IAEA, Vienna, 10-11 July 1995
Rapport GA-12/275

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LABORATOIRE DE PHYSIQUE DES PLASMAS

GAPHYOR DATA CENTER 1994-1996

Status Report and Projects

presented at the 13th Atomic and Molecular Data Centers Network Meeting IAEA, Vienna, 10-11 July 1995, Rapport GA-12/275

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Centre de Données GAPHYOR, Laboratoire de Physique des Gaz et des Plasmas, Université Paris-Sud Orsay
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e-mail 2 : delcroix@supelec.fr

GAPHYOR (GAz-PHYsics-ORsay) Data Center produces a Database on the properties of atoms, molecules and neutral or ionized gases ; as of June 15th 1995 the GAPHYOR file included about 450 000 entries covering mainly the 1970-1995 period. During the last two years it has moved from a mainframe computer to an Unix work-station. A complete restructuration of Data was performed at this occasion. GAPHYOR includes now a good deal of Numerical Data, completing its traditional bibliographical and factual information. The paper publications are now :
- GAPHYOR UPDATE : a yearly publication including the last entries (last issue UPDATE 94 published in January 1995)
- GAPHYOR HANDBOOK : a yearly publication including a selection of best entries in the whole Database. It is divided in two volumes : Volume 1 for Standard Data (atoms and small molecules) and Volume 2 for Special Data (multicharged ions, iso-electronic series, molecular clusters, gas-surface interactions). The last issue is HANDBOOK 95, Vol 1 and Vol 2, published in June 1995.

On-line dissemination (interrupted during the period of migration and restructuration) will start again before the end of 1995. But before that the Data will be available on Internet (WWW), and an Internet forum of cooperation with other Data Centers and individual users will be organized to improve the quality of the Database.

Le Centre de Données GAPHYOR (GAz-PHYsique-ORsay) produit une Banque de Données sur les propriétés des atomes, des molécules et des gaz neutres ou ionisés ; au 15 Juin 1995 le fichier GAPHYOR comprenait environ 450 000 enregistrements couvrant principalement la période 1970-1995. Pendant les deux dernières années GAPHYOR a migré d'un centre de calculs vers une station de travail sous Unix. Une restructuration complète des données a été réalisée cette occasion. GAPHYOR contient maintenant de nombreuses données numériques, qui viennent compléter ses traditionnelles informations bibliographiques et factuelles. Les publications sur papier sont maintenant les suivantes :

- GAPHYOR UPDATE : une publication annuelle contenant les entrées récentes (dernière parution : UPDATE 94 publié en Janvier 1995)

- GAPHYOR HANDBOOK : une publication annuelle contenant une selection des meilleures données de la base complète. Elle est divisée en deux volumes : Volume 1 pour les Données Standard (atomes et petites molécules) et Volume 2 pour les Données Spéciales (ions multichargés, séries iso-electroniques , amas moleculaires (clusters), interactions gaz-surface). La dernière parution est HANDBOOK 95, Vol 1 et Vol 2, publié en Juin 1995.

Le service de consultation en ligne (interrompu pendant la période de migration et de restructuration) reprendra avant la fin de 1995. Mais auparavant les données seront consultables sur Internet (WWW), et un forum de coopération avec les autres Centres de Données atomiques et moléculaires (et avec les utilisateurs individuels) sera organisé sur Internet afin d'améliorer GAPHYOR et de mieux le faire connaître.

July 5, 1995

Contents

1 Some Statistics

As of the 15th of June 1995, the total number of entries in the files was about 455 000 distributed as shown in Table 1.

Sections	1 structures	2 photon coll.	3 electron coll.	4 at./mol. coll.	5 macro. prop.	Σ
Standard Data	215 845	22 601	21 091	103 111	24 367	387 015
Special Data	33 687	1 428	6 359	17 290	9 416	68 180
Σ	249 532	24 029	27 450	120 401	33 783	455 195

Table 1: Statistics of Standard and Special Data (June 15th 1995)

2 Collection of new Data

The regular collection of Data from the current litterature is made by a group of experts in Physics and Chemistry, namely :

M. Aubès, M. Yousfi
Centre de Physique Atomique, Université Paul Sabatier, Toulouse
J. P. Booth
Laboratoire de Spectrométrie Physique, Université de Grenoble
M. Costes, J. Masanet
Laboratoire de Photophysique et Photochimie Moléculaires, Université Bordeaux 1
J.L. Delcroix
Centre de Données GAPHYOR, Laboratoire de Physique des Gaz et des Plasmas, Université Paris-Sud Orsay
A.M. Diamy, C. Lalo
Laboratoire de Chimie Générale, Université Pierre et Marie Curie, Paris
F. Emard-Katsonis, K. Katsonis, A. Ricard
Laboratoire de Physique des Gaz et des Plasmas, Université Paris-Sud
A. Faenov, M. Magulov
VNIIFTRI, Moscou, Russie
V. Hrachova
Dept. of Electronics and Vacuum Physics, Karlova Univ., Praha, République Tchèque
R. Hrach
Fac. Mathematics and Physics, Karlova Univ., Praha, République Tchèque
P. Veis
Dept. of Plasma Physics, Fac. Mathematics and Physics, Comenius Univ., Bratislava, Slovaquie

The Journals which are regularly analyzed are shown with an asterisk in Table 4.

3 Handbook

The Handbook is a synthetic yearly publication designed to help anybody who is interested in a new field of research. It can also be used as a help to on-line retrieval. It is a selection taken from the whole GAPHYOR Database. The selection criteria depend on quality and actuality of data. More precisely the selection is made as follows :

- **Assigning a value index** to every GAPHYOR record. This index is the sum of six partial indexes (cf. Sections 11 and 9) which take account of the quality of bibliographical, factual, and numerical data.

- **Multiplets.** A catalog of the "multiplets" included in the Base is then produced. A multiplet is the set of entries having the same structure : same values of elements, reactants, processes.

- **Selection.** The selection of entries is then made in two steps :

  - For every multiplet one selects the entry having the highest value index. One registers moreover the multiplicity MULT i.e. the number of entries in the multiplet. This number is printed in the last column of the Data Tables of the Handbook.

  - To decrease the global volume of the selection one eliminates all the entries whose value index is smaller than a given minimum value. The minimum value in Handbook 95 has been fixed at 165 in Volume 1 and 110 in Volume 2.

- **Separation in two volumes.** Volume 1 includes Standard Data, i.e. those related to atoms and small molecules, following the general philosophy of GAPHYOR. Volume 2 covers Special Data related to some fields extending the general scope of GAPHYOR :

  1. Multicharged ions
  2. Iso-electronic series
  3. Clusters
  4. Gas-Surface interactions

Finally, Table 2 shows some statistics linking together the Handbook 95 and the whole Database. The average multiplicity is about 2.8 in Volume 1 and 2.6 in Volume 2. These low values result from a large number of cases with MULT=1 (unusual processes) and of a small number of cases with MULT> 10 (well known processes). For Sections 2, 3 and 4 describing Collisions and Reactions (cf. paragraph 6.2) the Handbook covers about 50% (in Volume 1) and 90% (in Volume 2) of the topics (multiplets) included in the Base. The *coverage in Sections 1 (structures) and 5 (macroscopic processes) are much smaller*, especially in Volume 1. This was a deliberate choice in this 1995 Handbook.

Sections	1 struct.	2 phot.coll.	3 electr.coll.	4 at.mol.coll.	5 mac.prop.	Σ
BASE (Vol.1)						
Entries	215 845	22 601	21 091	103 111	24 367	387 015
Multiplets	71 430	7 318	3 891	48 874	8 580	140 093
Multiplicity	3.0	3.1	5.4	2.1	2.8	2.8
HANDBOOK (Vol.1)						
Selected multiplets (IV165)	2 828	3 383	1 892	28 377	622	37 102
Selection (IV165)	4%	46%	49%	58%	7%	26%
BASE (Vol.2)						
Entries	33 687	1 428	6 359	17 290	9 416	68 180
Multiplets	14 080	807	2 688	8 368	745	26 688
Multiplicity	2.4	1.8	2.4	2.1	12.6	2.6
HANDBOOK (Vol.2)						
Selected multiplets (IV120)	7 969	701	2 510	7 149	559	18 888
Selection (IV120)	57%	87%	93%	85%	75%	71%
BASE (Total)						
Entries	249 532	24 029	27 450	120 401	33 783	455 195

Table 2: Statistics of entries and multiplets.

4 Update

GAPHYOR UPDATE is now published once a year : It includes the new entries registered during the last year. The last published issue is UPDATE 94 (published in January 1995). This includes 28 230 entries. Note that this Update was produced during the difficult period of mutation of GAPHYOR : it may have a number of imperfections somewhat higher than wishable. Note also that during this period the up-dating was somewhat slow. One must moreover understand that the feeding of the Database is not made only once a year, but permanently, and the up-dating was much more efficient in 1995, with the result that UPDATE 95 will be about twice larger than UPDATE 94.

5 Dissemination of data

5.1 Retrieval by e-mail (expert's reports)

This mode of consultation revealed itself as the most efficient during the last two years : the user explains its problem by e-mail ; the GAPHYOR team defines the nature of needed data, performs locally the corresponding retrievals, and send the results to user by e-mail.

5.2 On-line retrieval

During the period of mutation (1994-1995) the on-line retrieval service was interrupted, because the convivial software of retrieval formulation (and on-line help) had to be completely rewritten. The present plans are to open it again before the end of 1995.

5.3 Distribution through Internet

The GAPHYOR work-station is connected to Internet. To open its files to users of this network, the present projects are as follows :

- Communication. A small number of atomic and molecular Databases are presently registered in a few specific points of access of Internet. The best point of access for plasma physicists is at Weizmann Institute in Israël. We have recently introduced GAPHYOR into this group. Other points of access, corresponding to other domains of research related to GAPHYOR, will be installed (molecular physics, chemical kinetics, lasers, astrophysics, fluid mechanics, atmospheric chemistry and pollution...)

- Opening of an ftp. server

  1. *Transfer of ftp. files.* The GAPHYOR server will be consulted using MOSAIC or NETSCAPE. The introduction page will describe the scope of GAPHYOR and will give a simplified overview of its internal organization. The whole base will be divided into a limited number of elementary files (a few hundred) each of them having a reasonable volume (to facilitate transfers, storing and possibly local treatment). The sections and the ordering will be the same as in UPDATE. The users will be authorized to save those files on their local site.
  2. *Control of access.* Access will be controlled for reasons of security as well as for the payment of an annual subscription fee (cf. Section 5.4).

- Opening of a forum. This will be used for communication with users and with other Atomic and Molecular Data Centers. Il will probably be used also for the expert's reports (see Section 5.1 above) and for a permanent critical review of GAPHYOR data . The access conditions to this forum will be defined within a few months from now.

5.4 Payments policy

The availability of GAPHYOR on Internet will lead to changes in thepayment policy for our services. After approval by our sponsoring agencies, the new fees should be as follows :

- *Annual subscription fee for unlimited Internet retrieval* : 1000F (HT)
- *Expert's report by e-mail* : $200 + 2n$ F (HT) where n is the number of delivered records.
- *Update 94* : 850F (HT)
- *Handbook 95, Volume 1* : 700F (HT)
- *Handbook 95, Volume 1* : 500F (HT)

5.5 Security and patrimonial protection problems

Offering the Database on the network could generate problems of informatic security. Its liberal distribution by ftp transfer could generate problems of protection of patrimony (minimized by the fact that the Database is continuously evolving through permanent introduction of new data). These two kinds of problems will be studied before the end of 1995.

5.6 Retrieval and Document order form

To order for one of the GAPHYOR services please use enclosed order form just before Data Tables.

6 New structure of Data

Every GAPHYOR entry includes the fields shown in Section 8. It is written on a line as :

/se/M1,M2,M3/pr/M4,M5,M6/
/info/enva/val/rem/
/an/jo,vo,page/au1,au2,...au10/nastci/

The meaning of all these descriptors is given below. But in the Handbook (see Section3 some fields have been eliminated and the format of a multiplet is written on a line as :

/se/M1,M2,M3/pr/.../
/info/enva/val/rem/
/an,jo,vo,page/au1/MULT/

6.1 Chemical elements

The ordering of the file is based on the periodic classification of elements. For the needs of GAPHYOR, the traditional list of families has been slightly modified as follows :

H H D T Ap (antiproton)
R He Ne Ar Kr Xe Rn
1A Li Na K Rb Cs Fr
2A Be Mg Ca Sr Ba Ra
3A B Al Ga In TI
4A C Si Ge Sn Pb
5A N P As Sb Bi Po
6A O S Se Te
7A F Cl Br I At
3B Sc Y La Ac
4B Ti Zr Hf
5B V Nb Ta
6B Cr Mo W
7B Mn Tc Re
8A Fe Co Ni
1B Cu Ag Au
2B Zn Cd Hg
8B Ru Rh Pd
9A Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu
8C Os Ir Pt
9D Th Pa U
9E Np Pu Am Cm Bk Cf Es Fm Mv
9F No Lw Ff(104) Gg(105) Hh(106)
Ii(107) Jj(108) Kk(109) Ll(110)
EE Ps (positronium e^+e^-),
Mu (muonium μ^+e^-), Um (antimuonium μ^-e^+)
NN Aa Bb Cc Dd : General papers
PA (Fields and particles) :
M(unspecified reactant)
hv(photon) ef(electric field) bf(magnetic field)
emf(electromagnetic field)
e (electron), mu(meson μ), neu(neutron)
ionized gas, plasma

Elements Aa Bb Cc Dd (family NN) are used to code general results which are a priori valid for all the elements. Aa is also used for iso-electronic series (cf. Section 6.9).

6.2 Sections SE

SE written at the beginning of the line can take the values 1 to 5 following the scheme :

1. Properties of atoms and molecules
2. Photonic collisions
3. Electronic collisions
4. Collisions between atoms or molecules
5. Macroscopic properties

6.3 Initial state M1 M2 M3

The initial state can include 1, 2 or 3 reactants M1, M2, M3 which can be atoms, molecules (possibly ionized), electrons, photons, and other members of the family PA (fields and particles).

Atomic and molecular reactants Standard reactants are atoms or small molecules. They are coded following the scheme :

/n form ix/s/

which exhibits the 5 following fields :

- form *Chemical formula.* The chemical formula is written :

  /AA*l*BB*m*CC*n*DD*p*/

  where AA,... DD are chemical elements written in the order of the table of paragraph 6.1.
  The numbers l, m, n, p specify the formula, with the rules : 1 to 4 elements in the molecule, no more than 8 atoms in the molecule.

- i *Index of ionization* which gives the state of ionization of the molecule with the possible values :

0	neutral
+	singly charged positive ion
2+...99+	positive ion with 2...99 charges
n+	unspecified charge positive ion
2-...9-	negative ion with 2...9 charges
n-	unspecified charge negative ion

  Note that in the Volume 1 the ionization index in the initial state is limited to the upper value 2+. Multicharged ions with $q > 2$ are in the Volume 2.

- x *Index of excitation.* This specifies the state of excitation by a chain of characters built from the elementary characters $n, p, r, v, *, m, y, z, ?$ with the meanings :

n	isotopic effect
p	polarized reactant
r	rotational excitation
v	vibrational excitation
*	electronic excitation
m	metastable state
y	Rydberg state
z	collective excitation
?	unspecified excitation

- s *Internal structure* which specifies some aspects of the structure of the reactant : holes in inner shells, electrons replaced by a μ meson. It is a chain of characters built from the following elementary ones :

K	hole in K shell
L	hole in L shell
...	
H	hole in unspecified shell
...	
MU	electron replaced by a μ meson
1,2...	multiplicity of terms above

  for atoms having 1, 2, or 3 holes with no more than two in the same shell.

- n multiplicity of the reactant. When a same reactant is multiple, it is written only once and the index n written before the formula specifies its multiplicity. One can write an unspecified multiplicity as "n" (e.g. for multiphotonic effects).

Electrons, photons, fields, particles

The following notation is used for particles or fields :

e	electron
hv	photon
mu	meson μ (Mu designates the Muonium atom)
neu	neutron
ef	electric field
bf	magnetic field
emf	electromagnetic field
M	unspecified reactant.

The μ meson is just a heavy electron ; muonic collisions are then put in section SE = 3.

Remarks

- *More than three molecules in the initial state.* When there are more than three molecules in the initial state one keeps as M1, M2, M3 only the three most significant and the entry is given a descriptor INFO=4 .
- *Unspecified second or third body.* One finds in the litterature reactions written with an unspecified second or third body designated by the symbol (M). In GAPHYOR this is coded as M.

6.4 Final state M4 M5 M6

Sections 2, 3, 4

In Sections SE = 2, 3, 4 (collisions and reactions) one designates as M4, M5, M6 the particles existing after the collision. But in the Handbook this final state is ignored and just written as "..."

Sections 1, 5

- *In section 1* (structures) one means by "initial state" the atom or the molecule whose properties are described. The final state is then used to give some additional informations, but it is ignored in the Handbook.
- *In section 5* (macroscopic processes) initial state designates the base gas in which the macroscopic process occurs. The code for M1, M2, M3 can then assume the following forms :
  - neutral gases : a set of atoms or molecules
  - partially ionized gases : a set of neutral atoms or molecules (as for neutral gases). There is usually in the "final" state some additional information, for example the unspecified form *"ionized gas"* which just means that the gas is partially ionized. But this is again ignored in the Handbook.
  - fully ionized gases (or strongly ionized) : a schematic code *"plasma"* which just means that the base gas is a plasma.

Processes in two or three steps

- *Two steps.* To describe a two-step process, the entry is given a descriptor INFO=2
- *Three steps.* To describe a three-step process, the entry is given a descriptor INFO=3.

More than three particles in final state

In some cases the final state (not shown in the Handbook) includes more than 3 particles. In such cases the entry is given a descriptor INFO=7.

6.5 Process PR

- *The full list* of processes, ordered by section, is given in Section 10, together with their codes.
- *Hierarchy of processes.* In some cases the process can correspond to two or more values of PR, each of them describing one of its aspects. (*Example* : Dissociative ionization : IN or DS). A choice is then made between the possible values of PR by applying rules of hierarchization. The general idea is to give priority to the description of changes in electrical charges, then to change in structures of molecules, and finally to changes in states of excitation. Whence the priority rules :

$$IN, AT, DT > DS, DX, AS, > EX, XX$$

6.6 Additional informations

The descriptor INFO is used to specify some importants aspects of the process or of the publication. It is a chain of characters built from the following elementary ones :

- Type of Data :

S	Total and transport cross sections (absolute values)
W	Differential cross sections (absolute values)
K	Reaction rate constants (absolute values)
U	Oscillator, line, or collision strength
P	Probabilities of transition or collision
<	Radiative lifetimes

- Nature of Data :

R	Review data
E	Experimental data
T	Theoretical data
D	Data deduced from other Data
X	Purely bibliographical review

- Energy domains :

L	Thermal energies (E < 10 eV CM system)
J	Medium energies (10 eV < E < 10 keV CM system)
H	High energies (E > 10 keV CM system)

- Additional informations :

2	Two-step process
3	Three-step process
I	Iso-electronic series
4	Four-body reaction
7	More than 3 molecules in the final state
8	Clusters
/	Gas-surface interactions

6.7 Numerical Data

The numerical Data are given in three fields :

- **ENVA** which gives the energy or energy range covered by the numerical Data.
- **VAL** which gives the values them-selves (lifetimes, cross-sections, reaction rates, ...)
- **REM** which gives additional informations.

These three fields are printed together (including also INFO) and separated by a /.

6.8 Ordering of Data

The ordering of Data in the Handbook is made by a rather elaborate algorithm to follow as well as possible the physical feeling of users. Let us just explain it here by a few simple rules :

- *General organization by number of elements and families* : The Handbook is organized, as shown in Table of Contents, first by number of elements in the sytem, and then by families of the periodic classification.
- *Organization by Sections* : For a given family (e.g. Noble gases), or a given group of families (e.g. Hydrogen + Carbon family), the entries are first ordered by Sections (cf. Paragraph 2.2).
- *Organization within a section* : In a given section, the first entries listed are those where the first molecule (see below the order of molecules) includes the first element of the first family (e.g. H in the Hydrogen family H, D, T). They are ordered by increasing number of this first element
- *Writing of a molecule* : the elements in a molecule are written in the order of Section 2.1. Examples : H2O ; H4C ; NaCl ; ClBr.
- *Order of molecules in initial state* : the first molecule contains the first element but with the minimum number of atoms of it. Examples . H2O,Ar ; HO,H2O
- *Ordering of two molecules with the same formula* : the neutral comes before the ion. Example : H2,H2+. Ground state comes before excited states. Example : He+,He+*.
- *Photon and electron in initial state* : Photon and electron come after atomic or molecular reactants. Example : H+,hv,e

6.9 Special Data

The second volume (Special Data) includes the four following chapters extending in some way the usual scope of GAPHYOR :

Multicharged ions Positive ions of charges 2+, 3+...99+ are described with the same notations as for Standard Data. But one has also included synthetic entries grouping a homonuclear sequence of positive ions with for instance the notation :

$$\mathbf{Ar/n + (02 - 12)}$$

Iso-electronic series An iso-electronic series is written as :

$$\mathbf{Aa(He)Z(02 - 12)}$$

which describes the Helium series from $Z = 2$ (Li) to $Z = 10$ (Ne).

Clusters A cluster is a big molecule including a group of identical atoms or small molecules ("motif") usually bound to a core which may be itself a small molecule or an atom. The core is written first, followed by the "motif" between brackets. Examples :

$$\mathbf{He(H2O)3/+, He(H2O)3(H3N)4/+, (C)60}$$

Note that in the second case there are two motifs while in the third one there is no core.

Gas-Surface interactions For gas-surface interactions we use the following notations :

(AA)s	solid AA
(AA-BB)s	alloy with AA dominant.
(AA/BBm)s	molecular solid
(AA)a(BB)s	AA adsorbed on solid BB

The structure index s is used to describe roughly the structure of the solid with the notations :

G	amorphous solid (like glass)
M	mono-crystal
P	poly-crystalline solid
L	liquid

Note that a *liquid* surface is written like a solid, for example (Hg)s, but with an L as the structure index

6.10 Bibliography and Multiplicity : AN JO VO PAGE AU1 MULT

The journal is coded on 4 characters following the code given in Section 5. The descriptor **JO** is also used to code references which are not regular journals using the following values .

THES Doctorate thesis or PHD
THE3 3rd cycle, engineer, or master thesis
REPT report
BOOK book
CONF conference

with the rules of priority :

CONF > BOOK > REPT > THES, THE3 For the first three cases the reference is completed in VO.

The GAPHYOR file keeps for every paper up to 10 names of authors, but in the Handbook one has kept only the first author **AU1**.

A descriptor **NASTCI** is used in the Base to localize the laboratory of the first author. It is omitted in the Handbook and replaced by **MULT** which gives the number of entries in the considered "multiplet".

8 Annex 1 : Examples

Descriptor	Meaning	Examples
SE	Section	1, 2, 3, 4, 5
M1(n1/form1/i1x1/s1)	Initial state reactant	
n1	Multiplicity of a reactant	21, n
form1	Chemical formula	Si1Br4, e, mu, neu, hv, M, (He)(H2O)4, (N)a(Fe-Co)s
i1	Ionization	0, +, 12+, n+, - , 8-, n-
x1	Excitation	vrnp,*mvrnp, *yvrnp
s1	Internal structure	K1, K1L1, H1, MU1, G, M, P, L
M2(n2/form2/i2x2/s2)	cf. M1	cf. M1
M3(n3/form3/i3x3/s3)	cf. M1	cf. M1
PR	Process	DS (Dissociation)
M4(n4/form4/i4x4/s4)	Final state reactant	cf. M1
M5(n5/form5/i5x5/s5)	cf. M1	cf. M1
M6(n6/form6/i6x6/s6)	cf. M1	cf. M1
INFO	Data, energies,...	SWKUP<RETDXLJH23I47
ENVA	Limit values of energies	1-10 eV
VAL	Numerical values	$4.10E-12*0.45\,cm3\,s-1$
REM	Remarks	(free text)
AN	Year of publication	92
JO	Journal	PR/A
VO	Volume	45
PAGE	Page	2544
AU1	First author	Dupont J.L.
NASTCI	Place (laboratory of AU1)	USCABE
MULT	Number ot entries in a multiplet	1, 2, 83

9 Annex 2 : Value indexes

One has seen in Section 3 that the Handbook is a selection taken from the whole GAPHYOR Database, and that the selection cnteria depend on quality and actuality of data. More precisely the selection is made as follows :

- Assigning a value index to every GAPHYOR record
- Production of a catalog of "multiplets" and selection
- Selection of the best entry in every "multiplet"
- Elimination of entries below a minimum value index
- Separation in two volumes

The basic quantity in this program is then the value index assigned to every entry. Let us now define the rules choosen for it : the value index is the sum of six partial indexes as shown in Tables 3 and 4 which take account of the quality of bibliographical (Vjo, Van, Vau), factual (Vse, Vin), and numerical (Vnu) data.

Bibliographical						Factual				Numerical	
An	Van	Journal	Vjo	Authors	Vau	Sect.	Vse	Info	Vin	Data	Vnu
95	45	JCP	92	10 aut.	45	2	50	r	10	Energies	25
94	42	JPC	91	9 aut.	40	3	50	e	10	Values	50
...	...	PR/A	90	...	...	4	50	s k <	5	Remarks	25
85	15	CHPL	89	5 aut.	25	5	20	p u l	5		
84	12	JP/B	88	4 aut.	20	1	0	w	2		
83	9	JACS	87	3 aut.	15						
82	6	JRD	86	2 aut.	10						
81	3	...	...	1 aut.	5						
Max	45		92		45		50		25		100

Table 3: Value indexes for the three categories of Data in an entry

10 Annex 3 : Processes list

Section 1. Structures

EN Energy levels , wave functions
EA Unstable energy levels
EI Energy of isomerization
VR Potentiel curves, structure of molecules
DP Dipolar moments
NP Multipolar moments
PE Electric (or magnetic) polarizability
PF Dynamical polarizability (frequency funct.)
TR Radiative transition (probability,...)
XX Change of excitation (non-radiative)
IN Autoionization
DT Autodetachment
DS Autodissociation
DG Autodesorption

Section 2. Photonic collisions

SN Effective absorption, total diffusion
AN True absorption
SC Angular diffusion (scattering)
EL Elastic diffusion (Thomson, Rayleigh)
DO Depolarization, Change of polarization
NL Non-linear effects
EX Photoexcitation
ER Emission of line
DX Photodeexcitation (stimulated emission)
XX Changeof excitation
FF Free-free absorption (inv. bremsstrahlung)
IN Photoionization
IM Creation of an ion pair (positive-negative)
DT Photodetachment
DS Photodissociation
DG Photodesorption
EE Photoemission of electrons (ions) by solids

Section 3. Collisions of electrons

SN Total cross sections
SM Transport cross sections (momentum, ...)
SC Angular diffusion (scattering)
PR Unknown products
EL Elastic collision
DO Depolarization, Change of polarization
EX Excitation
ER Emission of line
DX Deexcitation
XX Change of excitation
BS Bremsstrahlung
IN Ionization
IM Creation of an ion pair (positive-negative)
DT Detachment
AT Attachment
RC Recombination (unknown mechanism)
RR Radiative recombination
RD Dielectronic recombination
RE e-e-i recombination
RO e-i-o recombination
RS Dissociative recombination
DS Dissociation
DG Desorption
EE Emission of electrons by a solid
PU Emission of neutrals or ions by solids (sputtering)

Section 4. Atomic and molecular collisions

EN Energy or enthalpy of reaction
KE Constant of chemical equilibrium
SN Total cross sections
SM Transport cross sections (momentum, ..)
SC Angular diffusion (scattering)
SP Stopping power
PR Unknown products
EL Elastic collision
DO Depolarization, change of polarization
EX Excitation
ER Emission of line
DX Deexcitation (quenching)
XX Change of excitation
TE Excitation transfer
IN Ionization
IM Creation of an ion pair (positive-negative)
DT Detachment
TI Ionizing charge transfer
RI Recombination ion-ion
CX Charge transfer
XD Dissociative charge transfer
CA Capture of electrons
SR Loss of electrons (stripping)
DS Dissociation
IR Interchange reaction (of one or several atoms)
IA Associative interchange reaction
ID Dissociative interchange reaction
AS Association
DG Desorption
AD Adsorption
EE Emission of electrons by a solid
PU Emission of neutrals or ions by solids (sputtering)

Section 5. Macroscopic properties

ST Statistics of levels
FT Thermodynamic functions
VA Amplitude of vibration
ZT Function of partition
CO Correlations
PV Compressibility, equation of state
PE Dielectric and magnetic constants
DN Diffusion
VI Viscosity
CT Thermal conductivity
TD Thermal diffusion
DM Diffusion of metastables
RN Relaxation in gas neutral or ionized gases
LW Line broadening and shift (collisional effects)
LA Gas laser
PI First coefficient of Townsend
DT Detachment
AT Attachment
RC Recombination (unknown mechanism)
FE Distribution function of electrons
ME Mobility of electrons
CE Electrical conductivity
DE Diffusion of electrons
MD Characteristic temperature of electrons (D/μ)
PC Power delivered by electron-neutral collisions
FI Distribution function of ions
MI Mobility of ions
DI Diffusion of ions
DA Ambipolar diffusion
DG Autodesorption

11 Annex 4 : Publications Code

JOUR			Vjo	JOUR			Vjo
AAMP	Adv. atom. molec. phys.	US	0	*JPHT	J. Photochem.	SW	37
ACHP	Adv. chem. phys.	US	0	*JPJ	J. Phys. Soc. Jap.	JA	55
*ADND	Atom.data and nucl.data tables	US	84	*JQS	J. Quant. Spect. Rad. Transf.	US	69
*APJ	Astrophys. J.	US	49	*JRD	J. Phys. Chem. Ref. Data	US	86
*APJS	Astrophys. J. Sup.Ser.	US	9	*JVSA	J. Vac. Sci. Technol. A	US	16
APL	Appl. Physics Letters	US	51	*JVSB	J. Vac. Sci. Technol. B	US	2
APOP	Appl. Opt.	US	40	*KNCT	Kinetics and Catalysis	IS	43
*APPA	Acta Phys. Pol. A	PL	18	KVYE	Khim. Vys. Energ.	SU	5
*APSL	Acta Phys. Slov.	CS	7	*LTFS	Litov. Fiz. Sbor.	SU	17
*ARPC	Annu. Rev. Phys. Chem.	US	39	*MOL	Molecular Phys.	UK	82
*ASAR	Astron. and Astrophys.	DE	24	NJDC	Nouveau J. de Chimie	FR	38
*ASAS	Astron. and Astrophys. Suppl. Ser.	DE	8	OAS	Opt. and Spectroscopy (OASK transl.)	SU	79
*BBUN	Ber. Bunsengesellsch. Phys.Chem.	DE	50	*OASK	Opt. i Spektr.	SU	79
*BCSJ	Bull. Chem. Soc. Jap.	JA	58	OPTC	Opt. Communic.	NL	52
*BEPL	Beitr.Plas.Phys.(Contr.Plas.Phys.)	DE	35	PCPP	Plasma Chem. and Plasma Process	UK	10
*CHPH	Chem. Phys.	NL	81	PH/A	Physica A	NL	59
*CHPL	Chem. Phys. Lett.	NL	89	*PL/A	Phys. Lett. A	NL	65
*CJCH	Canad. J. Chem.	CD	63	PPCF	Plasma Phys. Contr. Fusion	UK	0
*CJP	Canad. J. Phys.	CD	74	*PR/A	Phys. Rev. A	US	90
*CR/2	Comptes-rend.Ac.Sc.2 (ex CR/B)	FR	48	*PRL	Phys. Rev. Lett.	US	72
CR/B	Comptes-rend.Ac.Sc.B (now CR/2)	FR	48	*PSC	Physica Scripta	SD	75
*CZJB	Czekosl. J. Phys. B	CS	11	*RMPH	Rev. Mod. Phys.	US	19
DOKL	Dokl Akad.Nauk. (DOKL Transl.)	SU	25	SJPP	Sov. J. of Plasma Phys. (FIZP transl.)	SU	14
*DOKN	Dokl.Akad.Nauk.	SU	25	*SPCA	Spectrochem. Acta A	UK	44
*EUPL	Europhysics Lett.	SW	29	SPTP	Sov. Phys. Tech.Phys (ZTF transl.)	US	34
*FIZP	Fiz. Plazmy	SU	14	SSRP	Surf. Sci. Reports	NL	20
*FRDD	Faraday discussions chem. Soc.	UK	46	STBN	Struct. and Bondg.	DE	13
HTSU	High Temperatures (TPVT transl.)	US	26	*TEKH	Teor. Exper. Khim.	SU	33
*IJCK	Int J. Chem. Kinet.	US	64	THCA	Theor. Chem. Acta	DE	62
*IJMS	Int. J. Mass spec. ion. phys.	NL	83	*TPVT	Teplofiz. vys. temp.	SU	26
IJPB	Indian J. Phys B	IN	15	USPK	Usp. Fiz. Nauk. (USPN Transl.)	US	30
IJPP	Indian J. pure applied phys.	IN	0	*USPN	Usp. Fiz. Nauk.	SU	30
*IJQC	Int. J. Quant. Chem.	US	57	*ZETL	Zh.Eksp. i Teor.Fiz. Pis'ma v Redak.	SU	23
*IJQS	Int. J. Quant. Chem. Symp.	US	42	*ZETP	Zh.Eksp.i Teor.Fiz.	SU	66
*INOR	Inorg. Chem.	US	67	*ZFKH	Zh. Fiz Khim.	SU	61
IVZF	Izv.Vys Uchebn.Zaved.Fis.	SU	3	ZN/A	Z. Naturforschung A	DE	41
IVZK	Izv.Vys.Uchebn.Zaved.Khim.Tech.	SU	1	*ZNKH	Zh. Neorg. Khim	SU	45
*JACS	J. Amer. Chem. Soc.	US	87	ZP/A	Z. Phys. A	DE	0
JAPH	J. Appl. Phys.	US	60	*ZP/D	Z. Phys. D	DE	80
*JCP	J. Chem. Phys.	US	92	*ZSKH	Zh. Strukt. Khim.	SU	47
*JCPB	J. Chim. Phys. Chim. Bio.	FR	68	*ZTF	Zh. Tekhn. Fiz.	SU	34
JCSF	J. Chem. Soc. Faraday Trans.	SF	77	BOOK			
JDP	J. Physique	FR	70	HCIO	Janev R K, Ph.high.charg.ions, Berlin	DB	0
*JDP2	J. Physique 2	FR	70	PHIA	Marrus,Ph.high.ion.at.NATO/asis/b201	US	0
*JDP4	J. Physique 4 (ex JDPC)	FR	56	REPT			
JDPC	J. Physique Colloques (now JDP2)	FR	56	CAMD	Bull.atom.mol.Data res. Beijing	RC	0
*JESP	J. Electron Spectr. Relat. Phen.	NL	54	IPPJ	Institute of Plasma phys. Nagoya	JA	31
JETL	Sov. Phys. JETP Letters	SU	1	*MAPL	Max Planck Inst. Garching	DE	4
JETP	Sov. Phys. JETP (transl ZETP)	US	66	*NIFD	Nat.Ins.Fusion sci.(Data rept.)Nagoya	JA	31
JFI	J. chem.soc.Faraday Tr.I (JCSF)	UK	0	*ORNL	Oak Ridge Nat. Lab.	US	27
JFII	J. chem.soc.Faraday Tr.II (JCSF)	UK	0	CONF			
*JGPR	J. Geophys. res.	US	28	AIPC	AIP Conf., e-mol.scatt, photoionization	US	0
*JJAL	Jap. J. Appl. Phys. Lett.	JA	6	AMDS	At.mol.data Space Astr., Buenos-Ayres	DB	0
*JJAP	Jap. J. Appl. Phys.	JA	1	AMFT	At.mol.data for Fusion, Cadarache	FR	0
*JMSC	J. Molec. Stuctures (theo-chem.)	NL	85	AMPI	Europ.st.conf.at.mol.phys.ion.gases	XX	0
*JMSP	J. Molec. Spectroscopy	US	78	*ATPH	Int.conf. Atom. Phys.	XX	12
*JMSR	J. Molec. Stuctures	NL	71	DIAM	Coll.Dyn.ions, atomes, molecules	FR	0
JNBS	J. of res. Nat. Bur. St.	UK	0	*EACC	I.conf.Phys.electr.atom.Coll.(contr.pap.)	XX	73
*JOSA	J. Opt. Soc. Amer.	US	76	*EACI	I.conf.Phys.electr.atom.Coll.(inv.pap.)	XX	36
*JP/B	J. Phys. B	UK	88	*GECO	Gaseous Electronics conf.	US	53
*JP/D	J. Phys. D	UK	32	*PIGC	I.conf.Phenom.ioniz.gases (contr.pap.)	XX	21
*JPC	J. Phys. Chem.	US	91	PLCH	Plasma Chem.(IUPAC Symp) Prog.rept.	XX	0

Table 4: Publications code (abstract) with journals value indexes Vjo : an asterisk means that this publication is regularly analyzed by one of GAPHYOR experts.

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Activity report at the Russian Scientific Centre "Kurchatov Institute" 1993/1995

V.A.Abramov
Institute of Nuclear Fusion
Russian Scientific Centre "Kurchatov Institute"
123182,Moscow,Russia

The present activities on the field of collection,dissiminati-on and evaluation of (A+M) data for fusion performed in the Institute of Nuclear Fusion of the Russian Scientific Centre"Kur-chatov Institute" are connected both the present tokamak research and the ITER design study and the DEMO design study.As previously, the Russian bibliography of (A+M) data for fusion are collected. THe corresponding collection is submitted to the "International Bulletin on Atomic and Molecular Data for Fusion".

Because of the interest to the innovation schemes of the liquid-metai limiter the data about the cross-sections and rates of dif-ferent elementary processes involving Li-ions have been calculated in the collaboration with Prof.L.A.Vainshtein.

The calculations of the radiative cooling rates for Ne-seeded plasmas with taking into account the charge-exchange between different Ne-ions and neutral hydrogen atoms are in progress.The

electron density effects are also taken into consideration.

The analysis some processes from the point of view of the applicability for the ITER diagnostics is performed(V.A.Abramov).Now the activity concerning the data base for the JET diagnostics is in progress(V.A.Abramov,I.V.Moskalenko,Scheglov).

The group headed by Dr.V.A.Belyaev are performing the experimental study of the molecular hydrogen ions dissociation due to self-collision at low energies (less than 20 eV) on the DIVA device.

THe activities in the field of the plasma-surface interactions are carried out in the laboratory headed by Prof.M.I.Guseva.The self-sputtering of berillium at the low energies is under investigation.The special efforts will be done to study the angular dependence of the self-sputtering yield.

THe experimental program to study the vibrational state of hydrogen molecules and molecular ions after the reflection from the Be,C and W is initiated (the collaboration with the group headed by Dr.V.A.Kurnaev from the Moscow Engineering- Physics Institute). THe results of this program are very important for the ITER divertor design study.

On-going and future activities:

1) Data compilation for such impurities as Ne,Ar,W which are important for the accurate consideration of the radiative divertor for the ITER.

2)Calculation of the radiative cooling rates for Ne-seeded plasmas.These results are necessary to evaluate the possibility to have the transition from the H-mode to L-mode in the ITER because the threshold power for this transition depends on the energy flux

across the separatrix.

3)Evaluation of the excitation cross-sections (rates) for the vanadium ions.

4)Evaluation of the data for the angular dependence of the self-sputtering yield for some materials.

5)Compilation and evaluation data for some processes involving H and H_2

Progress Report on the A+M Data Activites at CRAAMD September 1993 – June 1995

Sun YongSheng
Institute of Applied Phydics and Computational Mathematics
Beijing, China

We (CRAAMD) have done the following jobs since last network meeting in September 1993:

A. For use of the ITER Divertor Physics Design

(1) "ALADDIN Format of Cross Sections for H^+, H_2^+, H_3^+, H, H_2 and H^- in H_2 for energies from 0.1eV to 100eV" was given by Wang Y.,Sun Y.S., Qiu Y.B. IAPCM, Beijing.

In this work, the recommended data published by Phelps(1990) and the Janev's fitting formula were used.

In detail, please see "Bulletin on A+M Data Research" No.1, 17(1995), CRAAMD–AM–6.

(2) "Cross Sections for Electron Collisions with Hydrogen Molecules and Molecular Ions" were compiled and evaluated by Zhou Z.F., Xu Z., Chen J., Liu Y.Y.

Department of Modern Physics, Univ. of Scie. and Tech. of China, Hefei City, Anhui Province.

In this paper, the data of elastic scattering, excitation, dissociation, ionization, attachment, and recombination of hydrogen molecules H_2 and molecular ions (H_2^+, H_3^+) by electron impact (Until 1993) were compiled and evaluated.

See "Bulletin on A+M Data Research" No.2, 1(1995), CRAAMD-AM-7.

We hope that our works above will be of help to the A+M Data Centre Network.

B. For use of plasma physics research, our following papers have been published (in English, IAPCM, only):

(1) Qiu Y.H., Li S.C., Sun Y.S.
Dielectronic Recombination into Excited Levels of Ni-like Titanium from F-like Low-lying States
Phys. Scripta. Vol.47(1993)192

(2) Qiu Y.H., Li S.C., Sun Y.S.
Dielectronic Spectra for Ne-like Titanium from F-like Low-lying States
At.Data.Nucl.Data Tabs. 55(1993)1

(3) Sun Y.S., Meng X.J., Li S.C.
Electron Conductive Opacities for Partial Ionization Gases
JQSRT. Vol.51(1994)411

(4) Chen G.X., Fang Q.Y., Cai W.
Theoretical Simulations of Ni-like Laser Lines
Chin.Phys.Lett.,Vol.11, No.9(1994)533

(5) Chen G.X.
Core-polarization on Hyperfine Interaction Constants in Metastable State $3d^2$ of ^{45}Sc II
Phys.Lett.A 193(1994)451

(6) Yuan J.K., Sun Y.S., Zheng S.T.
Differential Cross Sections for the Elastic Scattering of Electrons in Hot Plasmas
J.Phys.B: Mol.Opt.Phys.28(1995)457

(7) Zhao L.B., Li S.C
Variation of Satellite Intensity Factors with n in the $1s^2 2s\varepsilon l_c \succ 1s^2 3dnl \succ 1s^2 2pnl$ Dielectronic Recombination of Lithium like Ions
Chin.J.A+M Phys. Vol.12, No.1(1995)99
(8) Chen G.X., Fang Q.Y., Cai W.
Wavelengths of Five Ni–like Laser Lines
Chin.J.A+M Phys. Vol.12, No.1(1995)91
(9) Yuan J.K., Sun Y.S., Zheng S.T.
Average Atom Model in Hot Plasmas
Chin.J.A+M Phys. Vol.12, No.2(1995)118
(10) Yuan J.K., Sun Y.S., Zheng S.T.
Inelastic Electron–Ion Scattering in Hot Dense Plasma
Submitted to J.Phys.B
(11) Yuan J.K., Sun Y.S., Zheng S.T.
Calculation of the Electrical Conductivity of Strongly Coupled Plasmas
Submitted to Phys.Rev.E

Data Collection at IPP-Garching

W.Eckstein
Max-Planck-Institut für Plasmaphysik, Garching, FRG
EURATOM-Association

Sputtering and Reflection

Plasma edge codes for fusion plasmas ask for a complete set of sputtering yields dependent on incident energy and angle and different bombarding species. Especially for new divertor designs not only the sputtering by hydrogen isotopes and selfsputtering but also by noble gas species is of importance.

Computer simulation with the binary collision program TRIM.SP (version TRVMC) is applied to create sputtering yield and sputtered energy data for energies up to 1 keV and 9 angles of incidence 0, 15, 30, 45, 55, 65, 75, 80, 85 degrees. The number of incident angles and the values are fixed; the number of incident energies is chosen so that the lowest yields given are about 10^{-5}, still lower values are put to zero. The data are given in the form of matrices (fixed energies in lines, fixed angles of incidence in columns). Similar matrices are determined for both particle and energy reflection coefficients. The matrices are stored at /afs/ipp/u/wge/trim.data/sputter.data and refl.data. So far, matrices for H, D, T, C, Ne. and Ar on C have been produced. As examples, the matrices for carbon selfsputtering yields and the three-dimensional plots of the sputtering yields and particle reflection coefficients for D, C, and Ne bombardment are given.

For the calculations the krypton-carbon interaction potential [1] and an equipartition of the Lindhard-Scharff [2] and the Oen-Robinson [3] inelastic energy loss models are applied. A target density of 1.85g/cm^3 and a surface binding energy of 7.41 eV are assumed for carbon. The data apply for a nearly flat surface.

In addition, the same program has been changed to determine energy and angular distributions of sputtered atoms with the same algorithm [4] as has been used for backscattered atoms [5,6]. Calculations are in preparation in a collaboration with the IPP

in Jülich.

References

1 W.D.Wilson, L.G.Haggmark, J.P.Biersack: Phys. Rev. B **15**, 2458 (1977)

2 J.Lindhard, M.Scharff: Phys. Rev. **124**, 128 (1961)

3 O.S.Oen, M.T.Robinson: Nucl. Instrum. Methods **132**, 647 (1976)

4 G.Bateman: Appl.Phys.Rep. No. 1, Princeton, USA (1980)

5 W.Eckstein, D.B.Heifetz: J. Nucl. Mater. **145 – 147**, 332 (1986)

6 D.Reiter, W.Eckstein, G.Giesen, H.J.Belitz: Jül- 2605, Jülich, FRG (1992)

Figure Captions.

Fig. 1. Sputtering yield of D on C

Fig. 2. Sputtering yield of C on C

Fig. 3. Sputtering yield of Ne on C

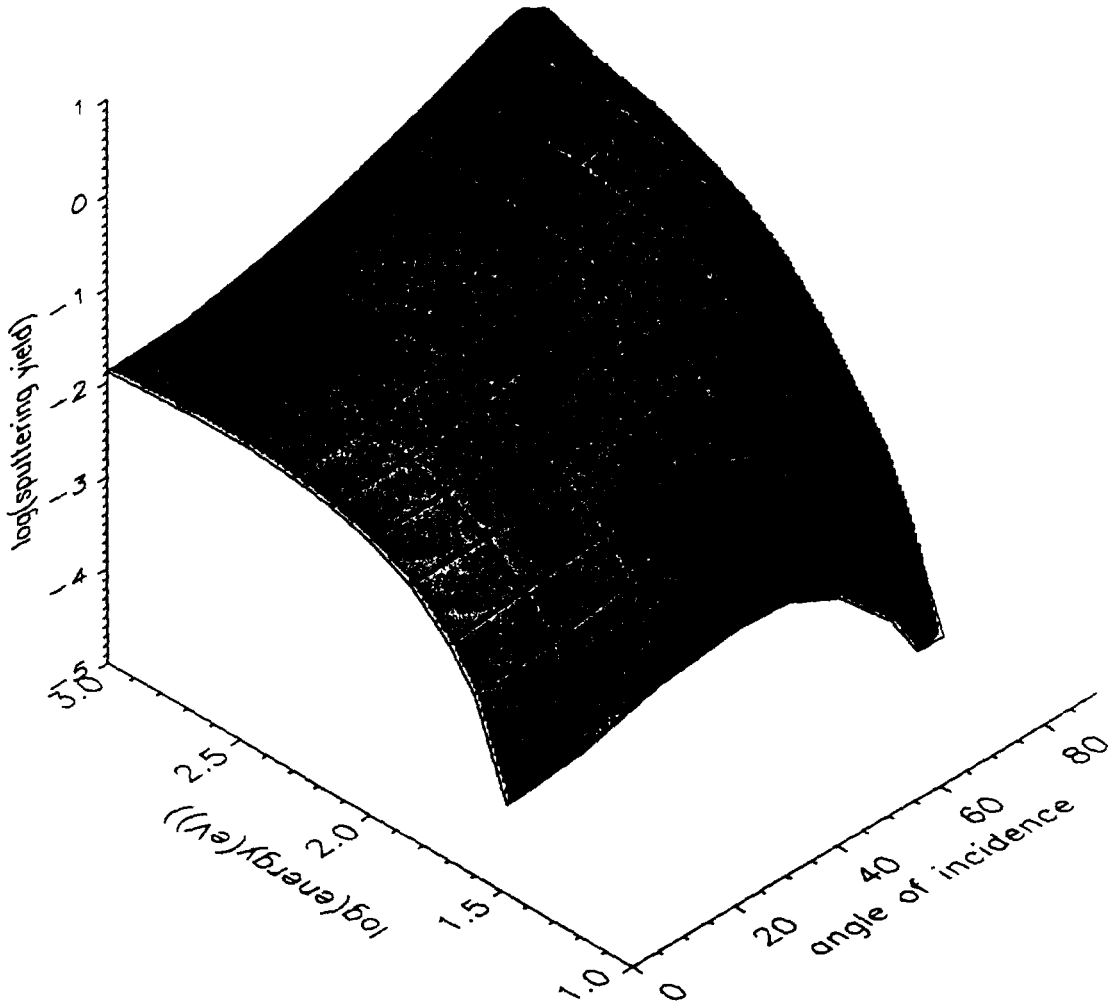
Fig. 4. Particle reflection coefficient of D on C

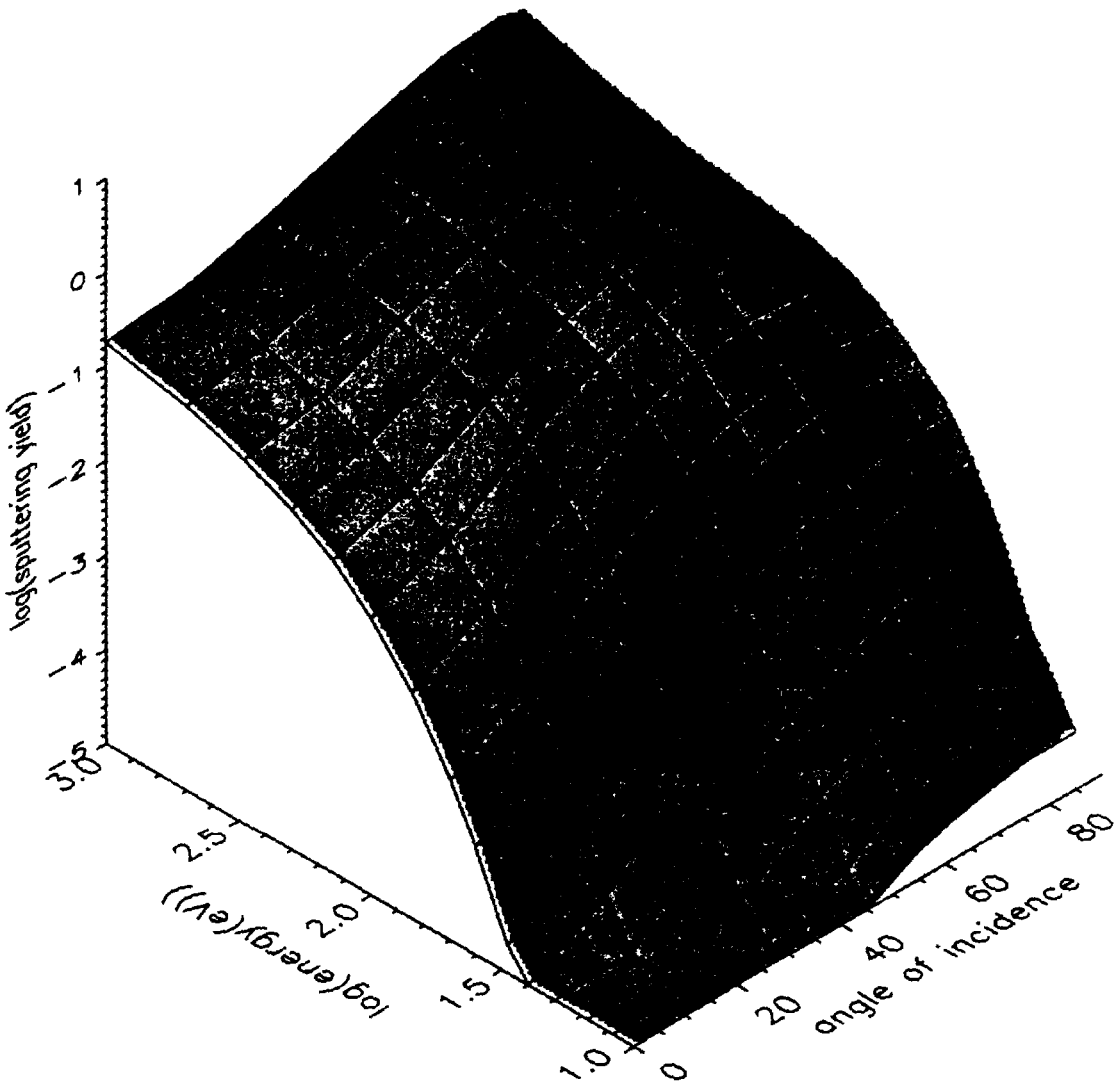
Fig. 5. Particle reflection coefficient of C on C

Fig. 6. Particle reflection coefficient of Ne on C

c sputtering yield : C -> C
c z1= 6 , m1= 12.01 , z2= 6 , m2= 12.01 , Es=7.41 , rho=1.85 g/cm**3
c ne=14, na=9

	0	15	30	45	55	65	75	80	85
8	.00000	.00000	.00000	.00000	.00000	.00000	.00001	.00001	.00001
10	.00000	.00000	.00000	.00001	.00002	.00003	.00004	.00004	.00004
12	.00000	.00000	.00000	.00002	.00005	.00007	.00008	.00009	.00009
15	.00000	.00000	.00002	.00009	.00015	.00020	.00024	.00026	.00026
20	.00000	.00001	.00008	.00036	.00067	.00118	.00173	.00195	.00205
25	.00000	.00003	.00028	.00128	.00290	.00502	.00661	.00713	.00712
30	.00002	.00010	.00081	.00395	.00802	.01305	.01553	.01552	.01603
40	.00014	.00060	.00373	.01556	.02852	.04060	.04158	.03997	.03845
50	.00052	.00189	.01038	.03582	.05806	.07504	.07570	.07032	.06366
70	.00257	.00731	.03009	.08402	.13420	.16270	.15060	.12770	.11010
100	.00884	.01962	.06527	.16550	.24500	.28910	.24490	.19920	.15350
140	.02132	.03949	.11120	.25210	.37350	.44260	.36530	.26040	.18250
200	.04137	.06756	.16310	.34920	.51560	.63300	.51400	.35290	.21120
300	.07163	.10630	.22650	.45980	.68250	.86290	.74160	.49430	.24220
500	.11620	.16130	.30540	.59840	.89090	1.17800	1.15200	.79230	.30140
1000	.17780	.22790	.39330	.73750	1.09900	1.55300	1.77100	1.44800	.49210


log(sputtering yield)
1
0
-1
-2
-3
-4
-5
3.0
2.5
2.0
1.5
1.0
log(energy(eV))
0
20
40
60
80
angle of incidence


log(sputtering yield)
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1.0
log(energy(eV))
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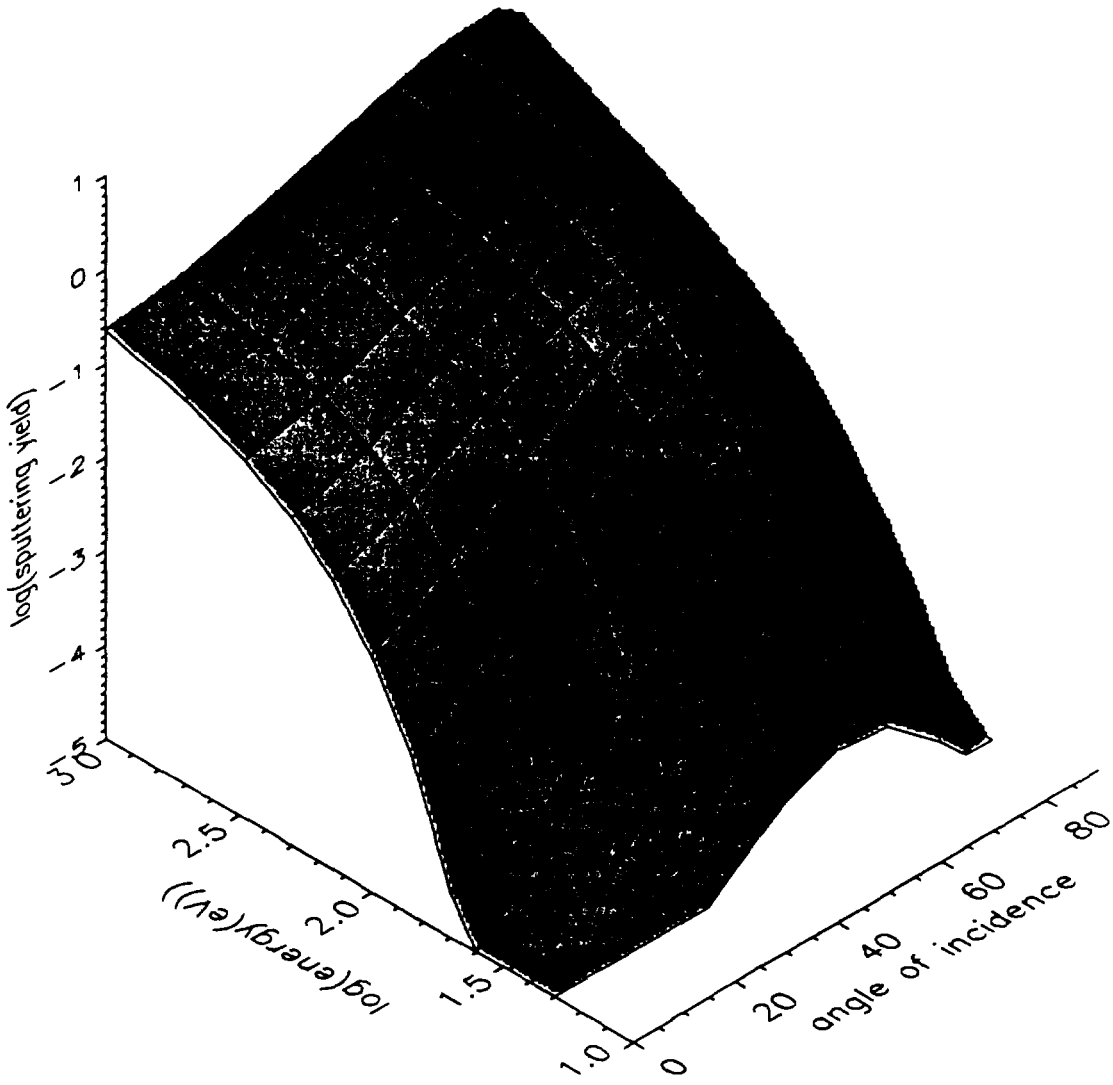
60
80
angle of incidence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log(energy(eV))
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angle of incidence
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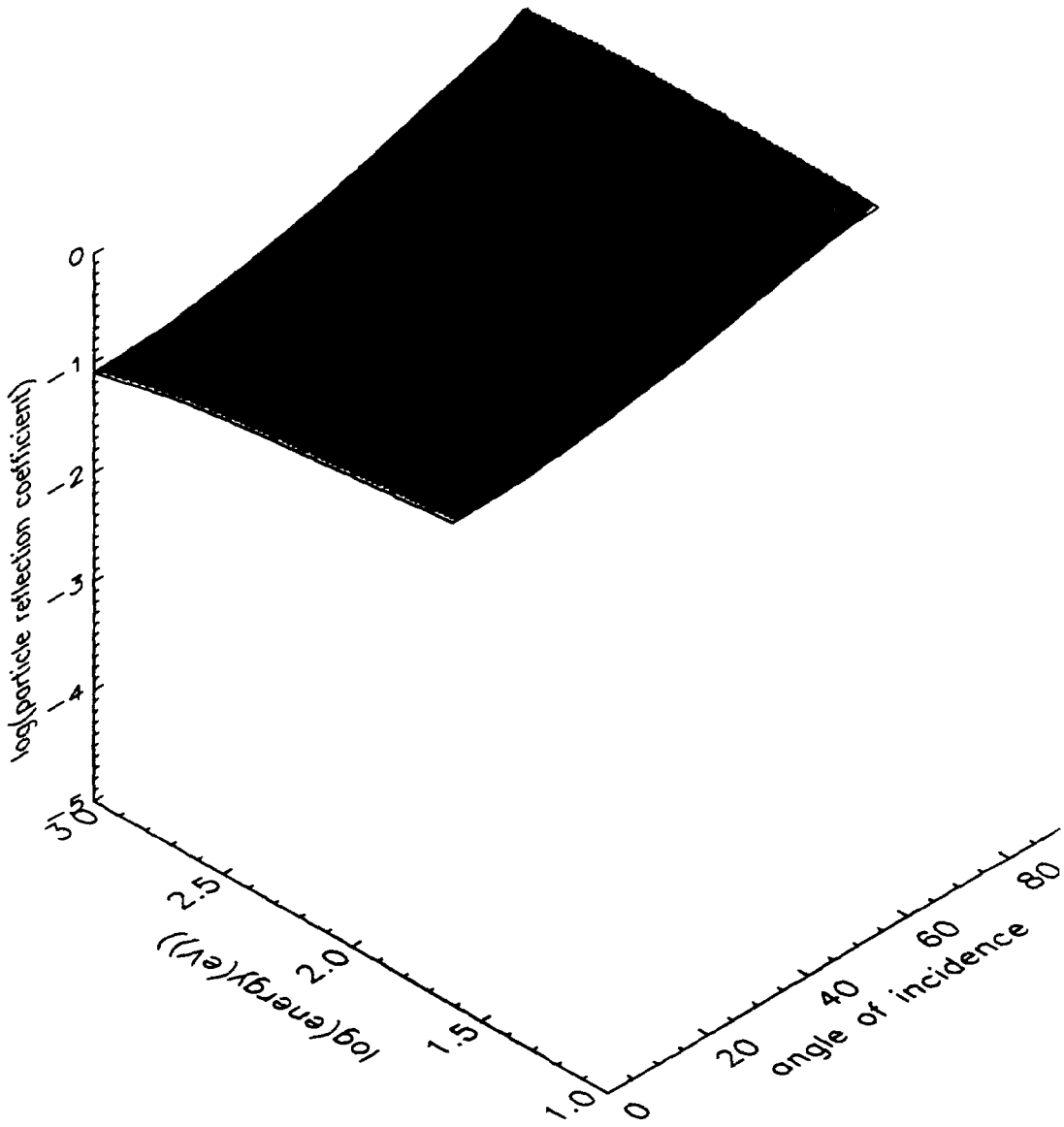
log(particle reflection coefficient)
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-1
-2
-3
-4
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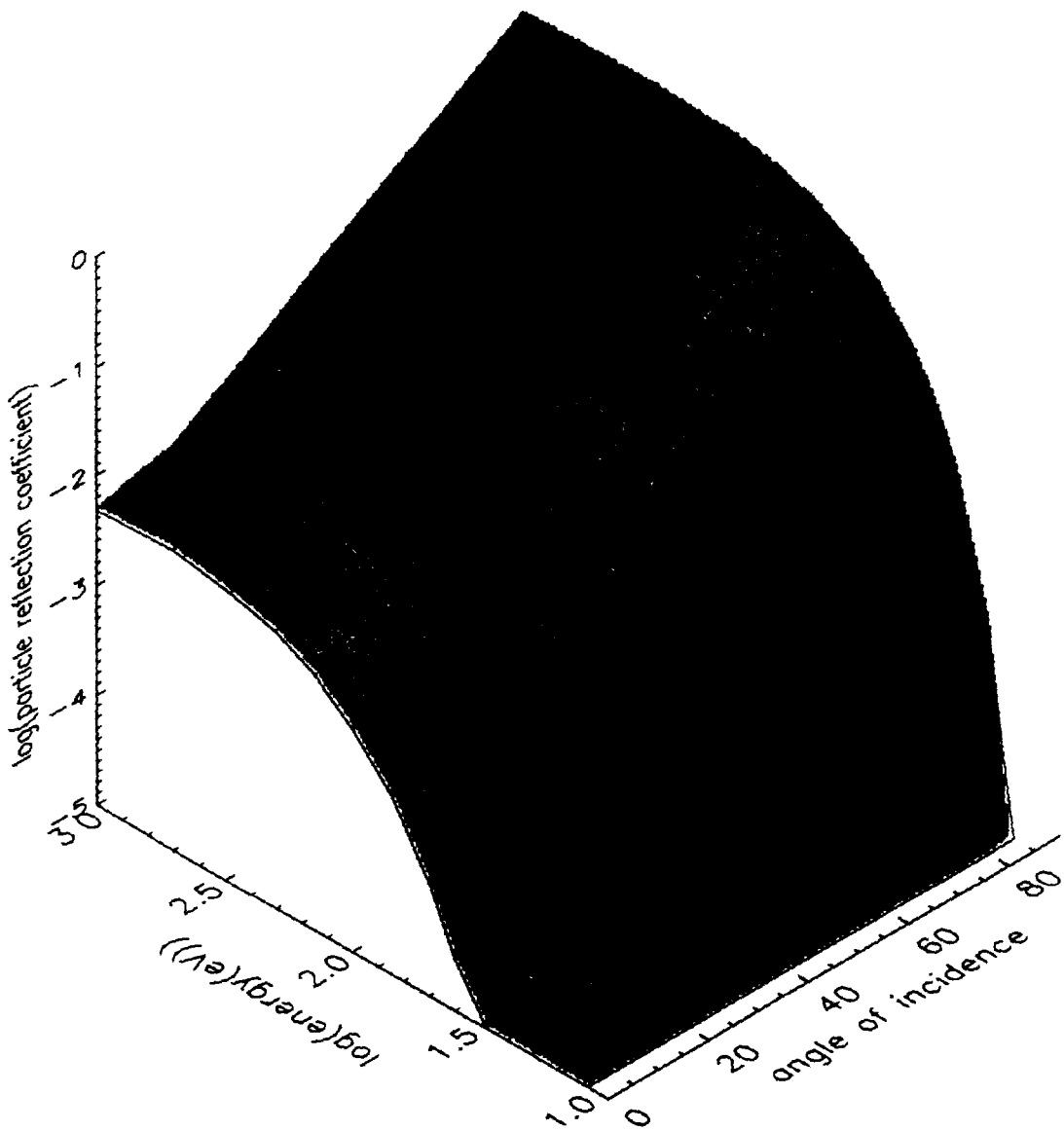
3.0
2.5
2.0
1.5
1.0
log(energy(ev))
0
20
40
60
80
angle of incidence


log(particle reflection coefficient)
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-3
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3.0
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2.0
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log(energy(eV))
0
20
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60
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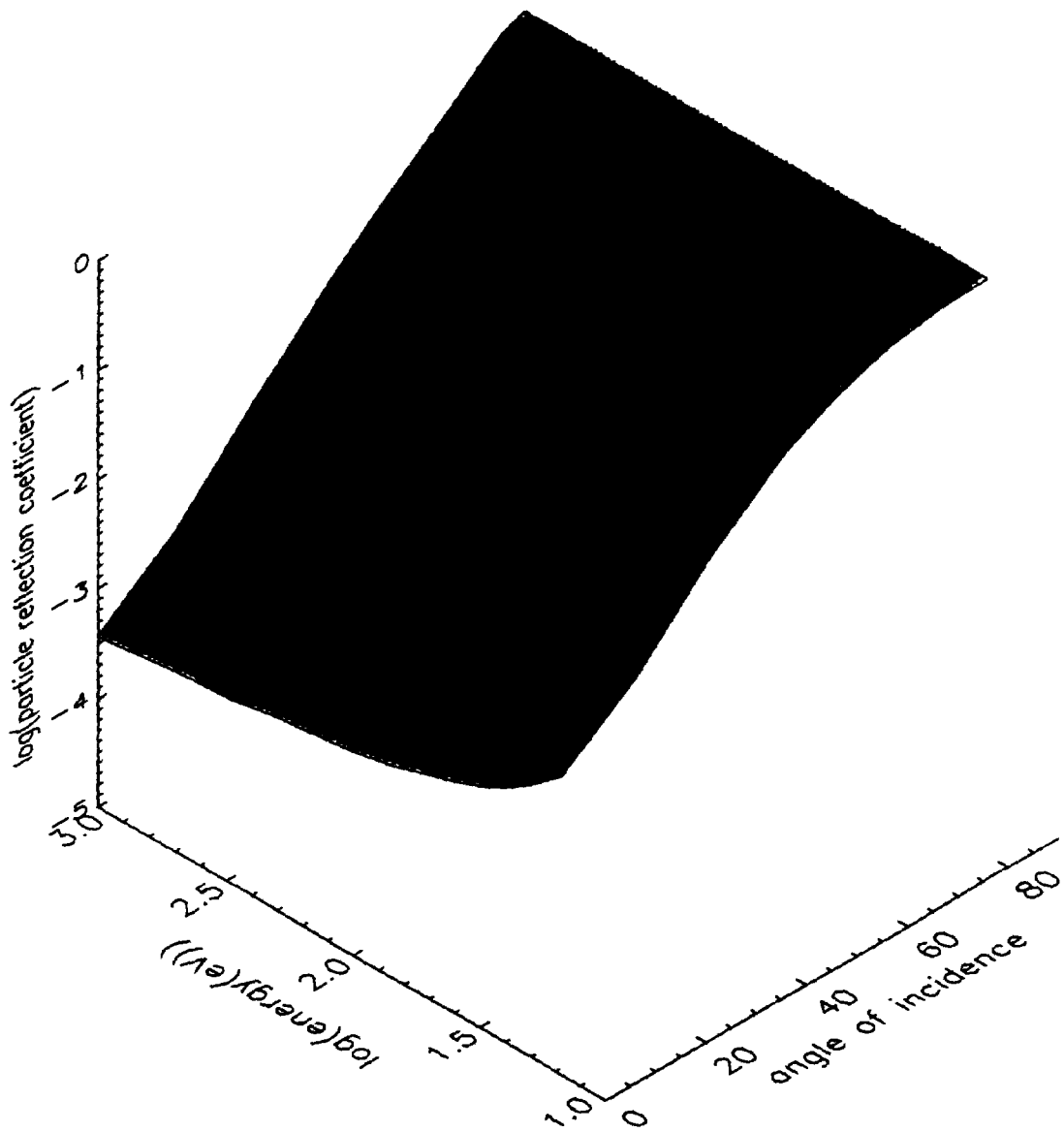
angle of incidence


log(particle reflection coefficient)
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log(energy(ev))
0
20
40
60
80
angle of incidence

Activities of A+M Data Study on Relating to Fusion Plasma at CNDC

Jinzhang Yao

The compilation and evaluation on particle reflection and physical sputtering from solid surfaces have been continued. And the calculation for radiative loss of plasma fusion has been developed at CNDC / A+M Unit.

Reflection

Particle and energy reflection coefficients for a large number of projectile–target combinations are evaluated. In present evaluation of reflection coefficients, the data source is taken from experimental measurements up to the end of 1994,new data calculated with improved bipartition model of ion transport which is partly taken into account angular correlation of energy loss and the influence of surface barrier by Luo, and the data calculated by modified empirical formula. The empirical formula is shown as

$$Q_e = \frac{\frac{0.705}{f}}{(1+(\frac{\varepsilon}{0.047})^{0.547}+(\frac{\varepsilon}{0.619})^{1.5})}$$

$$R_e = Q_e - exp(-\pi\varepsilon(M_1+M_2))$$

$$R_n = \frac{R_e}{r_e}$$

$$r_e = \frac{1}{(1+(\frac{\varepsilon}{0.133})^{0.285})} + \frac{0.530}{(1+(\frac{\varepsilon}{85})^{-1.46})}$$

$f = F(Z_1, Z_2, M_1, M_2, \varepsilon)$

refers to IPPJ–AM–41

The reduced energy is

$$\varepsilon = \frac{0.032534 M_2 E_0(eV)}{Z_1 Z_2 (M_1 + M_2)(Z_1^{\frac{2}{3}} + Z_2^{\frac{2}{3}})^{\frac{1}{2}}}$$

Our recommended data are determined to fit composite data optimal weights by Spline function. The recommended data substitute into the scale expression

$$R_n(or R_e) = \frac{A_1 ln(A_2 \varepsilon + e)}{1 + A_3 \varepsilon^{A_4} + A_5 \varepsilon^{A_6}} (1 - \frac{A_7}{\varepsilon})$$

The optimal values of parameters $A_1, A_2, \ldots\ldots A_7$ can be produced by method of generalized least–square. For instance, the results of D^+– C and D^+–Ni combinations are shown in fig.1 a,b,c,d.

Sputtering

Physical sputtering yields for a great number of projectile–target combinations have been evaluated at normal incidence. The data source are taken from in the possession of publications. We calculated the sputtering data using Bohdansky formula, and put the results calculated into data source for evaluation. The recommended data are determined to fit data with optimal weights by Spline function. Our recommended data compare with the results calculated by TRIM–91 code as seen in fig.2.

Radiative loss

We calculate the radiative loss for plasma impurity by modified corona model with metastable state effects. The results indicate that radiative power loss is necessarily taken to account under the electron temperature from 1 eV to 100 keV in design and operation to the local power balance and the total energy loss in plasma fusion device. As an example, the result of carbon plasma impurity is shown in fig.3.

Recent publications

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Communication of Nuclear Data Progress N0.10 (1993) 112
Yao jinzhang and Yu hongwei
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Zheng–Ming Luo, Bin Jiang and Qing Hou
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Acta Physica Sinica Vol.43 N0.1 (1994) 118
Luo Zheng–ming and Li Tai–Hua
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Yao Jinzhang, Yu Hongwei and Fang Shaohong
7) Single parameter description of the transport of light ions with low energy, Acta Physica Sinica Vol.43 N0.3 (1994) 505
Luo Zheng–Ming and Hou Qing
8) Reflection of light ions from heavy element targets, J. Appl. Phys. 75 1994) 1 , Zhengming Luo, Wengfeng Wu and Qing Hou
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Yu Hongwei and Yao Jinzhang
11) Calculations of range distributions by using the scaling property of ion transport, Acta Physica sinica Vol. 43 N0.3 (1995) 471
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12) Theoretical calculations of energy transfer from noble gases to surfaces, J. Appl. Phys. Vol. 74 N0. 10 (1995) 6007
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14) Analytic fitting to the Mott cross section of electrons
Radiat. Phys. Chem. Vol. 45 N0.2 (1995) 235
Teng Lijian, Hou Qing and Luo Zhengming
15) Single parameter expression for ions reflection from surfaces
Z. Physik B to be published , Luo Zhengming , Hou Qing and An Zhu
16) Radiative loss for Carbon plasma impurity, Commun. of Nucl. Data Prog. N0.13 (1995) 135, Yao jinzhang and Tian Wei

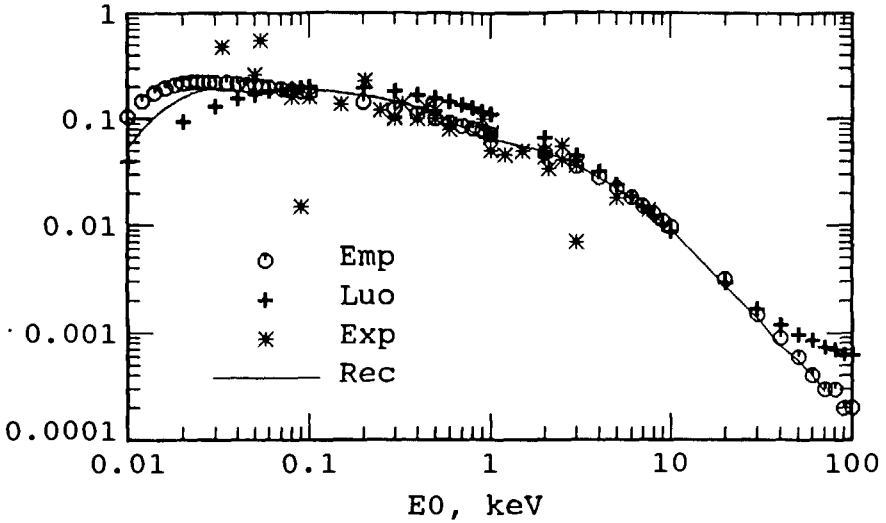

Fig.1a Rn vs E0 for D+ on C solid surface

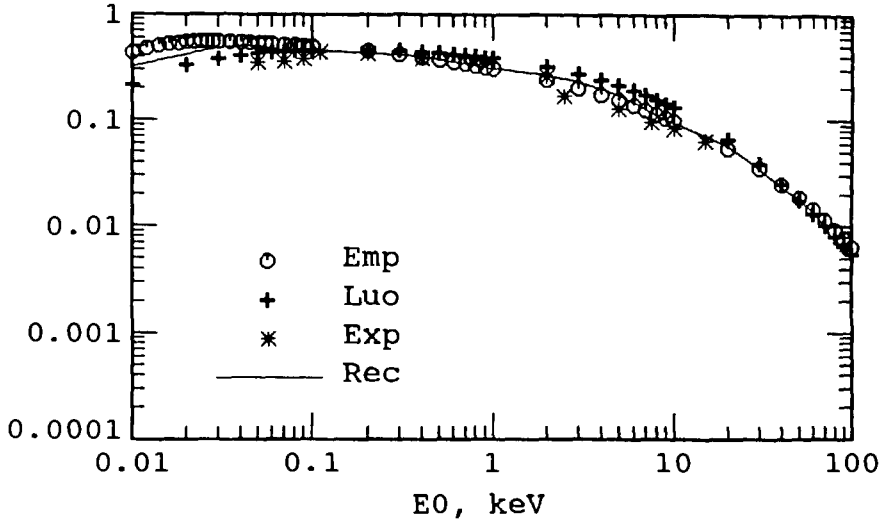

Fig.1c Rn vs E0 for D+ on Ni solid surface

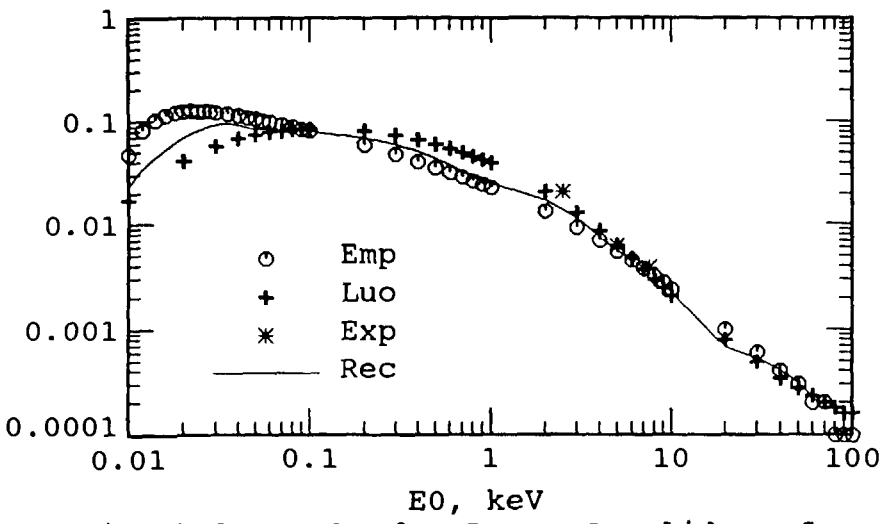

Fig.1b Re vs E0 for D+ on C solid surface

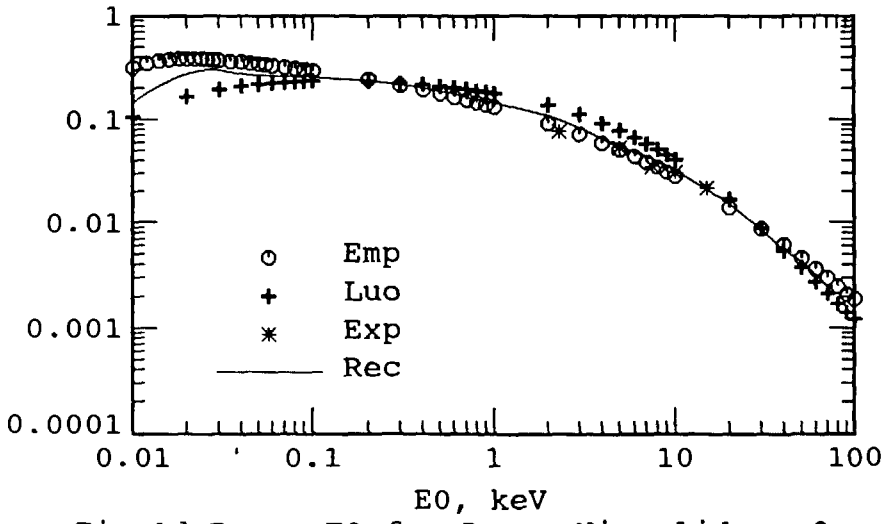

Fig.1d Re vs E0 for D+ on Ni solid surface

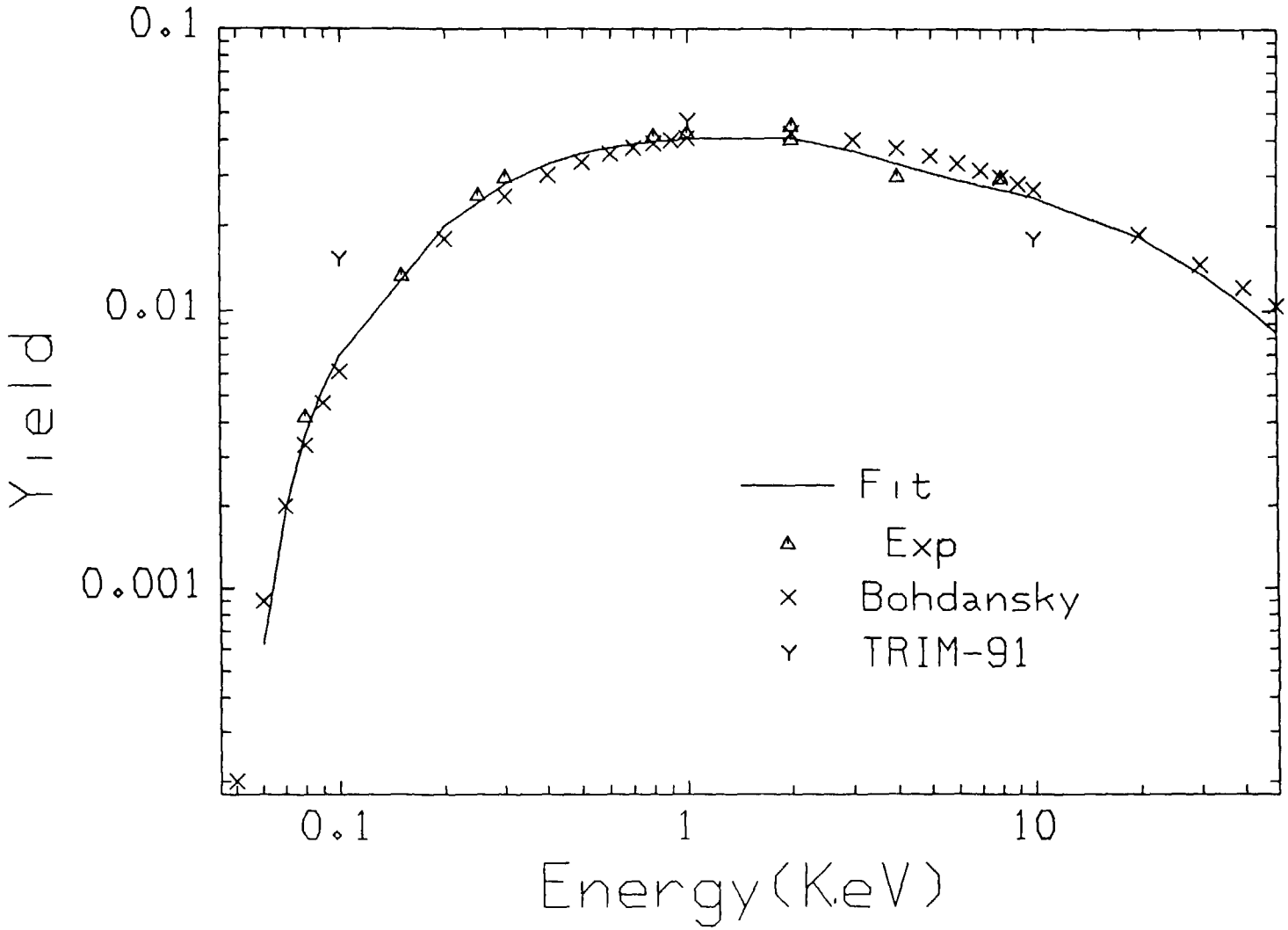

Fig.2) Sputtering Yield of Ni by D+

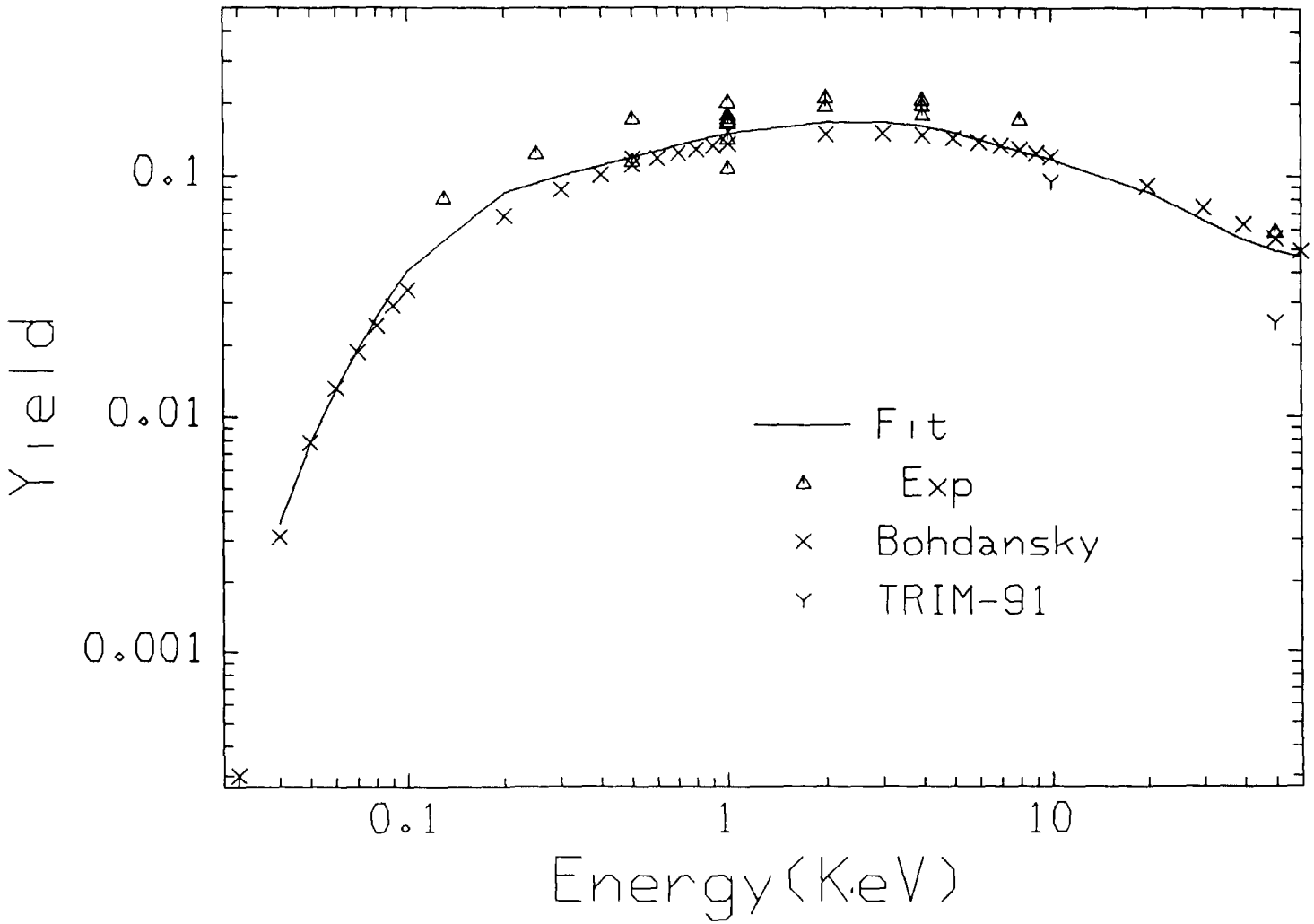

Fig.2 Sputtering Yield of Ni by HE4+

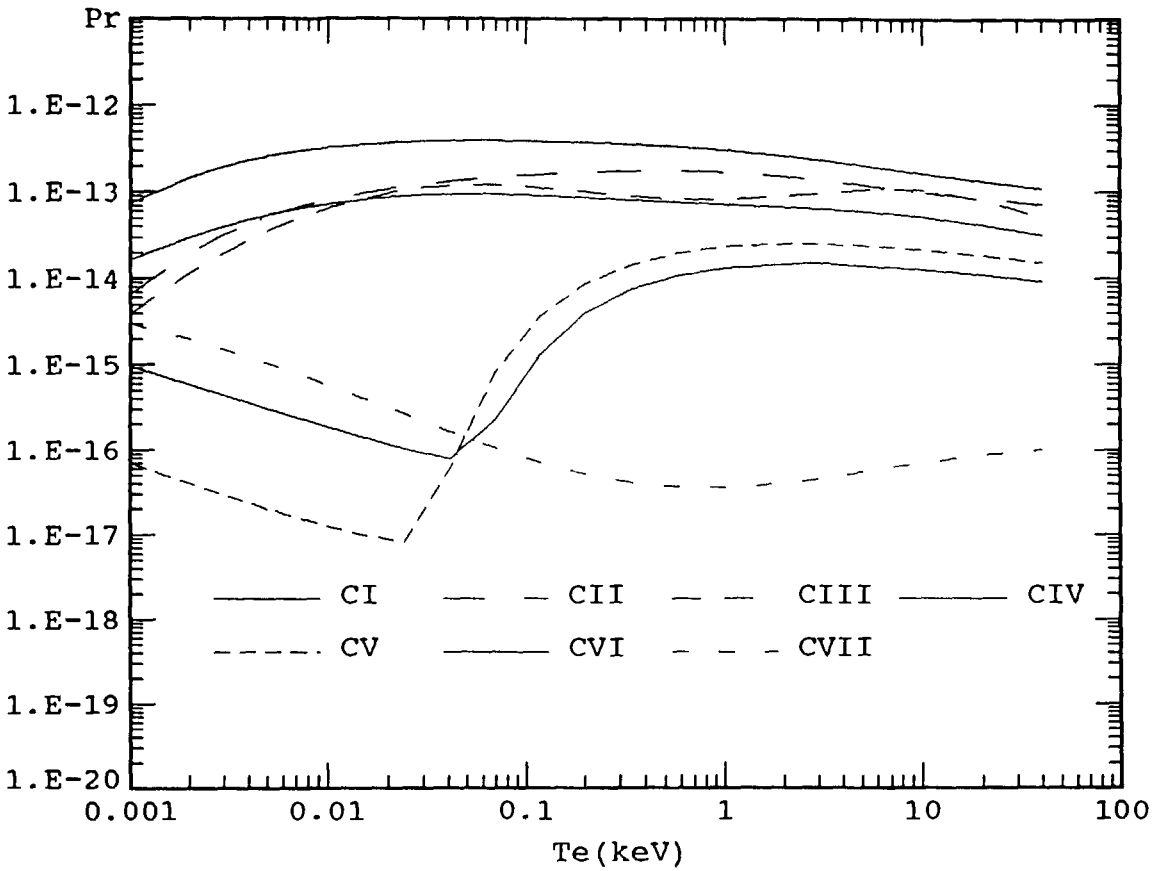

FIG.3 Radiative Loss Coefficients
for Carbon Plasma Impurity

PROGRESS ON ATOMIC AND MOLECULAR DATA ACTIVITIES AT ENEA AND OTHER RESEARCH INSTITUTIONS IN ITALY.

by E. Menapace

Reference: Scientific Data (*) Programme and Services
at ENEA Innovation Department - Applied Physics Division (INN.FIS)

Main items:

i) Electron impact excitation cross sections of vibrationally excited molecules.
(Bari University, CNR (**) and ENEA; cooperation with IAEA - A+M Unit).

ii) Molecular spectroscopic data with reference to vibrational-rotational structure.
(ENEA INN.FIS in cooperation with CNR and JAERI, Trento University).

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*) Including nuclear, atomic and molecular data.
(**) National Council of the Research (Italy).

iii) Low energy interactions (elastic and inelastic) of protons on metal surfaces by Molecular Dynamics approach.
Tritium migration data.
PKA spectra from neutron elastic and inelastic reaction with structural materials.
(ENEA INN.FIS and INN.NUMA*).

iv) Review of fields of interest on atomic and molecular data by the community involved in the applied research.
(Different Institutions).

v) Scientific Data Services and relationships with the international initiative of the IAEA - Atomic and Molecular Data Unit.
Suitable format rules and standards for data presentation.
(ENEA, Ref. as in the title).

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* Innovation Department, Advanced Materials Division.

i) Excitation cross sections for electron-impact induced transitions.

In the energy range from threshold to 200 eV, the above cross sections have been calculated for vibrationally excited H_2 and D_2 molecules with explicit summation over the final vibrational states and assuming their rotational degeneracy. The total excitation (including electronic exitation and dissociative electronic excitation) cross sections for each individual initial vibrational state, defined by the quantum number v_i (v_i cover the range O-14 for H_2 and 0-20 for D_2), are represented by analytical expressions containing a finite number of fitting parameters.

This representation is compatible with the prescriptions by the ALADDIN system structure and formats.
The analytical fits represent the calculated data with an accuracy better than 0.1%.

The figure 1 shows the cross section as a function of collision energy for X->B transition in a typical nondissociative process for H_2 molecule. The figure 2 reports a comparison between H_2 and D_2 dissociative cross sections for X->B transition as a function of the vibrational quantum number for a fixed value of the collision energy (40 eV).

Dissociative excitation cross sections for a number of electronic transitions have been obtained by using the semiclassical Gryzinski method.

Ionization and dissociative ionization cross sections have been calculated by utilizing the Gryzinski method for a number of relevant processes.
The accuracy of the obtained cross sections has been successfully cheeked by comparison with experimental data reported in literature for v_i=o case.

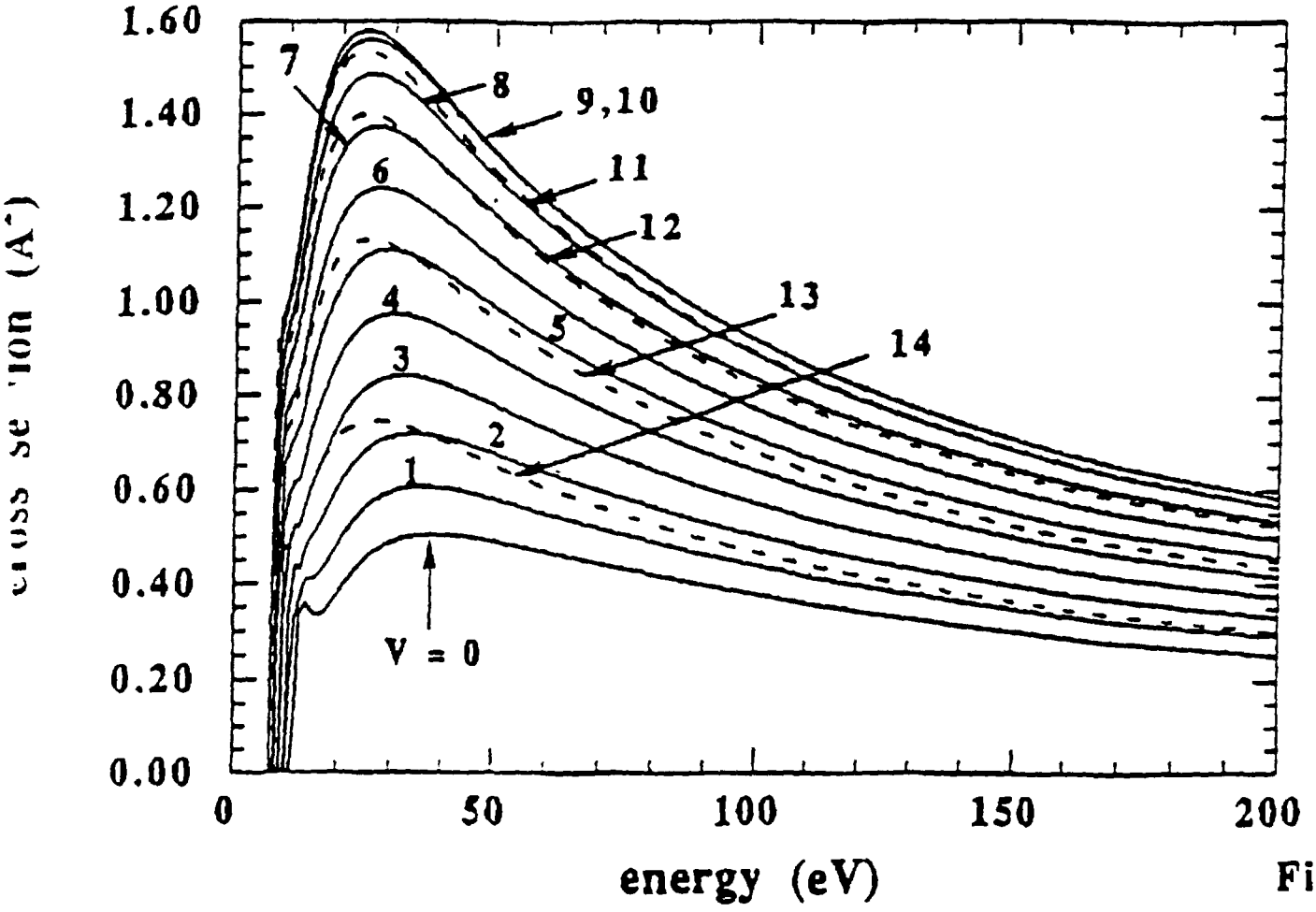

1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
0
50
100
150
200
energy (eV)
7
8
9,10
11
12
13
14
6
4
5
3
2
1
V = 0

Fig.1

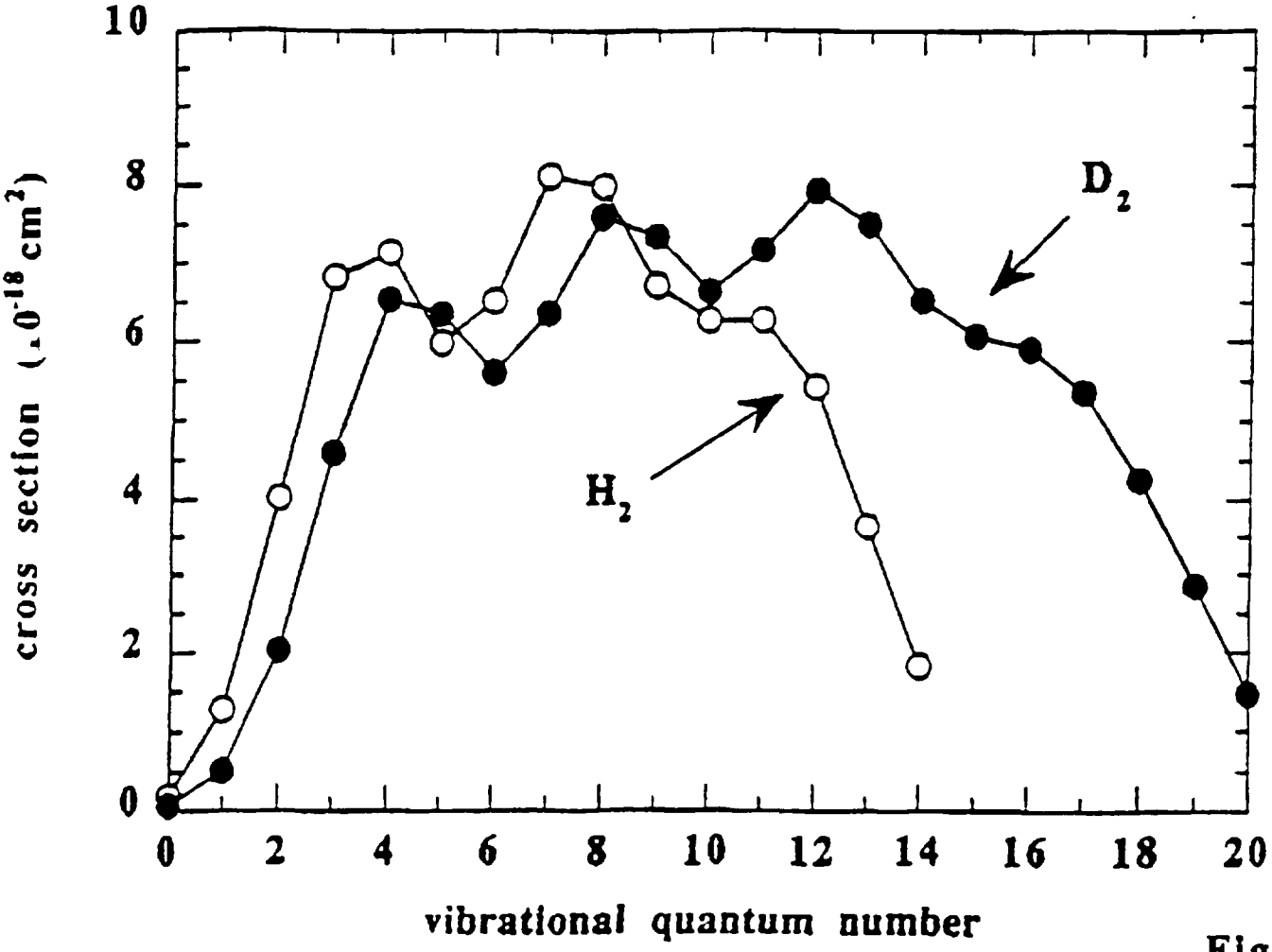

10
8
6
4
2
0
0
2
4
6
8
10
12
14
16
18
20
cross section ($\cdot 10^{-18}$ cm^2)
vibrational quantum number
D_2
H_2

Fig.2

A cooperation has been established with Dr. Janev (IAEA, A+M Data Unit), and results have been published as INDC (NDS) - 333 Report, where the fitting coefficients for the considered processes are given in tabular form, suitable for ALADDIN format data base preparation.

Excitation cross section calculations for electronic transitions of H_2 and D_2 molecules initially in electronic excited states have been initiated. This kind of process, until now negleted in plasma modeling, can play an important role in the kinetic of edge plasma fusion.

Finally atom-atom direct and momentum transfer cross sections for processes involving excited hydrogen atoms have been recently considered. It is expected that these cross sections could be quite higher than the corresponding ones referred to H atoms in their ground state.

(M. Capitelli, M. Cacciatore, R. Celiberto, C. Gorse and collaborators, CNR and Bari University)

ii) Molecular spectroscopic data (i.e. energy level spectra and transition probabilities) are calculated by applying the Vibron Model (VM), which has been studied in analogy with the Interacting Boson Model, developed for the description of collective degrees of freedom in nuclear excitations.
Algebraic techniques are successful in predicting the molecular spectra at least when some amount of experimental information in available at the purpose of calibrating the required algebraic parameters.
In particular:

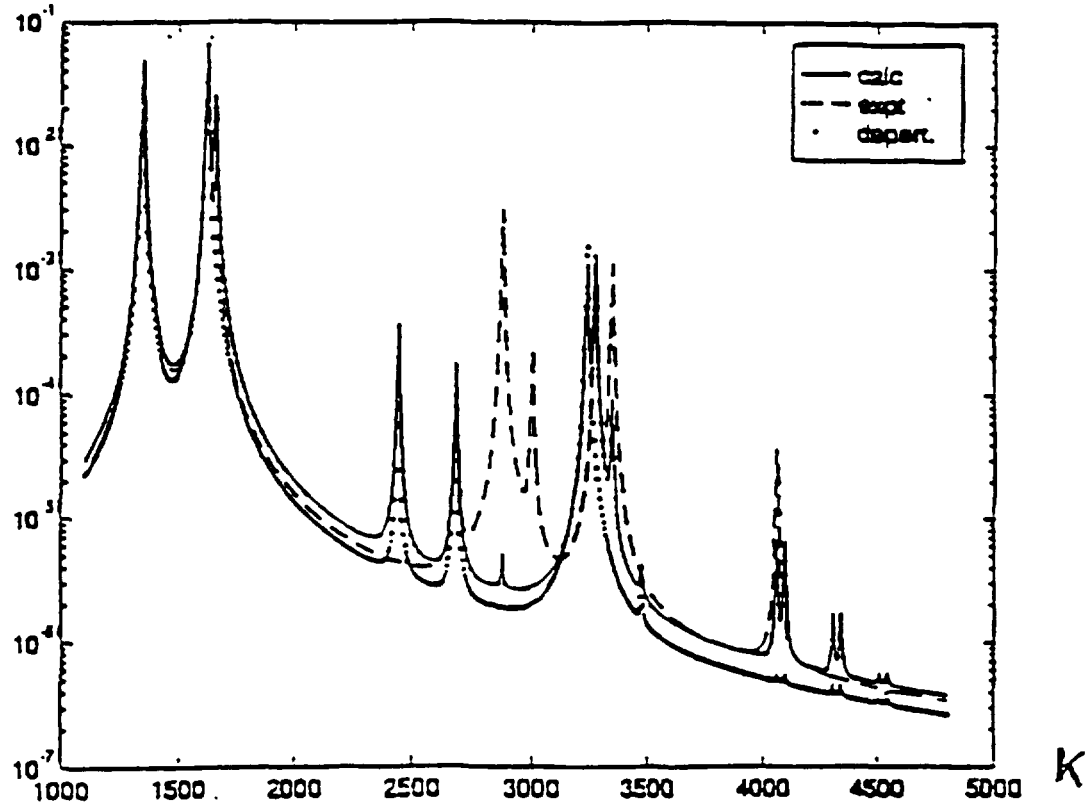
• The work was completed (according to the programme from previous Meeting contribution) concerning calculations for the bent molecule HCO and its deuterated pair DCO and the theoretical estimate of the mean field for the VM modelisation and dipole-moment function of diatomic molecules. The results of both topical calculations have been published and are available by the authors (A. Mengoni, ENEA INN.FIS in cooperation with T. Shirai, JAERI).

• Analogous algebraic techniques have been applied to the study of rotovibrational spectra of molecules of different complexity, taking advantage of the fact that such models can be easily adapted and used by means of rather simple computer routines.

These calculations are presently applied to a systematic analysis of molecules like methanes ($CH_{4-x}D_x$) and ethylenes ($C_2H_{4-x}D_x$), as a result of the fact that algebraic hamiltonian parametexs are characterized by some amount of "conservativity" with regard to isotopical substitutions. In the following figure some results are presented for ethylene, showing reasonable agreement with experimental data.

A specific application has concerned the molecule C_2H_2 and its isotopic species giving rise to a systematic description of the roto-vibrational spectra, as an important application of the development of the three-dimensional algebraic (VM) model for rather small molecules with the inclusion of rotational excitation and their coupling with the vibrational part of the spectrum.
For such molecules, roto-vibrational spectra in the infrared regime are of noticeable interest, in view of the complex features involving a large number of interacting levels.

On the other side systematic calculations have been performed for monofluoroacetylene and fluorobenzenes, as molecules of main interest for enviromental studies (see point iv below).



nparison between experimental, calculated and deperturbed Raman spectra of ethylene in the region of ong Fermi resonances (see Z.Phys.D (1995), in press)

The calculated values on the above molecules are being made available as numerical spectroscopic data to the ENEA Scientific Data service for the representation, in the planned working programme, within the ALADDIN system for the purposes of the international exchange initiatives coordinated by the IAEA Atomic and Molecular Data Unit. (S. Oss, Trento University).

- Vibro-rotational spectra of simple molecules have been measured by IR spectroscopy high resolution techniques and spontaneous or induced Raman spectroscopy.
Among these molecules the most interesting, for the purposes of the IAEA Atomic and Molecular Data Network, are CO, CO_2 and CH_4, C_2H_2, C_2H_4.

Biatomic radicals such as OH, CH, C_2 are of relevance too. Even more complex molecules like benzenes with different isotopic composition (e.g. D instead of H) were considered.

Advanced computer simulations have been performed in the analyses, using appropriate Hamiltonians, including both global (vibrational) and local (rotational) perturbations.

In particular the experimental data were fitted by Watson approach for asymmetrical rotors. Coriolis and Fermi interaction between different vibro-rotational bands were considered.
These results were aimed for applications in different fields, as pointed out in the following point iv).
(R. Fantoni, F. D'Amato - INN.FIS in collaboration with M. Snels - CNR Institute for Molecular Spectroscopy).

– A specific activity concerned the calculations of energy levels of quantum systems through the statistical analysis of the phase space with application to:
• energy level estimate of multielectron atoms expressed through simple analytical formulas, allowing a good agreement with the experimental spectroscopic data;
• homonuclear and heteronuclear diatomic molecules or radicals, by calculating the binding energy, binding lenght and fundamental vibrational energy, in particular for H_2, C_2, CH, CO, HF, HBr, HI, in good agreement with existing experimental values.
Activity is in progress to extend the approach also to more complex molecules of relevance as plasma impurities. (S. Tosto, ENEA INN.NUMA).

iii-a) The actions are in progress for including in a data base the particle and energy reflection coefficients, wich were already calculated (see previous contributions) by Molecular Dynamics method with regard to slow protons ($1eV \leq E_{in} \leq 50$ eV) on Fe {100} surface and to helium atoms (0.1 eV $\leq E_{in} \leq 50$ eV) on Ni {100} surface at finite temperature ($T = 0.3$ Tm), where Tm is the bulk melting temperature. (V. Rosato, A. Ventura, ENEA INN-NUMA and INN-FIS).

This work is directly related to the one of the ENEA Scientific Data service as indicated in the following point v).

- Detailed and extensive molecular dynamics studies on the interactions of vibrationally excited molecules H_2 and D_2 in collision with Cu surfaces, by considering inelastic and reactive processes such as: vibrational and rotational relaxation, dissociative chemisorption and atom recombination.

A classical description is assumed for the translational and internal motion of the molecules, whereas the motion of atoms and electron in the solid is quantized. Quantum tunneling effect in the reaction dynamics has been also considered.

The dissociation probability for H_2 and D_2 and the vibrational and rotational distributions of inelastically scattered molecules (from the wall) have been calculated as a function of the incident molecule kinetic energy.
Relevant results are shown in the following table A for D_2.
In table B typical isotopic effects are presented.

On a different side vibrational energy exchanges (V-V and V-T) in gas phase collision between vibrationally excited H_2 molecules have been calculated within a semiclassical time-dependent "conpled states" method, where the translational and rotational motion are treated classically, while the vibrational motion of H_2 is quantized.
The rate constants were obtained by averaging over a thermal distribution of translational energies.
A good agreement was obtained with the recently determined experimental rates for v=1 and v=2 states. In the following figure 3, a comparison is shown of the V-T rates for D_2 with the corresponding ones for H_2 at 500K.
(M. Capitelli, M. Cacciatore and collaborators - CNR and Bari University)

Table A : Dissociation probability, Pdiss, energy transfer to the surface phonons <Eads>, average values of final vibrational <v> and rotational <j> for reflected (non reactive) collisions as a function of the initial vibrational/rotational state (v,j) and kinetic energy Ei of D_2.

(v, j)	E_i(eV)	P_{diss}	⟨v⟩	⟨j⟩	$\langle E_{ads}\rangle$(eV)	N_t
(1, 0)	1.55	0.00	0.73	3.0	0.139	100
(1, 0)	1.70	0.05	0.83	3.4	0.149	100
(1, 0)	1.80	0.14	0.66	3.7	0.168	120
(1, 0)	2.00	0.33	0.45	6.7	0.200	120
(1, 0)	2.50	0.61	0.90	7.0	0.238	135
(2, 0)	0.50	0.00	2.0	0.5	0.035	25
(2, 0)	1.00	0.00	1.9	2.1	0.079	100
(2, 0)	1.30	0.03	1.6	3.7	0.109	120
(2, 0)	1.55	0.18	1.4	5.7	0.135	100
(2, 0)	2.00	0.32	1.3	8.8	0.182	139
(5, 0)	0.50	0.00	5.0	0.5	0.035	40
(5, 0)	1.00	0.00	4.3	5.9	0.076	100
(5, 0)	1.55	0.55	3.1	9.2	0.145	159
(5, 0)	2.00	0.92				116
(5, 5)	1.00	0.00	4.6	9.4	0.075	100
(7, 0)	0.50	0.00	7.0	0.5	0.035	24
(8, 0)	0.50	0.00	8.0	0.7	0.035	24

N_t is the number of trajectories and the probability for reflection is $1 - P_{diss}$.

Table B : Isotope effect on sticking probability, Pdiss, final vibrational and rotational states of the reflected molecules and energy transferred to the surface <Eads> as a function of the initial kineti energy Ei. The initial (v,j) state for H_2 and D_2 is (0,0).

E_i/eV	P_{diss}	⟨v⟩	⟨j⟩	$\langle E_{ads}\rangle$/eV	N_t
H_2					
1.55	0.11	0.70	3.4	0.070	100
1.70	0.25	0.68	3.3	0.079	100
1.80	0.29	0.48	4.4	0.090	120
2.00	0.50	0.37	5.3	0.098	120
2.50	0.81				135
D_2					
1.55	0.00	0.73	3.0	0.14	100
1.70	0.05	0.83	3.4	0.15	100
1.80	0.14	0.66	3.7	0.17	120
2.00	0.33	0.45	6.7	0.20	120
2.50	0.61	0.90	7.0	0.24	135

N_t indicates the number of trajectories.

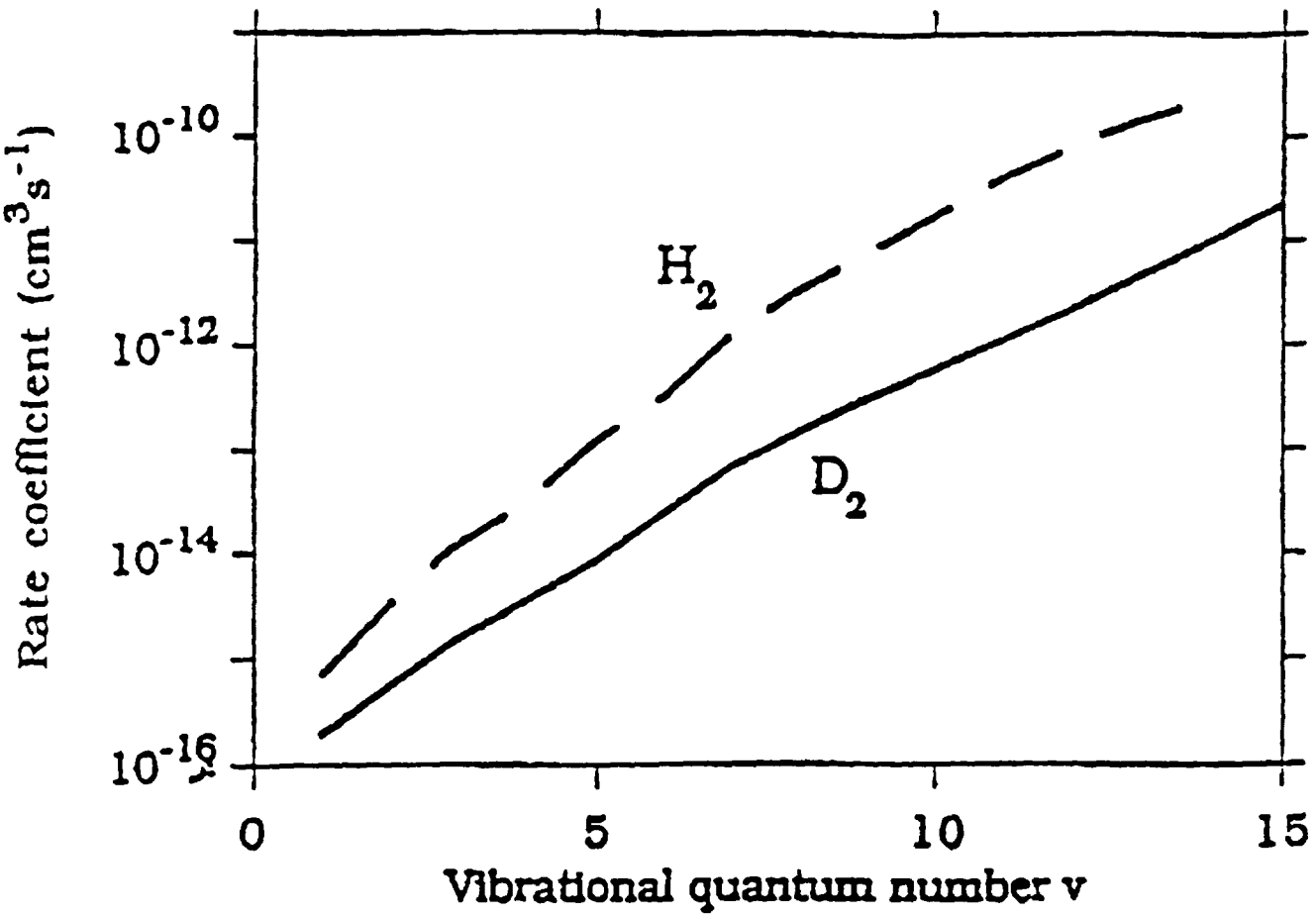


Fig.3: V-T rate coefficient at T=500K for the processes $H_2(v=1) + H_2(v) \dashrightarrow H_2(v=0) + H_2(v)$ as a function of the vibrational quantum number v

— Plasma-wall interaction with sputtering of neutral and excited particles has been investigated, in particular:

• With regard to the neutral sputtered species, in order to overcome the unsolved problems for the angular distribution determination by the usual Legendre expansion, an alternative approach has been undertaken based on the Chardresekar discrete stream technique.
First results indicate how to reproduce the correct angular distribution of the sputtered neutral species.

Concerning the excited (or ionic) species, in order to deal with new correct transport equations of general validity, then to define the proper boundary conditions for the excited species (for a correct kinematics of sputtered excited particles), a generalization of the Lindhard cross section for binary inelastic processed has been investigated, which will enable, as in the elastic case, to obtain analytical solutions for the transport equation.
(G. Falcone and collaborators, Bari and Calabria Universities)

— The topics concerning the migration of the interstitial Tritium in bulk Li_2O breeder, as a consequence of the T production via neutron induced reactions, have been investigated, as a matter of sinergystic approach related to both nuclear reaction and interatomic diffusion processes.

The most probable migration path is identified as a jump between nearest neighbour oxygen ions with an activation energy calculated by the model as the most crucial parameter in the diffusion coefficient. The value O.45 eV has been found.

In addition the binding energy of tritium to a lithium vacancy (tipically produced via a neutron reaction process) is found to be 1.3 eV.
(V. Rosato, A. De Vita, ENEA INN. NUMA in cooperation with the Cambridge University).

iii-b) PKA spectra related to energy transfer by neutron scattering on structural materials.

(M. Pescarini, S.A.M.M. Siddiqui, ENEA - INN.FIS)

In the spirit of a specific indication by the IFRC-SC on Atomic and Molecular data, that "radiation effects should be considered in a synergistic approch with plasma material interaction data estimate", the "primary knock-on atom" (PKA) spectra calculation has been investigated starting from neutron scattering data on structural materials.

In particular the amount of dislocation cascade rates dipends upon the PKA energy, then the global effect estimate requires the calculation of the energy distribution of the PKA's.

Starting from the neutron data processing system NJOY, in particular the module HEATR, specific modifications have been performed to single routines, mainly DISBAR routine in order to calculate the PKA spectra and the first results were obtained with regard to neutron elastic scattering on Fe-56.

Results from calculation at 14 MeV incident neutron energy are presented in the following figure 4. At this energy the angular distribution is strongly anisotropic in the CM system and this fact gives rise to a low-energy maximum in the PKA spectrum.

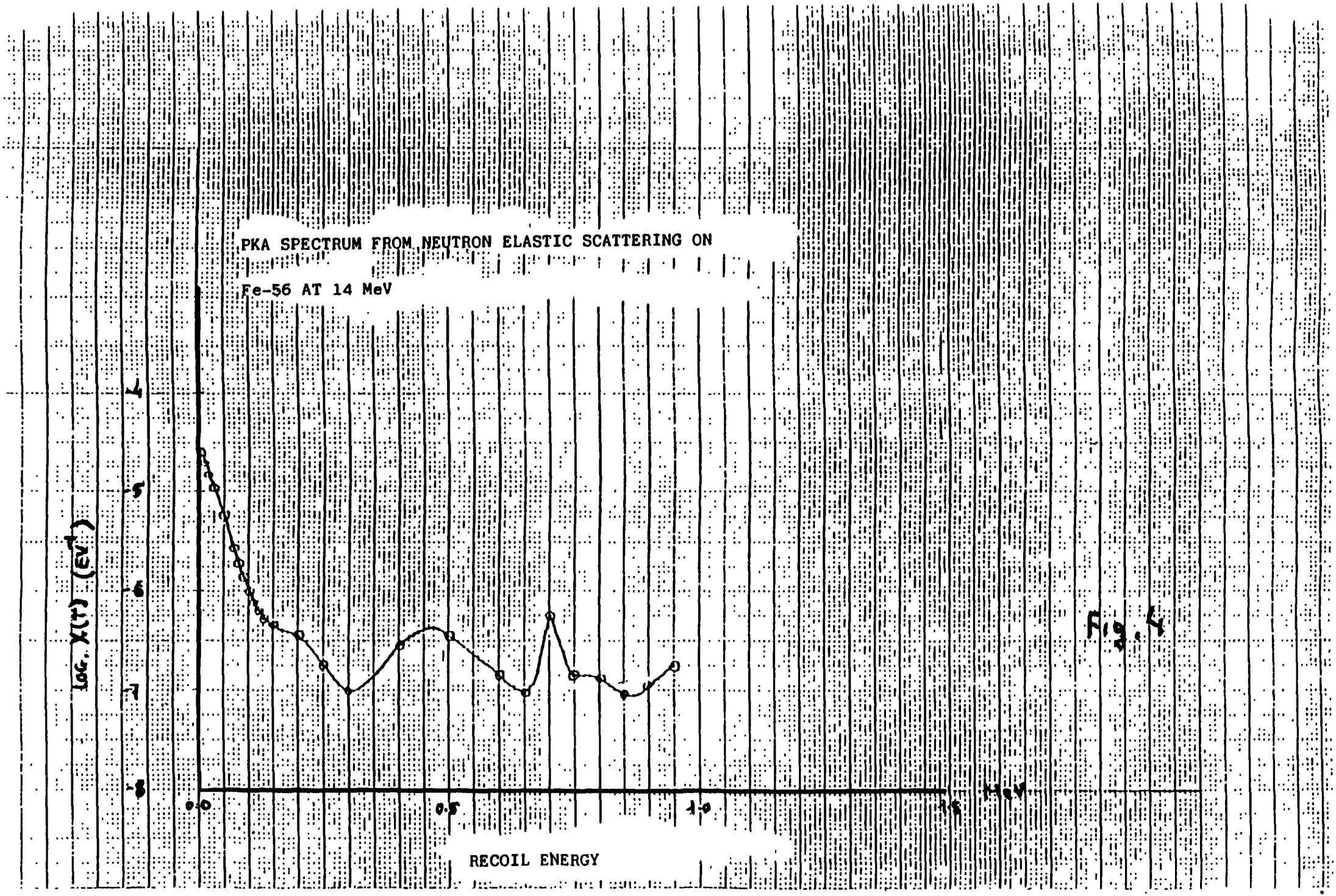

PKA SPECTRUM FROM NEUTRON ELASTIC SCATTERING ON
Fe-56 AT 14 MeV
Log. χ(t) (eV⁻¹)
-4
-5
-6
-7
-8
0.0
0.5
1.0
RECOIL ENERGY

Fig. 4

iv) The considered fields of interest for the applied research community with regard to atomic and molecular data are summarized in the following:

– by the Fusion programme at ENEA (Energy Department in collaboration with Innovation Department) and CNR:

• particle-surface data for plasma wall and divertor component materials, considering both interactions by low energy ions and atoms, from one side, and radiation damage studies, from the other side, starting from ions elastically or inelastically scattered by neutrons;

• electron-molecule interactions for H_2 and D_2 up to few hundreds eV incident energy, including estimate of cross sections for excitation and ionization (even dissociative) events;

• molecular spectroscopy data for diagnostics of plasma impurities as diatomic or triatomic molecules or radicals (HCO, DCO, CO, CO_2, CH, OH, C_2) or other simple molecules, like CH_4, C_2H_2, C_2H_4 etc;

– for application in PIXE analytical techniques:

• since an accurate knowledge of the L-shell X-ray line intensity ratios is needed, more precise data are requested, such as subshell fluorescence yields, intrashell radiative yields, Coster-Kronig transition probabilities and fractional radiative widths following L-subshell ionization, as from the recent Conference on PIXE (Padua, 27 to 30 May 1995);
[See fig. 5 on overall effect, by S. Fazinic at same Conference, including experimental data situation with respect to previous compilation and recent theoretical calculations].

– by research programmes on combustion processes and environmental studies and analyses:

• molecular spectroscopic data for small molecules (such as CO, CO_2, NO, NO_2, CH_4, C_2H_4,C_2H_2 etc) or radicals (OH, CH, NH, C_2) and more complex systems like benzenes (isotopically different), fluorobenzenes, monofluoroacetylene etc.

v) The functions by the Scientific Data services at ENEA INN.FIS and the corresponding actions have been:

• the monitoring of most relevant results produced at the different research Institutions and of the requirements and exigencies from the different applied fields, even in the frame of the international collaboration involving national programs; the critical review resulting from this action has been recently updated and summarized as described above;

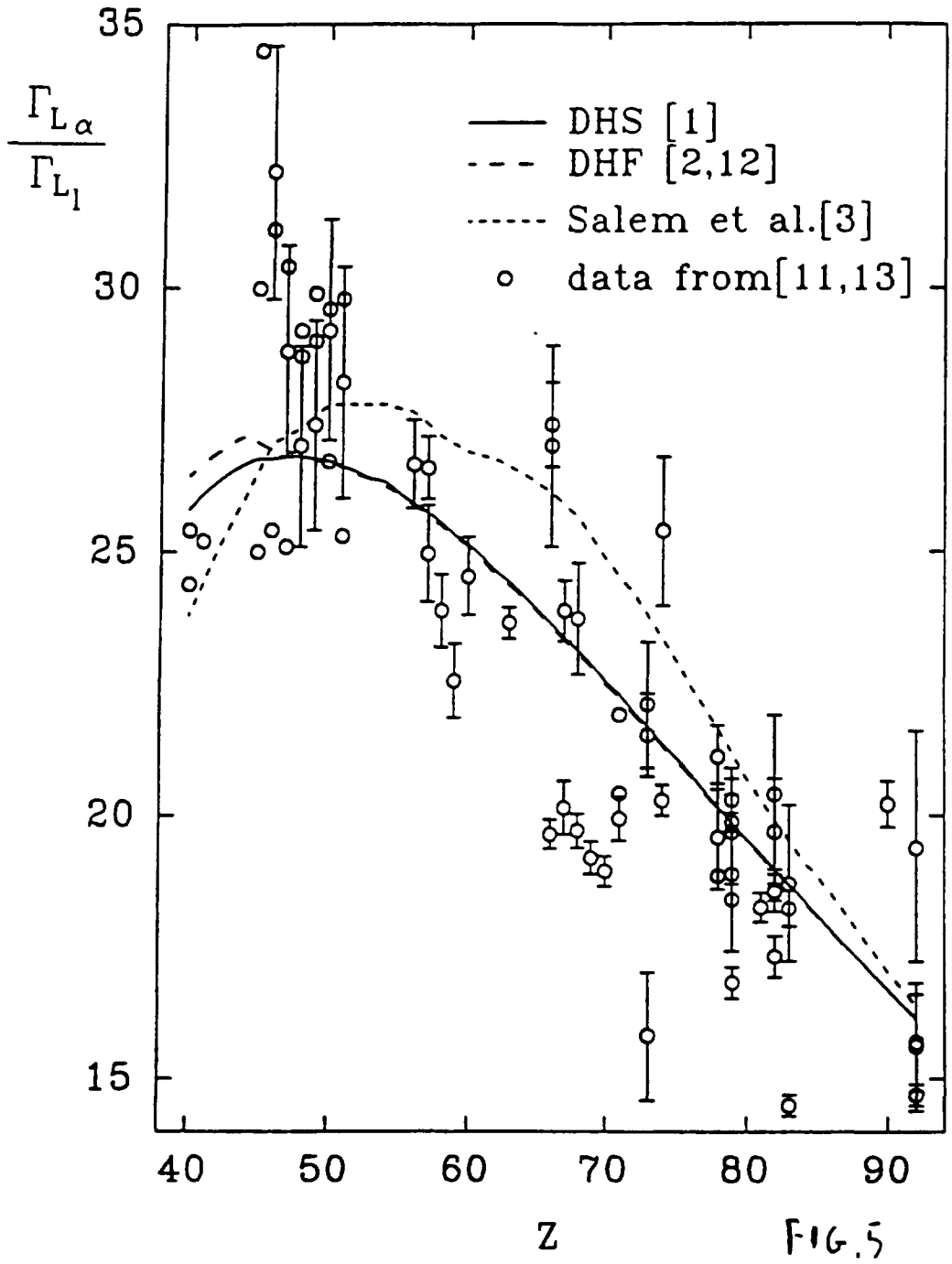

35
30
25
20
15
$\frac{\Gamma_{L\alpha}}{\Gamma_{L_1}}$
DHS [1]
DHF [2,12]
Salem et al.[3]
data from[11,13]
40
50
60
70
80
90
Z

FIG. 5

• the presentation and discussion of this kind of reviews in the frame of the international Network on Atomic and Molecular Data organized by the IAEA (A+M Data Unit), according to the expressed interest for applications such as fusion programmes, radiation damage studies, technological (typically material) and environental applications; verification of fields of common interest with other Laboratories or Centers referring to the Network and of matter of desirable collaboration;

• to collect and disseminate data represented numerically with informatic procedures, as made available from the producing Laboratories and, in the same context, to encourage the representation according to the ALADDIN system standards and formats, by interacting with the IAEA Unit on the subject;

• to update, maintain and distribute the available data bases, according to the requirements of the research programmes, by discussing the critical selection according to the scientific and technical exigencies from the user community, and to promote well focoussed research activities by the data producer community, in cooperation with the international community through the IAEA (A+M Unit) coordination.
(G.C. Panini and E. Menapace, ENEA INN.FIS).

TROITSK ATOMIC DATA GROUP

Progress Report

1995

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Presented at the 13th Atomic and Molecular
Data Centres Network Meeting
Vienna, 10-11 July 1995

1. SOME HISTORY

Troitsk Atomic Data Group was formed in the late 80's at Kurchatov Institute of Atomic Energy (Branch), located in the town of Troitsk about 20 km from Moscow At that time, the group were concerned in research on the physics of high-temperature plasmas The group had to support the modeling and diagnostics of plasmas by reliable atomic data

2. OFFICIAL STATUS

Today, Troitsk Atomic Data Group is part of the Centre of Theoretical Physics and Computational Mathematics, a division of Troitsk Institute for Innovation and Fusion Research (TRINITI) which is a State Research Centre subordinated to the Ministry of Atomic Energy of Russian Federation

3. SCOPE OF ACTIVITIES

At the present time, the main scope of activities of the Troitsk Atomic Data Group falls into few clusters

1 Theoretical studies on the physics of electronic an atomic collisions
   - Direct and resonance (via autoionizing states) ionization of atomic systems by charged particle impact Study of a role of electron correlations in the ionizing collisions
   - Two-electron transitions in collision of atoms with charged particles The processes of two-electron excitation and excitation-ionization
   - Excitation of quasistationary states of atomic systems by proton, electron and ion impact
   - Effects of sign of projectile charge in atomic collisions Projectiles with electrons
2 Atomic data banks
   - Development of methods for processing of diverse atomic data on the basis of hierarchical approach, because it is hierarchical approach that corresponds to the logic of scientific research
   - Constructing new software for hierarchical data management on a personal computer and matching common requirements of work with numerous and diverse data
   - Filling the specialized banks of atomic data with values of cross sections and velocities of collision processes
3 Support of the research on the physics of high-temperature plasmas with reliable atomic data Systematic calculations of the collision and spectroscopic characteristics Derivations of most reliable values from the analysis of published experimental and theoretical results Use of data recommended by other data centres

4. INTERACTION WITH RESEARCH ON PLASMAS PHYSICS

The atomic data produced and recommended by our group have been used in the Centre of Theoretical Physics and Computational Mathematics (TRINITI) for the theoretical modeling of high-temperature, nonequilibrium plasmas of multicharged ions, for the description of shapes of spectral lines and for calculations of radiation transfer

The group is involved also in the analysis of the experimental emission spectra from hot plasmas Such plasmas is produced inside the installations of TRINITI within research projects on inertial and magnetic confinement fusion In particularly, the ratio of intensities of different spectral lines has been used for the diagnostics of electron density and temperature of plasmas (Installation "Angara-5" in collaboration with Ecole Politechnique of France and Imperial College of London Installations "Mishen" and "TIR" for laser fusion experiments Installation "Compact Torus")

There is a collaboration with Kurchatov Institute of Atomic Energy, All-Russian Institute of Experimental Physics, All-Russian Institute of Technical Physics The atomic data calculated and recommended by the group have been applied for the diagnostics and modeling of hot plasmas The collaboration with University Paris Sud is connected with research on short-wavelength lasers in recombinating laser plasmas

Nowadays the group participates in the project "Atomic and Radiation Processes in Plasmas, Gases and Solids" which is being supported by the United State and European Community through the International Science and Technology Centre The project focuses primarily on theoretical research aimed at the solution of a number of atomic physics and radiation problems that have both fundamental importance as well as significant application in the problem of controlled fusion, X-ray laboratory sources, astrophysics etc Scientists from six Russian institutes participate in this project (TRINITI, Lebedev Physical Institute, Kurchatov Institute, Institute of Experimental Physics, Institute of Technical Physics, Ioffe Physical-Technical Institute)

5. RESOURCES AND CAPABILITIES

5.1 Man Power

The permanent staff of TADG is 4 people. When it is necessary, more people can be drawn in cooperation to perform some special tasks The personnel has a good experience in the physics of atomic and electronic collisions and atomic spectroscopy to be involved in data evaluation and recommendation as well as literature searches for A+M data

5.2 Computational Power

Personal computers (IBM compatible) are generally used for our work, including both theoretical calculations and data processing In complex cases more powerful computer facilities of the computer centre of TRINITI can be used

5.3 Computational Codes

To calculate collision and spectroscopic characteristics, we employ our own programs, as well as some packages that are of wide usage in many physical laboratories The following quantities can be calculated by our group (names of the program packages in parentheses)

- Energy levels and transition probabilities (COWAN, GRASP, SUPERSTRUCTURE)
- Autoionization probabilities (COWAN, RMATRIX, DIANA)
- Spectral line shape of hydrogen-like ions in hot plasmas (DOMINO)
- Cross sections for excitation of atoms and ions by electron impact in the close coupling scheme (RMATRIX)
- Cross sections of direct and resonant ionization of helium by charged particles with allowing for Coulomb interaction in the final state Total and differential electron emission yield Cross sections of two-electron excitation (BEAR)

5.4 Software

We have developed original software to work with hierarchical data collections (Hi Base) No commercial products are incorporated in our database management system, which has already the history of several versions

6. PROGRESS

6.1 The Physics of Atomic And Electronic Collisions

We have elaborated a theoretical method for the description of the direct and resonance ionization of atoms by charged particles The consideration is based on the solution of multichannel equations in the diagonalized approximation with inclusion of state-to-continuum interference and Coulomb interaction in the final state (CIFS) between ejected electron, scattered charged particle and residual ion The approximate solution of the Faddeev-Merculiev equations for three-body Coulomb problem has been used for allowing for CIFS It was shown that CIFS influences considerably on the ionization processes in a broad region of collision kinematics As the projectile charge increases the role of CIFS becomes more important The explanation for a number of experimental results on electron emission spectra and differential electron emission yield at ionization of the helium atom by charged particles has been given

The role of electron correlations in the processes with two-electron transitions has been studied for the two-electron excitation of the discrete state of the beryllium atom and two-electron excitation of the autoionizing states of the helium atom The approximate solution of the four-body problem has been derived for the description of two-electron excitation of atom by charged particles We arrived at the connection of our results with few terms of Born series Preliminary calculations show that such approach is promising for studying of the role of electron correlations in collision processes

Our attention has been also directed on the study of the mechanisms of excitation of autoionizing states by particle impact It was found that the excitation via adjacent

continuum (reversed Auger decay) can be as efficient as mechanisms of direct excitation We studied the differences in the excitation of autoionizing states of the helium by fast particles of opposite charge We found that such differences are much more remarkable at excitation of autoionizing states that at excitation of discrete states

6.2 Atomic Data Banks

Several specialized banks of data on collision cross sections are being filled by the group today We make use of literature data and take into account some other compilations Now we have got

- Data on single and multiple ionization of atoms, ions and simple molecules by electron impact
  251 references, about 2400 reactions.
- Data on excitation of atoms and ions by electron impact
  244 references, about 2000 reactions
- Data on charge transfer in ion-atom collisions
  169 references, about 1100 reactions
- Database on spectroscopic and collision characteristics of helium are in the process in development

So far, atomic data to data users are distributed in the Hi Base format on diskettes There is also the possibility of text output in a standard format that can be interpreted by any applied program working with text files It is also possible to send such text files by e-mail The next generation of Hi Base that is to be completed in 1995 will have built in utilities for reading/writing data in the ALADDIN format

6.3 Hierarchical Data Processing

Methods of hierarchical data processing have not been extensively investigated in the database practice yet Our group has formulated the basic principles of hierarchical approach to database construction, and these ideas have been partially incorporated in our database management system (Hi Base) The system is capable of efficient work with large amounts of atomic and molecular data on IBM compatible personal computers under MS DOS Data can be stored together with bibliographical notes, and a number of search operations have been provided The system supports traditional way of particle specifications in atomic physics, including all the ion notations adopted (e g Ne-like Fe, Fe^{16+}, FeXVII), isotope indices, atomic state tags ets The system understands all the variety of energy units, including energies per/amu An interactive shell for viewing/editing a database requires no preliminary training to start with, and most data are checked for formal correctness at input A collection of data types built into Hi Base includes both general-purpose types (like integer, character string, etc) and special types useful in atomic physics (particle, energy, reaction, etc) Combining these primary data types in different aggregates (lists, structures, sets), we can construct a hierarchical pattern for any A+M process Adding a new reaction class, or new characteristics of a reaction, does not require changing data formats in already existing databases, since only relevant information is stored in a hierarchical database

7. TENTATIVE PLAN FOR 1995-1996

We will continue our studies on the theory of atomic and electronic collisions The existing atomic data banks will be extended All available atomic data presented in the ALADDIN format will be incorporated into our data base We are going to increase our efforts on data evaluation, recommendation and dissemination

New generation of Hi Base (version 2 0) is to be issued in 1995 This version will provide complete hierarchical treatment of bibliographical and reaction data, and conversion utilities from/to ALADDIN format are to be built into the system More powerful versions of Hi Base of the second generation should be appeared in 1996, with more reaction types and new conversion utilities Graphic data processing is to be built into Hi Base in versions 2 x, to store/view graphic data along with numerical values The possibility of data conversion between different data representations (e g analytical fit/table, or table/graph) is to be built into Hi Base Hi Base for Windows is to be issued in 1996

INTERNATIONAL ATOMIC ENERGY AGENCY

Atomic and Molecular Data Unit

Report of Activities: September, 1993 to July, 1995

Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (13th Meeting of the A+M Data Centres and ALADDIN Network)

Prepared by: J. Botero
July 11, 1993

AREAS OF INTEREST

- Atomic and Molecular Collisions
- Atomic and Molecular Structure and Spectra
- Plasma-Surface Interactions
- Material Properties

STAFF AND EQUIPMENT

- Staff
  - 3 Physicists
  - 2 Fellows
  - 1 Consultant (Programmer, 9 months)
  - 1 Secretary and Support
- Equipment
  - IBM RS6000/340
    - 64 Mbytes of RAM
    - 1 (2) Gbytes of Hard Disc
    - Operating System: UNIX
  - IBM RS6000/340
    - 64 Mbytes of RAM
    - 1 (2) Gbytes of Hard Disc
    - Operating System: UNIX

- 3 IBM PC 386
  - 8 Mbytes RAM
  - 40-80 Mbytes Hard Disc
  - Operating System: MS/DOS, MS/Windows
- Access to:
  - Vax 4000 (VMS)
  - IBM Main Frame (TSO)

- Communications
  - EARN/BITNET. rnd@iaea1, rng@iaea1
  - INTERNET
    - Anonymous ftp account: user "anonymous" or "ftp"
    - AMDIS on-line service: user "aladdin"
    - IP Address: ripcrs01.iaea.or.at (161.5.74.1)

PROJECTS

- Data Base Development
- Data Evaluation and Recommendation
- Coordinated Research Projects and Research Contracts

1. Data Base Development

   - Atomic and Molecular Data Information System (**AMDIS**): On-line computer access to atomic, molecular, plasma-material interaction and material properties data bases and to other information.

     - A+M Bibliographic Data Sistem (AMBDAS): The A+M Bibliographic Data System of the **IAEA** A+M Data Unit contains more than 33000 bibliographic entries with information relevant to fusion research and development. The on-line system gives acces to this bibliographic database with a menu-driven and user friendly evironment.

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Ju -95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

BIBLIOGRAPHIC RETRIEVAL SYSTEM

SELECTION CRITERIA

- Author
- Process
- Reactants
- Reference
- Year of Pub ication
- Energy/Te p.
- Method (Th/E|p)
- RETRIEVAL

HELP: Choose se ection criteria.

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Jul-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

BIBLIOGRAPHIC RETRIEVAL SYSTEM

PROCESS

Code (?)

Category

SELECT PROCESS

Category	Process
Structure an	B Line Shapes and Shifts
Structure an	GS Structure, Spectra
Structure an	I Interatomic Potentials
Structure an	P Polarizabilities, Electric mom
Structure an	S Energy Leves, Wavelengths
Structure an	T Transition probabil., Oscill.
Photon colli	GP Photon Collisions
Photon colli	PA Total Absor., Scat.

HELP: Select process that you want.

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Jul-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

BIBLIOGRAPHIC RETRIEVAL SYSTEM

REACTANT SPECIFICATION

	Reactant code (?)	Ionization state (Q) or isoelectronic se_. (I)	Limits Low.	Upp.	Excited state (Y/N)
First					
Second					

HELP: Insert/Select reactant code.

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Jul-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

BIBLIOGRAPHIC RETRIEVAL SYSTEM

ENERGY OR TEMPERATURE

Energy or Temperature :

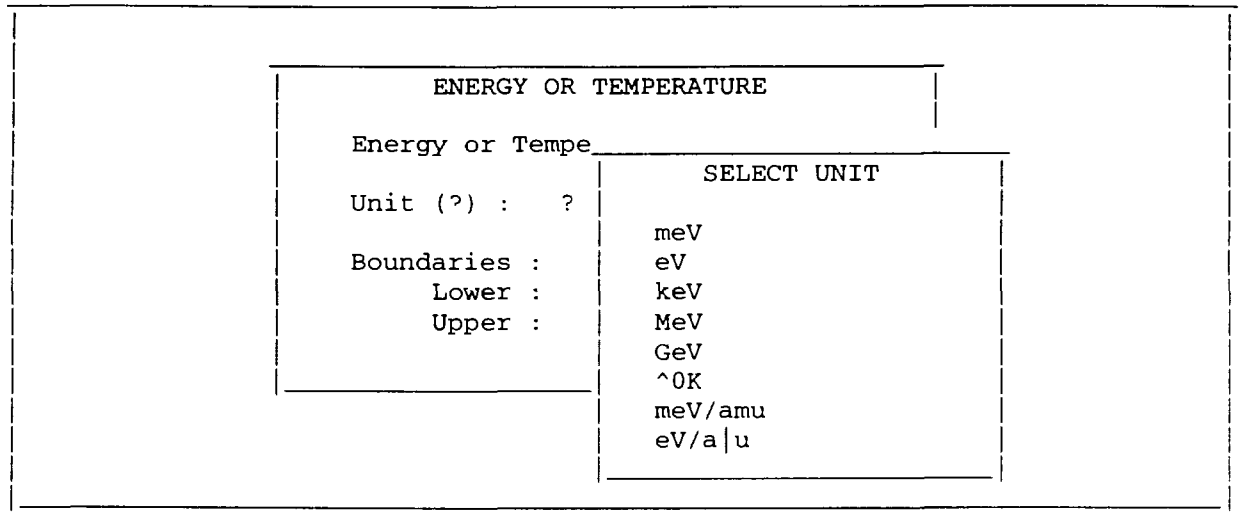
Unit (?) :

Boundaries :
Lower :
Upper :

HELP: Energy (E) or te|perature (T).

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Jul-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

BIBLIOGRAPHIC RETRIEVAL SYSTEM



HELP: Select process that you want.

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Jul-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

BIBLIOGRAPHIC RETRIEVAL SYSTEM

NUMBER OF BIBLIOGRAPHIC ENTRIES RETRIEVED : 7

NUMBER OF INDEXATION RECORDS RETRIEVED : 9

Output form ?

ASCII (Screen) ASCII (File) LATEX (File) RETURN

- ALADDIN interface and data base New on-line system, menu-driven and user frindly environment. A search-tree of hierarchical labels is built to do the search. New features have been implemented:
  * Text: Entries may be accompanied by a text file. This text file gives the information on the evaluation or recommendation procedure, availability of data, accuracy, references, etc. This still has to be implemented in most entries.
  * Figure: Users may choose to see a formatted figure with the data, labels, etc. These figures will be stored in a command file to be executed by the **xmgr** graphicd package. If the user has an X-terminal, the figure may be seen on the screen Otherwise it has to be written to a file using PostScript format. The file may be transferred to the user's computer using **ftp**. This has to be implemented in most entries
  * Source code Users may choose to get the C or Fortran code of the evaluating function This are stored in independent files and may be transferred along with the coefficients via **ftp**. This still has to be implemented in most entries.

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Jul-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

ALADDIN

SELECT SUBJECT AREA

- Collisional Data Base
- Plasma-Surface Interaction
- H Neutral Beam Data Base
- Elementary Process in H-He Plasmas
- test

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Jul-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

ALADDIN

HIERARCHICAL LABEL

??
? ASDET: Associative detachment:A + B[-] -> AB + e ?
? ASION: Associative Ionization:A + B -> AB[+] + e ?
? BEM: Spectral band emission:A + BC -> \lambda \lambda' ?
? CHEMION: Chem. ionization = Penning + associative + other ionization ?
? CX: Charge Exchange (Single), Total:A[+q] + B -> A[+(q-1)] + B[+] ?
? CX2: Double Charge Exchange Total:A[+q] + B -> A[+(q-2)] + B[+2] ?
? CXSS: State Selec. Elec. Capture, Single:A[+q] + B -> A[+(q-1)] + B[+] ?
? DEST: Destruction of Projectile or Target ?
? DEXC: Collisional De-Excitation (of target):A + B (*) -> A + B ?
? DEXC+STRIP: Projec. De-Excit. by Stripping:A(*) + B -> A[+](*) + B + C ?
? DIS: Direct (Impact) Dissociation:A + BC -> A + B + C ?
? DISCX: Dissociative Charge Exch.:A[+q] + BC -> A[+(q-1)] + B + C[+] ?
??

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Jul-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

ALADDIN

HIERARCHICAL LABEL

CX C [+1] H

?????????

ASD	*C	*[+1	*H ? [+0]	?A + B[-] -> AB + e
ASI	Fe	[+2	H{2?????????	A + B -> AB[+] + e
BEM	H	[+3	_____	ion:A + BC -> \lambda \lambda'
CHE	He	[+4]		ization = Penning + associative + other ionization
*CX:	H{2	[+5]		e (Single), Total:A[+q] + B -> A[+(q-1)] + B[+]
CX2	O	[+6]		Exchange Total:A[+q] + B -> A[+(q-2)] + B[+2]
CXS	_____	_____		Elec. Capture, Single:A[+q] + B -> A[+(q-1)] + B[+]

DEST: Destruction of Projectile or Target
DEXC: Collisional De-Excitation (of target):A + B (*) -> A + B
DEXC+STRIP: Projec. De-Excit. by Stripping:A(*) + B -> A[+](*) + B + C
DIS: Direct (Impact) Dissociation:A + BC -> A + B + C
DISCX: Dissociative Charge Exch.:A[+q] + BC -> A[+(q-1)] + B + C[+]

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Jul-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

ALADDIN

BOOLEAN LABEL

AND: XS ORNL-CFADC
NOT: EVAL 20/06/89

```
??????????????????
? A XS             ?
?                  ?
? N EVAL           ?
?   ACC=C          ?
? A ORNL-CFADC     ?
?   DOC=ORNL-6090  ?
? N 20/06/89       ?
??????????????????
```

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Jul-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

ALADDIN

SELECTED LABELS

HIERARCHICAL:
CX C [+1] H H ** **

BOOLEAN:
AND: XS ORNL-CFADC
NOT: EVAL 20/06/89

NUMBER OF ENTRIES SELECTED: 0

? Do you want to :
?
? Show Entries Change Labels New Search E|it

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Ju_-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

ALADDIN

SUMMARY OF SELECTED ENTRIES

```
CX  C [+1]  H [+0]
XS  EVAL  ACC=C  ORNL-CFADC  DOC=ORNL-6090  20/06/89
#CHEB
CX  C [+1]  H(2) [+0]
XS  EVAL  ACC=C  ORNL-CFADC  DOC=ORNL-6090  20/06/89
#CHEB
CX  C [+2]  H [+0]
XS  EVAL  ACC=C  ORNL-CFADC  DOC=ORNL-6090  20/06/89
#CHEB
CX  C [+2]  He [+0]
XS  EVAL  ACC=C  ORNL-CFADC  DOC=ORNL-6090  20/06/89
#CHEB
CX  C [+2]  H(2) [+0]
XS  EVAL  ACC=B  ORNL-CFADC  DOC=ORNL-6090  20/06/89
#CHEB
```

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Ju_-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

ALADDIN

FULL SELECTED ENTRY

```
$ CX2  H [+1]  H [-1]   H [-1]  H [+1]
& XS   EVAL  ACC=C  ORNL-CFADC  DOC=ORNL-6086  A-44  6/90  #CHEB %GRAFIC
^CODIGO @TEXTO
-74.0098  .227379  .0232305 -.388332 -.00604588  .0351500  .101175 -.132693

-.0302977                    59.        1100.
```

```
????????????????????????????????????????????????????????????????????
? Do you want to :                                                   ?
?                                                                    ?
? Ev.Func.    Text    Graphic   Source    Previous    Exit         ?
????????????????????????????????????????????????????????????????????
```

- New ALADDIN formated data
  - Particle interchange reactions involving plasma constituents, plasma impurities and H_2, D_2 and HD.
  - Collisional database for Lithium-beam interaction with fusion palsmas.
  - Radiative Losses and electron cooling rates of H, He, C, O.
  - Particle-impact induced electron ejectionfrom surfaces.
- Mantain the IAEA Bibliographic Data Base: 33500 entries, dating from 1950 to present. Contributors:
  - ORNL, USA
  - NIST, USA
  - GAPHYOR, France
  - Kurshatov Institute, Russia
  - NIFS, Japan
- Publish the International Bulletin on Atomic and Molecular Data for Fusion (new Format), published semiannually.

- Atomic Collision Database for Lithium Beam Interaction with Fusion Plasmas: IAEA INDC(NDS)-267. (Janev, Smith, Aumayer, Wutte, Schneider, Winter and Schewinzer).
- Particle Interchange Reactions Involving Plasma Impurity Ions and H_2, D_2 and HD: IAEA INDC(NDS)-310 (Armentrout, Illesca, Botero).
- PArticle-impact Induced Electron Ejection from Surfaces. IAEA INDC(NDS)-322. (Thomas)
- Analytical Representation of Electron Impcat Excitation Cross Sections of Vibrationally Excited H_2 and D_2 Molecules. IAEA INDC(NDS)-333 (Celiberto and Janev)
- Radiative Losses and Electron Cooling Rates of Hydrogen, Helium, Carbon and Oxygen. IAEA INDC(NDS)-311 (In press) (Marchand, Illescas, Bonnin, Botero)
- Material Properties Data Base. In progress. (Langley, Barabash)
- Plasma-Surface Interaction Induced Erosion Data Base: In progress. (Langley)

3. Coordinated Research Projects

   - Medium and High Z Impurities in Fusion Plasmas.
   - Plasma-Surface Interaction Induced Erosion of Fusion Reactor Materials.
   - A+M Data for Plasma Edge Plasmas.
   - Radiative Cooling of the Plasma Edge.
   - Reference Data for Thermo-mechanical Properties of Fusion Reactor Plasma Facing Materials.
   - Tritium Retention and Release of Fusion Reactor Plasma Facing Materials.

PRIORITIES IN DATA COMPILATION, EVALUATION AND GENERATION (FOR FUSION)

R.K. JANEV, IAEA

- STATUS OF PRIORITIES WITH RESPECT TO THOSE IDENTIFIED IN 1993 ALMOST UNCHANGED
- SMALL SHIFTS AND DATA NEEDS EXTENSIONS RESULTING FROM THE ADOPTED "DYNAMIC GAS TARGET" DIVERTOR CONCEPT FOR ITER (WITH ENHANCED SUPPLEMENTARY IMPURITY RADIATION COOLING)
- PRIORITIES RELATED TO IAEA RESEARCH COORDINATION PROGRAMMES (RELATIVE PRIORITIES)
- REDUCTION OF PRIORITY LIST DUE TO ACCOMPLISHED WORK

A. SPECTROSCOPIC DATA

- COMPLETE SPECTROSCOPIC CHARACTERIZATION OF Ne-, Ar-IONS (DIVERTOR COOLING)
- SPECTROSCOPIC INFORMATION FOR LOW-q METALLIC HIGH-Z IONS (W, Mo, IMMEDIATE NEEDS, V, LONG-TERM NEED)
- SPECTROSCOPIC CHARACTERIZATION OF
  - H_2 (H_2^*), H_2^+ H_3^+ AND ISOTOPIC VARIANTS (NEEDED FOR ESTABLISHING A COLLISIONAL-RADIATIVE MODEL FOR H_2)
  - IMPURITY PLASMA EDGE MOLECULES (CO, CO_2, HYDROCARBONS)

B. ATOMIC COLLISION PROCESSES

1. PLASMA EDGE REGION

- ELECTRON - $H_2(v)$, $H_2^+(v)$ COLLISION PROCESSES (ALL)
  - IN PARTICULAR - DISSOCIATIVE CHANNELS
    - RECOMBINATION
    - ATTACHMENT
- ELECTRON - LOW-q IMPURITY ION PROCESSES (HIGH-Z IONS)
  (EXCITATION, IONIZATION, RECOMBINATION, INCLUDING METASTABLE ION STATES)
- ION-MOLECULE (PARTICLE INTERCHANGE) REACTIONS INVOLVING HYDROGEN AND HELIUM
  - IN PARTICULAR THOSE LEADING TO FORMATION OR DESTRUCTION OF H_2^+ AND H_3^+,
- ELASTIC, MOMENTUM TRANSFER ETC COLLISIONS INVOLVING HYDROGEN AND HELIUM IONS AND NEUTRALS
- THREE-BODY RECOMBINATION

2 CORE PLASMA REGION

- ELECTRON-IMPACT PROCESSES, WITH HIGH-q, HIGH-Z IONS (W, Mo, V), INCLUDING MULTIPLE ELECTRON PROCESSES

- He^{2+}-A^{q+} COLLISIONS CHARGE EXCHANGE, EXCITATION
  H^{+}-A^{q+} COLLISIONS FINE STRUCTURE EXCITATION

C. PARTICLE-SURFACE INTERACTIONS

- SPUTTERING, REFLECTION THRESHOLD REGION,
  SURFACE ROUGHNESS EFFECTS

- CHEMICAL EROSION, RES, EVAPORATION

- QUANTUM PROCESSES ON SURFACES
  MOLECULAR (MOLECULAR ION) FORMATION/DESTRUCTION
  (WITH IDENTIFICATION OF PRODUCT CHARGE/QUANTUM STATE)

- PARTICLE STICKING

PSI and Materials Data Base at IAEA

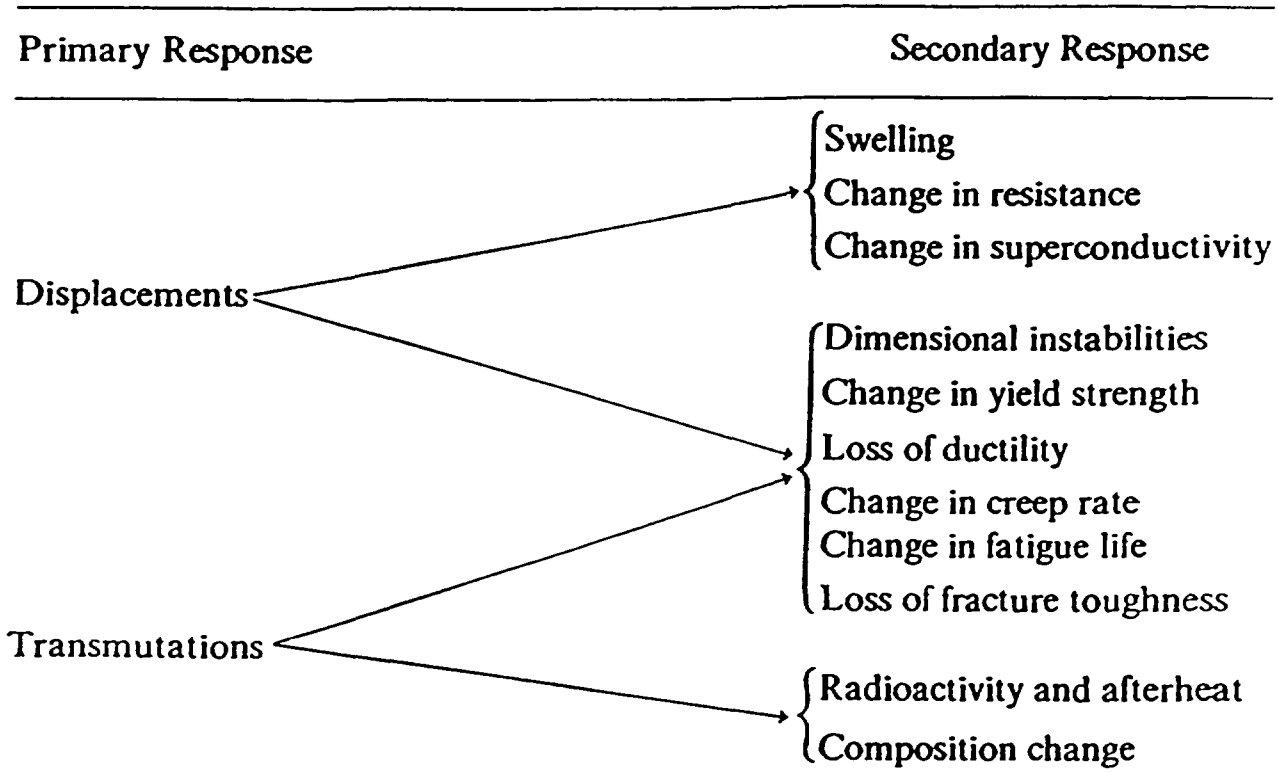
R.A. Langley

IAEA Coordinated Research Program

Objectives:

1) to encourage awareness of reactor designers to the problems involved in the selection process for plasma facing materials
2) to coordinate the anticipated experimental and theoretical work
3) to encourage the individual funding organizations to support the individual scientific groups in their work
4) to provide partial financial support to individual groups through the IAEA Research Agreements program
5) to collect and evaluate the data for presentation to the reactor designers

Physical and Mechanical Property Changes



Coordinated Research Programme Plasma-Interaction Induced Erosion of Fusion Reactor Materials

Initial Objectives:

1. Generation of experimental and theoretical data for all plasma-wall interaction processes contributing to the erosion of candidate fusion reactor materials

2. Compilation and critical assessment of the existing data on plasma-wall interaction induced erosion processes

3. Preparation of recommended sets of erosion data for candidate fusion reactor materials

Current objectives:

Erosion properties of Be, B-, Si-, Ti-doped graphites and certain high-Z materials (V,W,Mo)

Participants:

A. Haasz	/ Canada
W. Eckstein	/ Germany
K. Morita	/ Japan
L. Zhengming	/ China
E. Vietzke	/ Germany
M. Guseva	/ Russia
Y. Hirooka	/ USA
J. Brooks	/ USA

Coordinated Research Program Collection and Evaluation of Reference Thermo-mechanical Properties of Fusion Reactor Plasma Facing Materials

Objective: create (collect and critically assess) a materials database for fusion which includes thermo-physical and thermo-mechanical properties for plasma facing materials

Participants:

P. Fenici	/ Italy
S. Suzuki	/ Japan
V. Barabash	/ Russia (consultant)
I. Mazul	/ Russia
M. Pick	/ UK
T. Burchell	/ USA
J. Davis	/ ITER / USA
P. Smith	/ ITER / USA

Materials

Be, C, Ti, V, Mo, W

Carbon based materials considered

Pyrolytic graphite
Nuclear grade graphite
Doped graphites
Carbon fiber composites
Carbides

Example: Nuclear grade graphite, e.g. AXF-5Q

$\rho \simeq 1.8$ gm/cm^3 (ρ_T=2.26 gm/cm^3)
Porosity surface area: 1 m^2/gm

Metals

Beryllium (unirradiated)

Favorable consideration
- Low Z
- Thermomechanical properties

Unfavorable consideration
- Low melting point
- High erosion rate

Beryllium easily forms an oxide layer
- This has rendered the results of many measurements inconclusive.

Implantation of D into Be is similar to that of graphite (Wampler and Möller)
- 100% retention until saturation at about 0.3 D/Be at room temperature.

There appears to be little to no codeposition of H with eroded Be.

Bulk beryllium has little open porosity but retention in plasma-sprayed material has not been measured.

Molybdenum and tungsten

Favorable considerations
- Refactory
- Thermal properties
- Low sputtering coefficients for H and He
  - (high threshold energy)
- Low solubility in undamaged bulk

Unfavorable considerations
- High Z
- Sintered and radiation damaged material are expected have significantly higher retention of H.

Table 1: Material Properties

Common Information	Coating & Cladding	Structural
Description	x	x
Production history	x	x
Baseline Physical Properties		
Melt Temp	x	x
Vapor Pressure (T)	x	
Heat of Fusion	x	
Heat of Vaporization	x	
Thermal Conductivity (T)	x	x
Density (T)	x	x
Coeft. of Thermal Expansion (T)	x	x
Electrical Resistivity (T)	x	x
Viscosity (T)	x	
Surface Tension	x	
Baseline Mechanical Properties		
Elastic Modulus (T)		x
Poison Ratio (T)		x
Ultimate Strength (T)		x
Uniform Elongation (T)		x
Total Elongation (T)		x
Reduction of Area (T)		x
Creep (T,G)		x
Fatigue (T,G)		x
Fracture Toughness (T)		x
Stress/Strain (@3T)		x
Fatigue Crack Growth (T)		x

(T) = as a function of Temperature

Table 1: (Contd.)

Radiation Effects (dpa, dpa/t,T)	Structural
Physical Properties	
Thermal Conductivity	x
Specific Heat	x
Coefficient of Thermal Expansion	x
Electrical Resistivity	x
Swelling / Density	x
Mechanical Properties	
Ultimate Strength	x
Yield Strength	x
Uniform Elongation	x
Total Elongation	x
Reduction of Area	x
Creep	x
Fatigue	x
Fracture Toughness	x
Residual Activity	x
Impact Toughness (DBTT) (W,Mo,V, Ferritic Steels)	x
Stress/Strain Curve	x
Corrosion / Chemical Effects	
Compatibility @ H_2O & other Coolants	x
Joints (dissimilar metals, e.g. Be/Cu,W/Cu, C/Cu)	x

dpa = displacements per atom
dpalt = displacements per atom per second
DBTT = ductile to brittle transition temperature

Table 2: Priorities of Materials Data Generation and Evaluation

Materials	
I. Plasma Facing Materials and In Vessel Structural Materials	
A. Low-Z Materials	
Be, CFC (+ Doped B, Si), Graphite	1
PG, C + Ti	2
C + B, SiC (Fibers), BeB	3
B. High-Z Materials	
W	1
Mo, Nb	3
C. Medium-Z Materials	
SS (316 LN Annealed), V-4Cr - 4Ti, Cu, Cr, Zr, Dispersion Strengthened Cu	1
Ferritic Steel, Inconel 625, Cu Be Ni	3
D. Advanced Materials	
Liquid Materials	2
II. Interface	
Brazes (Thixotropic)	
FGM (W ↔ Cu, CFC ↔ Cu)	2

CFC = carbon fiber composits
PG = pyrolytic graphite
FGM = Fuctionally Graded Material

Table 3: Suggested Data Quality Standards

Limited Use Data

1. Data are traceable to an individual, organization, or reference (both the data "Source" and "Digitizer" are identified)
2. After independent review, an identifiable authority approved the digitized version for inclusion in the database
3. Basis of the data is identified
   a. experimental measurements
   b. derived data - specify theoretical basis and data
   c. estimated data
4. Type of data is indicated
   a. original point values
   b. analyzed data
      b1. standard fit - specify fit and data
      b2. fit unknown

Qualified Data

1. Number of measurements and data sets stated
2. Nominal confidence limits estimated (i.e., 0.90, 0.95, *n*)
3. Traceable materials specification assures reproducibility
4. Testing methods are specified and conform to a standard
5. Data are traceable to a testing/data generating organization or individual

Highly Qualified Data

1. High confidence limits determined (i.e., 0.99, 0.95, *n*)
2. Perform minimum number of individual measurements
   a. from minimum number of sample lots
   b. from multiple suppliers (if appropriate)
3. Data determined for each variable (i.e., form, processing condition, size, and so forth) that significantly affects property
4. Independent testing performed (other than the producer and preferably by several testing labs)
5. A second, independent evaluation (evaluator identified)
6. All features explainable
7. Producer(s) identified

Taken from ASTM Manual Series: MNL 19 (1993) 21.

Coordinated Research Program
Tritium Retention in Fusion Reactor Plasma Facing Components

General Objective:

Determination of the retention and release characteristics for materials relevant to fusion research and for conditions relevant to fusion reactor operating parameters

Primary Focus:

ITER and its chosen materials and operating parameters but will include other materials of interest and expanded operation parameter space

Participants:

Tony Haasz	/ Canada
Egon Vietzke	/ Germany
Adolfo Perujo	/ Italy
Tetsuo Tanabe	/ Japan
Andrey Zakharov	/ Russia
Rion Causey	/ USA

First Meeting - fall 1995

Table 1. Availability of Experimental and Theoretical Data

	Material		
	Beryllium	**Carbon**	**Medium and High Z material (Ti, V, Mo, Nb, W)**
Physical Property			
Diffusivity	L	M	M
Solubility	L	M	M
Recombination rate coefficient	L	M[a]	L
Trapping	L	M	M
n-generated	L	M	d
He effects	L	d	M
Reflection	L[b]	M[c]	H

Degree of data availability

H = high

M = medium

L = low

a) limited to graphite

b) only calculations

c) extensive for some graphites

d) unknown

TABLE II. SELECTION CRITERIA FOR MATERIALS OF PLASMA FACING COMPONENTS

Criterion	General qualification	Materials[a]	
		Favoured	Unfavoured
A. Plasma facing materials			
(1) Potential for radiation losses	Low Z	Be, B, CBM	W, Mo, Ta, SS
(2) Erosion properties.			
— physical sputtering	Low	W, Mo, Ta, Nb, and	CBM
— chemical sputtering	Low	Be, B, Si, Ti doped CBM	—
(3) Disruption resistance:			
— thermal erosion	Low	High melting point	
— crack formation	Low	Ta, Mo, CFC	CAPG, PS, SS
(4) Thermomechanical properties			
— thermoconductivity	High	CAPG, PG, CFC, W	IG, SS
— thermal stress resistance	High	CFC, W, Mo	IG, SS
— fatigue lifetime	Long	Mo	—
— fracture toughness	High	SS, Ti, Al, CBM	—
— creep strength	High	Mo, V, Ti, SS	—
(5) Irradiation influence:			
— changes of physical properties	Low	W, Ta, Mo, SS	CBM
— swelling	Low	W, Mo, Ta	CBM
— changes of mechanical properties	Low	CFC, Ta	W, Mo
— neutron activation	Low	CBM, Be, V, Ti, Al	W, Mo, Ta
— helium production	Low	W, Mo, CBM, Nb, V	Be
— reduction of thermoconductivity	Low	—	CBM (?)
(6) Tritium retention	Low	W, Mo, Be, Ti, Nb	CBM
(7) Availability	High	All metals, CBM except CFC	
B. Heat sink and structural materials			
(1) Thermomechanical properties:			
— thermal stress resistance	High	DS Cu, Cu, Mo	SS, V
— fatigue lifetime	High	DS Cu, Mo	—
— creep strength	High	Mo, DS Cu	—
— fracture toughness	High	SS, DS Cu, Cu, Nb	Mo
(2) Irradiation influence:			
— changes of physical properties	Low	SS, Mo, DS Cu, Cu, Nb	—
— swelling	Low	DS Cu, Nb	SS, Cu, Mo
— changes of mechanical properties	Low	DS Cu, Nb	Mo, SS
— neutron activation	Low	LASS	Mo, Cu, Nb, SS
(3) Tritium retention/permeation	Low	—	—
(4) Compatibility with coolants			
— critical heat flux	High	Cu, DS Cu, Mo, Nb	SS
— erosion/corrosion	Low	DS Cu, SS, Mo, Nb	—
— ICSC	Low	Mo, DS Cu	SS
— hydrid formation	Low	Mo, Cu, DS Cu	Nb
(5) Availability	High	All materials	
(6) Fabricability:			
— welding	High	SS, Cu, Nb	Mo, DS Cu
— joining with PFM	High	Mo, Nb, Cu	DS Cu, SS

[a] CBM — carbon based materials
CFC — carbon fibre composite
CAPG — compression annealed pyrolytic graphite
PG — pyrolytic graphite
IG — isotropic graphite
SS — stainless steel
DS Cu — dispersion strengthened Cu alloys
LASS — low activation stainless steel
PFM — plasma facing materials

ITER MATERIAL DATA BASE ASSESSMENT FOR Be

Beryllium

- Baseline physical properties
  - Density ■
  - Melting temperature ■
  - Vapor pressure ▲
  - Thermal expansion ▲
  - Thermal conductivity ▲
  - Specific heat ■
  - Electrical Resistivity ▲
- Baseline mechanical properties
  - Elastic modulus ▲
  - Poisson's ratio ●
  - Fracture properties
    - Tensile ●
    - Bending ●
    - Compressive ●
  - Creep properties ●
- Chemical stability/compatibility
  - Composition/purity ■
  - Vapor pressure/transport ■
  - Compatibility
    - Water ●
    - SS ■
- Tritium solubility/transport
  - Tritium solubility ○
  - Tritium diffusivity ●
  - Adsorption/desorption properties
- Radiation effects
  - Physical properties ○
  - Swelling ●
  - Creep
  - Tritium trapping/transport ●
  - Helium trapping/transport ▲
  - Fracture properties ●

■——Adequate/good agreement
▲——Limited/general agreement
●——Limited/important discrepancies
○——Single set of data
Blank—Very limited/non-existent/high uncertainties