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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Consultants' Meeting on "Atomic and Plasma-Surface Interaction Data Needs for Plasma Disruption Modeling"

8-9 November 1993, Vienna, Austria

SUMMARY REPORT

Prepared by:

R.K. Janev, A. Hassanein, Yu. Martynenko and H. Bolt

January 1994

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

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Abstract

A brief proceedings of the IAEA Consultants' Meeting on "Atomic and Plasma-Surface Interaction Data Needs for Plasma Disruption Modeling" (November 8-9, 1993, Vienna) is provided. The main results of the meeting regarding the atomic and plasma-surface interaction data needs for a comprehensive modeling of plasma disruption erosion, including the vapor shielding effects, are described. The scope and potential participants of a Co-ordinated Research Programme, recommended for initiation by the IAEA in 1994, are also presented.

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Appendices

1. INTRODUCTION

On recommendation of the IAEA Technical Committee Meeting on "Atomic and Molecular Data for Fusion Reactor Technology" (Cadarache, October 12-16, 1992) and with the endorsement of the IFRC Subcommittee on Atomic and Molecular Data for Fusion (7th Subcommittee Meeting, Cadarache, October 16-17, 1992), the IAEA Atomic and Molecular (A+M) Data Unit organized on November 8-9, 1993, a small Consultants' Meeting on the "Atomic and Plasma-Surface Interaction Data Needs for Plasma Disruption Modeling" at the IAEA Headquarters in Vienna, Austria. The objectives of the meeting were to make a thorough analysis of the atomic and plasma-surface interaction physics content of the existing plasma disruption modeling codes from the point of their capabilities for predicting the material erosion during plasma disruptions with inclusion of the shielding effects of evaporated material cloud in front of the surface on the net erosion rates, and on the atomic and plasma-surface interaction data required for enhancement of the predictive power of modeling codes. The findings of the meeting would then serve as a basis for future Agency actions aiming at improvement of the required database.

Because of financial constraints, only three leading experts in the field were invited to participate in the Meeting: Dr. H. Bolt (KFA, Jülich), Dr. Yu.V. Martynenko (Kurchatov Institute, Moscow) and Dr. A. Hassanein (ANL, Argonne). Due to unexpected developments, Dr. Bolt was not able to participate in the meeting, but through intense commnication with him before and after the meeting, his views are fully represented in the present Report. The staff of the IAEA A+M Data Unit took also active participation in the meeting. The List of Meeting Participants and the Meeting Agenda are given in Appendices 1 and 2, respectively.

2. BRIEF MEETING PROCEEDINGS

After the introductory remarks of the scientific secretary (R.K. Janev) regarding the meeting objectives, the work of the meeting closely followed the adopted agenda. Drs. Hassanein and Martynenko described first the underlying physics and the structure of numerical code packages used in their research groups for plasma disruption modeling and for calculation of disruption erosion rates. The presentations were illustrated with code results on the eroded depth (evaporated mass) for various materials (Be, graphite, W) and various disruption conditions (deposited energy, pulse duration, etc), including comparison with plasma gun and electron beam experiments. Both of the described codes packages include vapor shielding effects on the net erosion rates. The presentations demonstrated that the code results are very sensitive to the parameters describing the plasma interaction with the solid surfaces, mechanisms of energy deposition, material response to the plasma action, and to atomic processes which define the radiative and transport properties of evaporated material cloud. After these presentations a detailed analysis of atomic (collision and radiative) and plasma-material interaction processes involved in the disruption erosion modeling was performed from the point of view of their completness, relative importance and the accuracy of the corresponding data included in the codes. This analysis has led to identification of the processes for which the data are either missing or of insufficient accuracy. Generation of such data (or their collection and critical assessment if they are available) and their implementation in the modeling codes would be a significant step in enhancing the predictive capability of the codes.

Some aspects of the discussions, including the meeting findings, conclusions and recommendations are presented in the remainder of this Report.

3. PHYSICS BASIS AND STRUCTURE OF CURRENT PLASMA DISRUPTION MODELING CODES

The underlying physics of plasma disruption modeling codes includes the following three essential areas: (1) plasma-material interaction, (2) plasma-vapor interaction, and (3) radiation hydrodynamics and transport. Each of these areas includes a number of outstanding physical problems which can be well defined in mathematical terms and are reflected in the disruption modeling codes. The main issues in plasma-material interaction area are the plasma energy deposition (involving amount and type of energy deposited, particle incidence angle, etc.) and the target thermal response (including the type and form of material release, melt layer behaviour, substrate thermophysical and thermomechanical behaviour). The plasma-vapor interaction physics includes aspects related to the plasma energy deposition in the vapor, plasma scattering (reflection) from the vapor cloud, vapor heating and conduction, and all processes associated with the plasma cooling in the vapor region. The area of radiation hydrodynamics and transport in the vapor cloud is particularly complex and includes a large variety of atomic collisional and radiative processes. The dynamics of plasma-vaport interaction is schematically shown in Fig. 1 (taken from the presentation of Dr. A. Hassanein). It is obvious that all three physics areas are mutually strongly coupled and form a complex self-consistent problem.

The presently available computer code packages for disruption modeling include all the physics relevant for description of disruption effects on the plasma facing materials, including the net material erosion. The most comprehensive package of codes is that developed at the Argonne National Laboratory (ANL), and its current improvements are done through close collaboration with several US, EC and Russian institutions. The largest part of the physics related to the disruption erosion is included in the ANL A^* Thermal-2 computer code. The structure of this code is shown in Fig. 2 (taken from the presentation of Dr. Hassanein). This code fairly successfully describes the experimental results on material erosion induced by plasma gun and electron beam (Fig. 3 and Fig. 4, respectively, taken from the presentation of Dr. Hassanein).

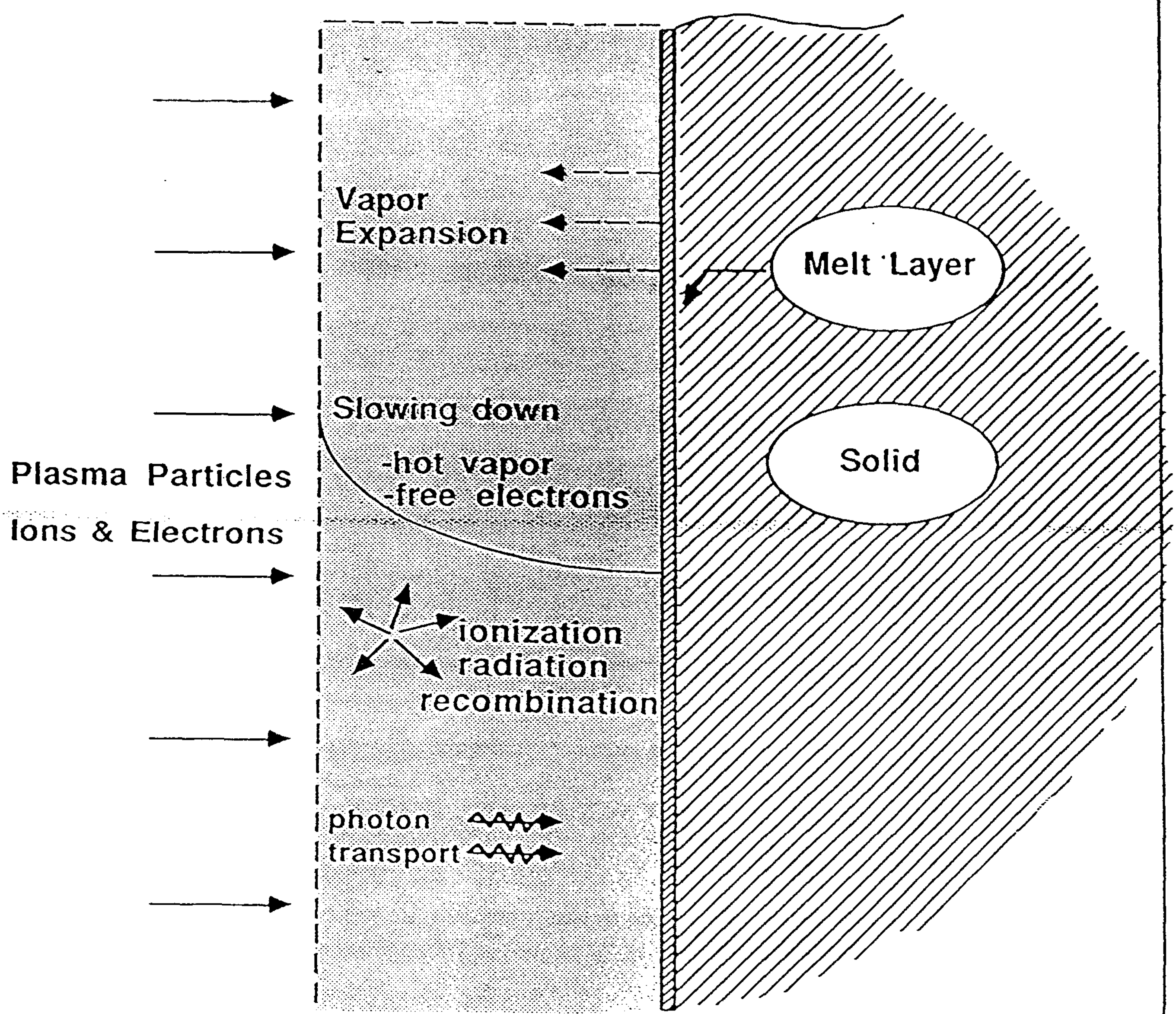
4. ATOMIC AND PLASMA-MATERIAL INTERACTION DATA NEEDS FOR IMPROVEMENT OF DISRUPTION EROSION MODELING

The detailed analysis of the status and the needs of atomic, plasma-material interaction and material properties data required in the numerical codes for disruption erosion modeling has revealed that improvements of the database are needed in all three physics areas mentioned in the preceeding section. The most needed types of data for each of these areas are listed below:

4.1. Plasma-Material Interactions

1) Thermophysical and thermomechanical properties data (as function of temperature (T), where applicable)
   - Melting temperature
   - Boiling temperature
   - Vapor presssure
   - Heat of fusion
   - Heat of vaporation
   - Thermal conductivity (T)

Dynamics of Plasma-Vapor Interactions



Materials and Components Technology

Fig. 1

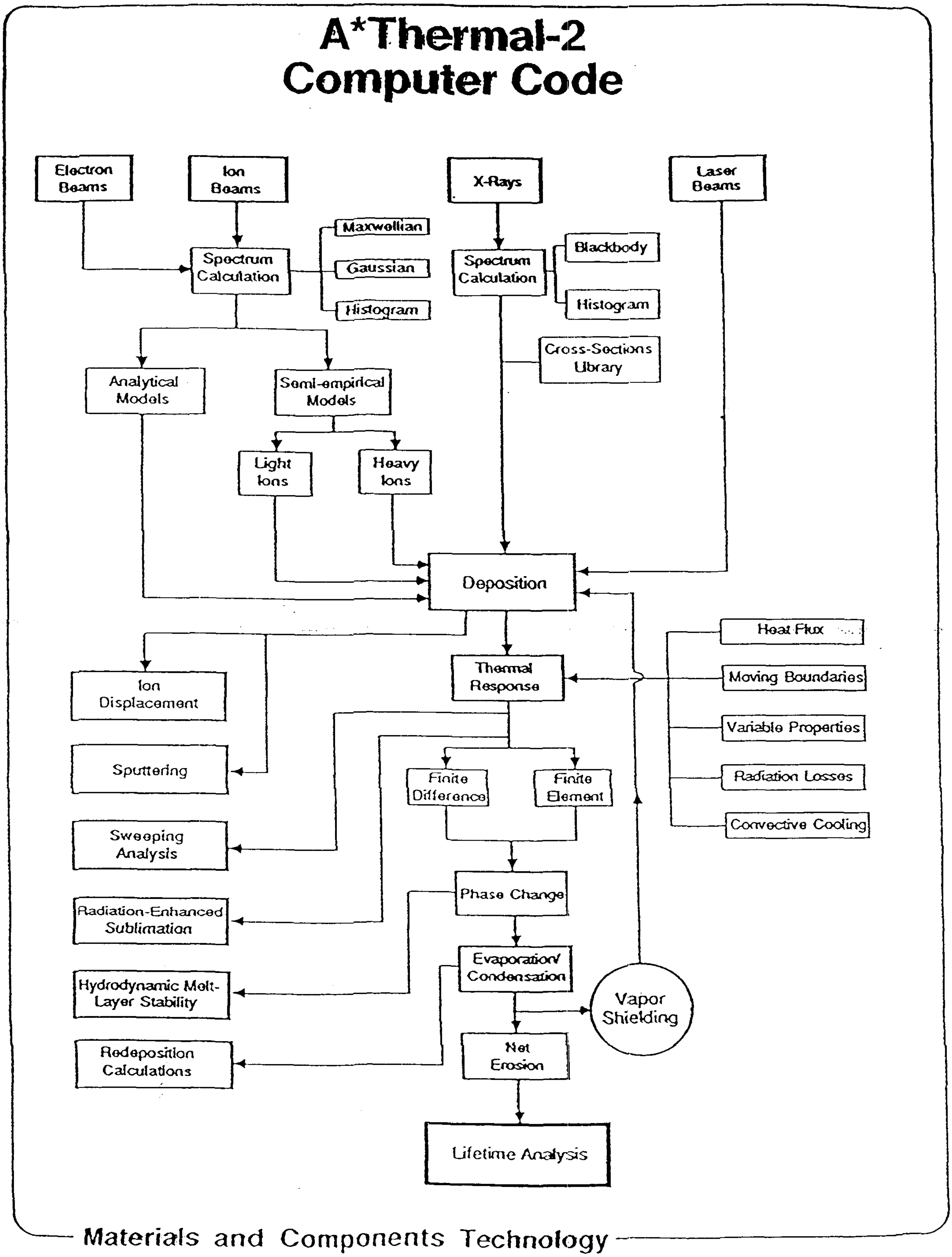
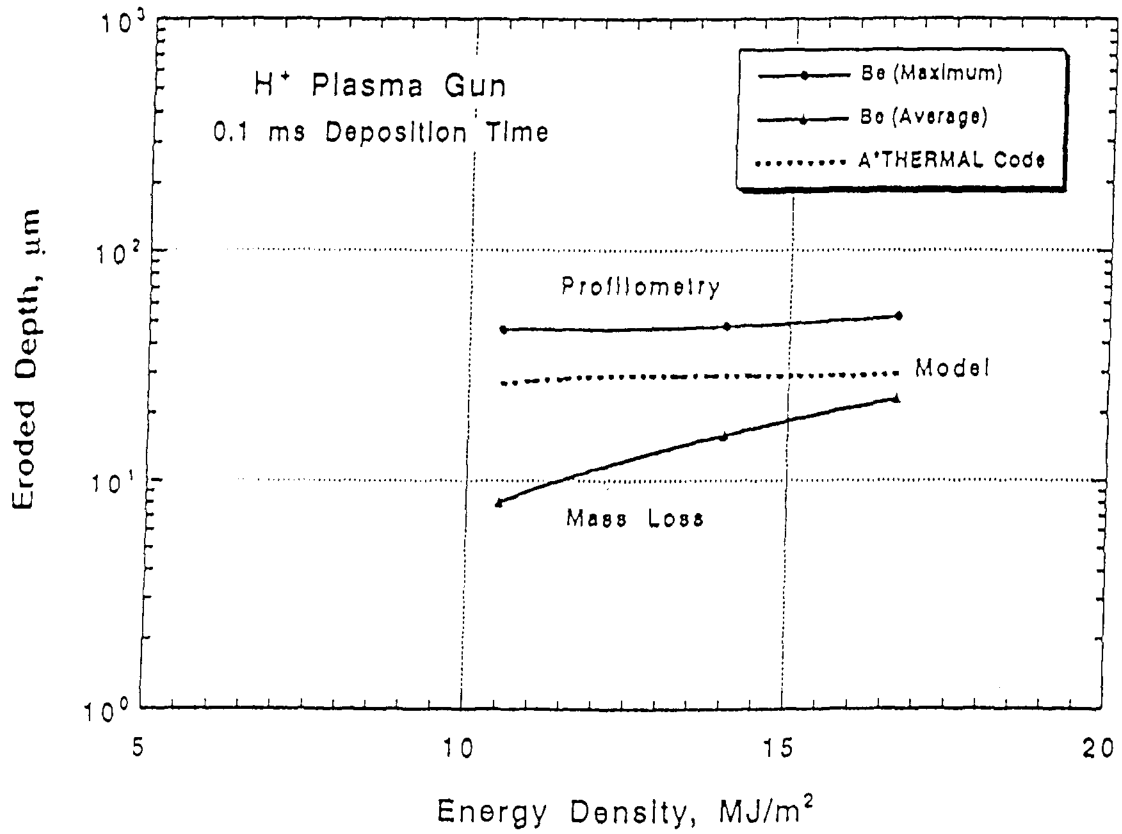
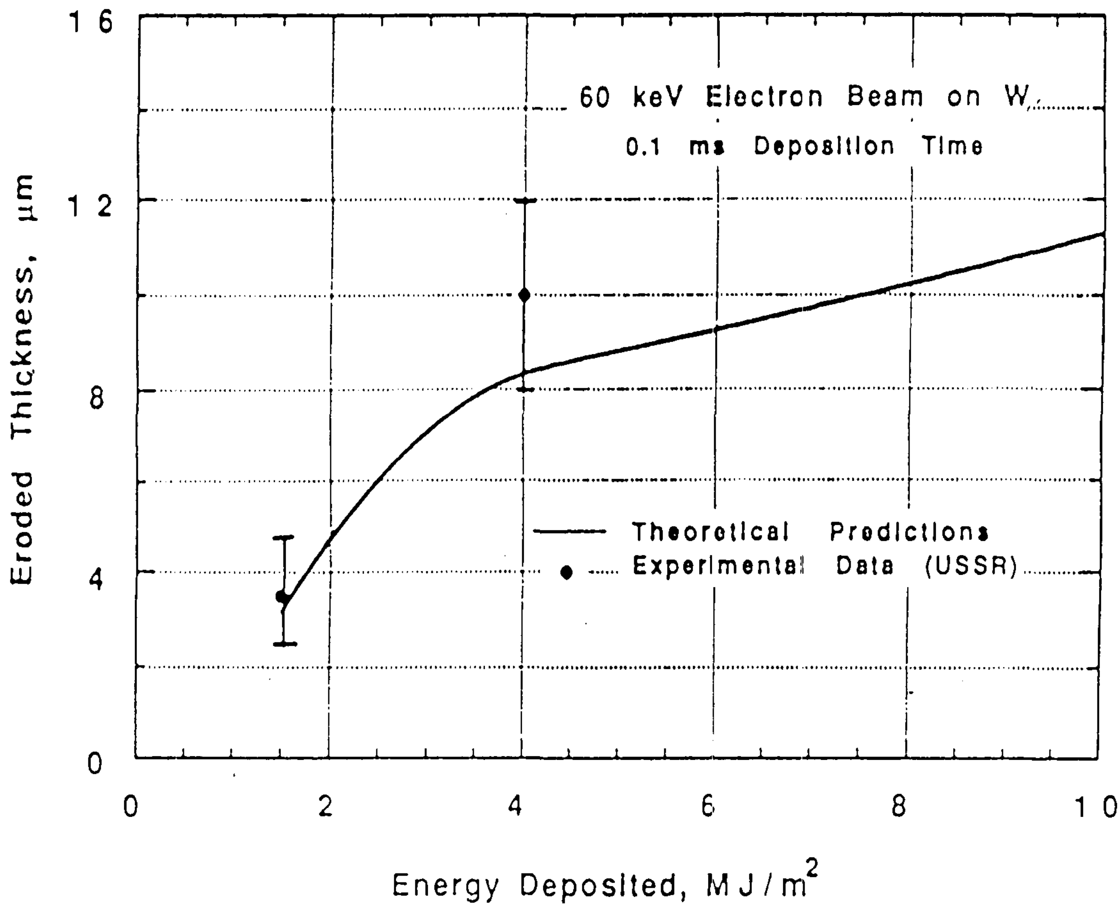

A*Thermal-2
Computer Code
Electron Beams
Ion Beams
X-Rays
Laser Beams
Spectrum Calculation
Maxwellian
Gaussian
Histogram
Spectrum Calculation
Blackbody
Histogram
Cross-Sections Library
Analytical Models
Semi-empirical Models
Light Ions
Heavy Ions
Deposition
Heat Flux
Thermal Response
Moving Boundaries
Variable Properties
Radiation Losses
Convective Cooling
Ion Displacement
Sputtering
Sweeping Analysis
Radiation-Enhanced Sublimation
Hydrodynamic Melt-Layer Stability
Redeposition Calculations
Finite Difference
Finite Element
Phase Change
Evaporation/ Condensation
Vapor Shielding
Net Erosion
Lifetime Analysis
Materials and Components Technology

Fig. 2



H+ Plasma Gun
0.1 ms Deposition Time
Be (Maximum)
Be (Average)
A*THERMAL Code
Profilometry
Model
Mass Loss
Eroded Depth, µm
Energy Density, MJ/m2

Fig. 3



Comparison Between Recent Experimental Data and Current Model Predictions

Fig. 4

- Specific heat (T)
- Density (T)
- Coefficient of thermal expansion (T)
- Electrical resistivity (T)
- Viscosity (T)
- Surface tension (T)
- Elastic moduli (T)
- Poison ratio (T)

2) Iradiated material properties
   (as function of T, flux and fluence)
   - Thermal conductivity
   - Specific heat
   - Coefficient of thermal expansion
   - Electrical resistivity
   - Swelling
3) Redeposited material properties
   - Structure
   - Thermophysical and thermomechanical properties (as in 1) above)
   - Irradiation effects (as in 2) above)
4) Particle and energy reflection coefficients
   From:
     - Solid targets
     - Liquid targets
     - Gas targets
5) Characteristics of incident energy during disruption
   - Form of deposited energy (electrons, ions, plasma)
   - Parameters (energy, distribution)
   - Angle of incidence

4.2. Plasma-Vapor Interaction

1) Plasma particle and energy deposition in vapor

- Reflection/scattering
- Stopping power at higher vapor temperature
  (i.e. effects of T on range of particles)

2) Vapor heating
   - Ionization/recombination coefficients (for all ionization stages)
   - Excitation/de-excitation (collisional and radiative)
   - Conduction
   - Effects of impurities
   - Magnetic field effects

4.3. Radiation Hydrodynamics and Transport

1) Spectroscopic information
   (for all ionization stages of ions)
   - Radiation spectra (wavelengths, energy levels)
   - Transition probabilities
2) Collisional information
   - Photoionization/photoabsorption
   - Excitation, ionization, recombination
   - Heavy particle collision processes
3) Composite radiative information
   - Line radiation/absorption
   - Stark and Doppler line broadening
   - Opacity and emissivity data (for various vapor temperatures and densities)

The materials for which the above data information is required include:

a) Low-Z materials:
   Be, CFC, PG, C+Ti, C+B, SiC, BeB
b) Medium-Z materials:
   V, SS, Ni-based, Cu
c) High-Z materials:
   W, Mo, Nb, Ta

The format of generated (evaluated, recommended) data should preferrably be in either analytic equation form (e.g. for the thermophysical properties as function of temperature, atomic reaction rates as function of plasma temperature, etc) or in table format (e.g. opacity, emissivity). The IAEA ALADDIN data format seems quite adequate for computer storage and manipulation (and exchange) of the data. For an easy implementation of the data into the modeling code, appropriate interfaces could also be developed.

Additional Comments

1. The efforts should be oriented towards modelling the energy deposition from an incident plasma rather than from either electrons or ions as done untill now.
2. The effect of recycling hydrogen on the gas shield formation in the first stages of the energy deposition should be looked at. Perhaps the recycling hydrogen contributes considerably to the formation of a gas cloud in front of the target.
3. Lower energy deposition scenarios with longer pulse durations should also be taken into account (e.g. 3 MJ/m^2 for 20 ms), since they are of main importance for the first wall.
4. Stopping power data for the outer zones of the vapour shield would provide a better modelling of the energy input in the periphery of the cloud. This energy input is of importance for the expansion behaviour of the outer zones of the cloud where most of the energy shielding takes place.
5. Opacity and emissivity data in the intermediate regime between LTE and coronal equillibrium are needed: An updated reference set of such data would be very helpful. With these data the effects at the cloud periphery and also the lower energy deposition scenarios with longer pulse duration can be treated.
6. Effects of the toroidal magnetic field on the expansion behaviour of the vapour cloud should be considered in a realistic geometry. Much of the shielding effect seems to be critically dependent on the magnetic field configuration.
7. For ITER the melt layer stability under disruption conditions should be looked at. Eventually data on viscosity and surface tension of molten metals (Be,W) should be included in a data base.

5. SCOPE AND OBJECTIVES FOR AN IAEA Co-ordinated Research Programme (CRP)

The volume of atomic and plasma-material interaction data required for improving the predictive capabilities of presently existing plasma disruption modeling codes is so large that a broad and well organized co-ordinated effort would be necessary to be undertaken in order to meet timely the needs of ITER EDA. The existing databases and data compilation/generation activities of the IAEA Atomic and Molecular Data Unit, as well as its established forms and experience in the co-ordination of worldwide data generation, compilation and evaluation efforts, represent a good basis for organization of an international database establishing programme for plasma disruption modeling. Such a programme would take advantage of the existing data information already available at the IAEA, of the data generation possibilities already existing within the other ongoing Agency co-ordinated research programmes in the areas overlaping with the needs of plasma disruption modeling database, and should address only those complementary database parts for which no adequate information is presently available. The Agency A+M Data Unit will then be responsible for the integration of the entire relevant information into one database, including its appropriate formatting and installing in the ALADDIN system.

The objectives of an IAEA Co-ordinated Research Programme (CRP) would be to:

- Establish a comprehensive and recommended atomic and plasma-material interaction database for use in plasma disruption modeling codes,
- Develop an in-depth understanding of plasma disruption effects on reactor plasma facing materials, in particular the vapor shielding effects,
- Develop an accurate tool to evaluate the erosion lifetime of ITER plasma facing components .

The composition of this CRP should include the most active groups in disruption modeling (ANL, Univ. of Visconsin, Kurchatov Institute, TRINITI, Efremov Institute, KFA Jülich, KFK Karlsruhe, JAERI), experimental disruption simulation (KFA Jülich, JAERI, Efremov Institute, TRINITI, SNLA), representatives of the A+M/PMI Data Centre Network, and the most active groups in atomic and plasma-material data generation.

It should be noted that the suggested CRP is currently not in the Agency programmes for 1994-1996, and its implementation would require either an additional, extrabudgetary contribution to the IAEA from the participating institutions (i.e. corresponding Member

States), possibly through arrangements with the ITER home teams, or participation in the co-ordinated research meetings related to this CRP at the expence of the participating institutions (or ITER home teams).

6. MEETING CONCLUSIONS AND RECOMMENDATIONS

1) Plasma disruption induced erosion of plasma facing materials is an important design parameter for the next step fusion devices, including ITER. Establishment of an appropriate computer package for accurate prediction of erosion lifetime of plasma facing components under off-normal events requires significants improvements of the atomic and plasma-material interaction databases incorporated in the computer codes, as well as of certain aspects of the disruption physics and dynamics.
2) The atomic and plasma-material interaction physics currently implemented in plasma disruption modeling codes requires further improvements both in terms of included processes and, even more so, in terms of the data accuracy.
3) In order to meet the design needs of next step devices, in particular ITER, in a timely fashion, it is necessary to undertake a well defined concerted international effort for establishing a comprehensive, internationally recommended atomic and plasma-material database for accurate modeling of the disruption effects on plasma facing components and their performance. The IAEA, with its existing databases, co-ordinating potential and data evaluation and processing capabilities, is extremely well suited to undertake and co-ordinate this effort.
4) It is, therefore, strongly recommended that the Agency initiates in 1994 a Co-ordinated Research Programme with the scope and objectives outlined in section 5 of this Report. If budgetary problems appear in connection with the implementation of the suggested CRP, their solution should be sought through various forms of external support to this programme.

Appendix 1

IAEA Consultants' Meeting on
"Atomic and Plasma-Surface Interaction Data Needs for Plasma Disruption Modeling"

8-9 November 1993, IAEA Headquarters, Vienna, Austria

LIST OF PARTICIPANTS*

Dr. Y. Martynenko	Scientific Research Centre, "Kurchatov Institute", Ploshchad I.V. Kurchatova, Moscow D-182 123182, RUSSIAN FEDERATION
Dr. A. Hassanein	Energy Technology Division, Argonne National Laboratory, 9700 South Cass Avenue, Bldg. 207, Argonne IL 60439, U.S.A.

IAEA

Dr. R.K. Janev	IAEA Atomic and Molecular Data Unit, Wagramerstrasse 5, P.O. Box 100, A-1400 Vienna, AUSTRIA
Dr. J. Botero	IAEA Atomic and Molecular Data Unit, Wagramerstrasse 5, P.O. Box 100, A-1400 Vienna, AUSTRIA

* **Dr. H. Bolt** (Institut für Reaktorwerkstoffe, Forschungszentrum Jülich GmbH, P.O. Box 1913, D-52425 Jülich, Germany) has actively participated in the outcomes of this meeting by an extensive correspondence with the Meeting Scientific Secretary on all the items of the Agenda.

Appendix 2

IAEA Consultants' Meeting on
"Atomic and Plasma-Surface Interaction Data Needs for Plasma Disruption Modeling"

8-9 November 1993, IAEA Headquarters, Vienna, Austria

MEETING AGENDA

Monday, 8 November

9:30 - 9:45	Opening Adoption of Agenda	Meeting Room: C-04-51
9:45 - 12:15 (*)	Characteristics of current computer codes for plasma disruption erosion modeling: (presentations)	
12:15-14:00	Lunch	
14:00-18:00 (*)	Atomic and plasma-surface interaction content in present discription erosion modeling codes (Analysis and quality assessment)	

Tuesday, 9 November

9:00-12:00 (*)	Atomic and plasma material interaction data needs identification for predictive disruption erosion modeling (including vapor shielding effects) (Data requirements specification; data implementation into codes)
12:00-14:00	Lunch
14:00-17:30 (*)	Required code improvements and data collection/generation actions for expanding the modeling code capabilites and establishing recommended disruption erosion databases for the ITER candidate PFC materials (Formulation of Meeting conclusions and recommendations)

(*) A 15 min. coffee break envisaged