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Assessment of Atomic and Molecular Data Priorities

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

4 – 5 December 2006

Prepared by

R.E.H. Clark

November 2007

IAEA Nuclear Data Section, Wagramer Strasse 5, A-1400 Vienna, Austria

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Abstract

The interaction of plasma particles with surfaces will be a vital aspect of the ITER machine and other future fusion devices. The Atomic and Molecular Data Subcommittee of the International Fusion Research Council had recommended that the Atomic and Molecular Data Unit hold a Technical Meeting (TM) to assess the current data priorities in this area. Accordingly, eleven international experts on particle-surface interactions participated in a TM at IAEA Headquarters, Vienna, on 4, 5 December 2006 to assess the data priorities. After a review of the current state of understanding on particle-surface processes involving various proposed materials under different conditions, a list of specific data needs for fusion-related materials was formulated. Areas in which a meaningful CRP could be established were also defined. The discussions, conclusions and recommendations of the TM are briefly described in this report.

November 2007

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Introduction

An IAEA Technical Meeting (TM) on "Assessment of Atomic and Molecular Data Priorities" was held on 4, 5 December 2006 at IAEA Headquarters, Vienna, Austria. The primary aims of this TM were to review the relevant on-going research activities of the participants, specify the data needs for plasma-surface processes identified with the operation of fusion devices, and assess the priorities for such A+M data.

Eleven international experts on particle-surface interactions participated in the TM (see Appendix 1). Each participant gave a summary of their areas of expertise and research activities, focusing on fusion-related materials. Subsequent discussions among the participants on A+M data priorities produced a final list of recommendations, including specific topics for possible Coordinated Research Projects (CRPs).

Meeting Proceedings

N. Ramamoorthy (Director, Division of Physical and Chemical Sciences) welcomed the participants on behalf of the IAEA. He noted that fusion research continues to advance, and is an important topic within the IAEA Nuclear Data Section. Significant political progress in the ITER project has generated extensive motivation for increased research to address atomic and molecular data needs, and he expressed confidence that the TM would provide valuable advice to the Atomic and Molecular (A+M) Data Unit on priorities. R. Clark (Scientific Secretary) reviewed the proposed agenda, which was accepted without change (see Appendix 2).

Each participant reviewed their capabilities and relevant research activities through detailed presentations at the meeting. These presentations were collected electronically and distributed on CD; brief summaries are given below.

D. Cowgill (Sandia National Laboratories, USA) summarized his work on transient trapping of helium by bubble formation in liquid metals. He discussed the Bubbles in Liquid Metals (BLM) model, based on He bubble evolution in tritium-containing materials. Flowing liquid metals have the potential to pump He by bubble formation, and this model has been developed and Sandia National Laboratories to predict significant bubble nucleation and growth under certain conditions. Low-flux experiments with a Penning trap are being udertaken to test and benchmark the model.

R. Majeski (Princeton Plasma Physics Laboratory, USA) reviewed on-going research into a liquid lithium wall for CDX-U and LTX. Initial experiments with liquid lithium PFCs – wet-mesh lithium rail limiters were described, as well as studies with a free-surface liquid lithium-filled tray limiter. Work on tray limiter and electron beam-induced evaporative coatings was discussed, along with area effects using liquid lithium. Aspects of the mechanical stability of liquid lithium during tokamak operations were presented, and high power density experiments with liquid lithium targets were defined. The next step involves the construction of the Lithium Tokamak eXperiment (LTX).

Igor Lyublinski (FSUE "Red Star", Moscow, Russian Federation) presented work on lithium capillary-pore systems as new plasma-facing materials (PFM) for fusion. These studies appear to provide a convincing basis for the proposed advance of liquid lithium PFM for adoption in steady state Li-tokamaks. Potential problems with such a tokamak need to be addressed, including wall and divertor plate erosion, "dust" accumulation and re-deposition, tritium recovery, low Z_{eff}, and heat removal in the steady-state regime and during disruptions. The liquid lithium approach requires further experiments, calculations, design research and technological development to address these issues.

G. Mazzitelli (Associazione EURATOM-ENEA sulla Fusione, CR Frascati, Italy) presented experimental results with liquid lithium as a plasma-facing component on FTU that support "lithization" as an effective tool for plasma operations. Experiments using a liquid surface in a tokamak were carried out on FTU that exhibited very promising results. An experimental campaign over the forthcoming 12 months will focus on studies of the peaked density profile discharges with an

I_p scan, and the behaviour of the liquid lithium limiter (LLL) with additional heating. Studies are underway on a new LLL with the ability to act as the main limiter. "Boronization" was found to be very effective in reducing the impurity content and the radiated power of the FTU plasma over the range of densities considered.

R. Doerner (Center for Energy Research, University of California – San Diego, USA) summarized outstanding research and development issues in mixed-material PMI. His assessment focused on our understanding of mixed Be/C and Be/W materials of relevance to ITER. Outstanding issues relating to co-deposition and erosion were enumerated, and future directions of the PISCES research programme were described.

I. Kupriyanov (Bochvar Research Institute of Inorganic Materials (VNIINM), Russia) discussed the main aspects of applying Be as a PFC material. The nuclear and physical-mechanic properties of beryllium have long been used to good effect in fission reactors, and more recently in the Joint European Torus (JET). Be will be used as a plasma-facing material in vessel components of ITER, and is under consideration in various forms for several designs of tritium-breeding blanket. However, beryllium possesses some disadvantages which restrict application in fission and fusion. The efficiency and variety of Be applications in future fusion devices will depend on understanding these disadvantages, and developing various ways of eliminating them.

A.A. Pisarev (Moscow Engineering and Physics Institute, Russia) discussed the thermal desorption of deuterium from various forms of graphite. Deuterium release is observed as D_2, HD, CD_4 and HDO, and the peak temperatures for the emission of various D and H containing gases exhibit a well-defined correlation. Three groups of peaks centered at 500, 800 and 1100K are observed after plasma implantation, and each group contains more than one peak. A single peak at 1100K is observed after ion implantation, and the peaks at 500 and 800K are observed after exposure to gas (also observed after exposure to an H atom beam, as described in the literature). Therefore, the 1100K peak found in plasma experiments may be connected with radiation damage, while the peaks around 500 and 800K may be connected with natural sites or pseudo "like-natural" sites produced by low-energy ions. Atoms, ions and gas all participate in trapping processes within plasma experiments. Peak positions have been found to be similar for three different plasmas and two materials: powdered graphite and CFC. The amplitudes of the peaks depend on the material and plasma parameters, while the structure of the surface depends on the material and plasma. Relief structure can be prominent, thin and non-uniform, and nanostructures with potentially high absorption can be formed on the surface. Both the trapping and release processes can be influenced by the topographic features of the surface.

P. Coad (EURATOM Association/UKAEA, Culham Research Centre, UK) presented work on erosion-deposition studies on JET, and plans for the ITER-like wall experiment. Erosion-deposition issues in JET include divertor asymmetry, and the modelling of transport and hydrogen isotope retention. Important scientific goals for the ITER-like wall experiment, scientific goals and material configurations were discussed - deposition and H-retention in JET occurs mostly at the inner divertor for normal discharges. Some erosion has been observed at the outer divertor, but the major location for such problems is the main chamber. Divertor conditions are more balanced and controlled for reversed field operations. ^{13}C puff experiments were carried out in 2001 and 2004, and a further campaign is planned for March 2007 to provide input data for modelling. JET is preparing for an ITER-like wall experiment from 2008 onwards to study retention and develop operational scenarios with a metal wall that will include Be tiles and coatings in the main chamber and a full W divertor (some solid W tiles, and the remainder to be coated with W). There is also a proposal to add C strike points at a later date.

V. Alimov (Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Russia) reported on deuterium retention in plasma-facing materials. A review has been undertaken of the available data for ITER wall materials, which highlighted specific data needs. Requirements for CFC have been identified with hydrogen isotope retention at irradiation fluences above 1026 D m^{-2}. Beryllium materials would benefit from quantification of hydrogen isotope retention after high-flux plasma exposure at temperatures above 500K, including the determination of the fluence, temperature dependence and D depth profiles in the bulk of the beryllium. Hydrogen retention by W materials will be affected by carbon and oxygen impurities in the plasma, and this behaviour requires detailed study. Hydrogen isotope retention and D concentrations in beryllium and tungsten carbides merit more comprehensive study. Data are also required to define hydrogen retention in Be-C, Be-W and C-W mixed materials, as well as to determine the dependence of the D concentration in the bulk as a function of the C concentration.

N. Ohno (Nagoya University, Japan) reported on high flux helium and hydrogen plasma exposure to bulk tungsten and tungsten-coated graphite. Tungsten W is one of the most important candidates for plasma-facing components in future fusion devices (ITER and Demo) because of various appropriate properties: high melting point, low gas retention and high threshold energy for physical sputtering. However, laboratory experiments show a potential problem exists of He hole/bubble and hydrogen blister formation on solid W by low-energy plasma irradiation, although this behaviour has not been observed in tokamak experiments (ASDEX-U and JT-60U). There are many important issues involving plasma-W interaction, for example, the difference between solid W and W-coated graphite, high-Z dust formation, and the influence of transient heat pulses on damaged W surfaces, as investigated by a linear divertor plasma simulator. Ohno focused on the properties of He bubbles and holes on the surface of bulk W, bubble formation on W-coated graphite, and damage by heat pulses as well as hydrogen blister formation.

A.A. Haasz (University of Toronto, Canada) described the effect of impurities on D retention in W, and D removal from C-D co-deposits. Deuterium retention in tungsten has been studied, including the impact of He on D trapping during sequential irradiation by He and D, simultaneous irradiation by He and D, and the effect of implanted C on D retention. Experiments have been carried out on the oxidative removal of deuterium from co-deposits: oxidation of DIII-D and JET co-deposits, and the effect of inherent impurities on co-deposit removal efficiency and sputtered W on D removal from laboratory-created films and DIII-D co-deposits.

Recommendations and Conclusion

Considerable discussion took place on the data requirements, based on the different materials proposed for ITER. After summarizing the recognized data needs, the participants formulated and agreed their recommendations and proposed areas that could benefit from a CRP initiative.

Liquid Metals:

Status of liquid metals, Ga, Sn and Li: Experimental data exist for a small tokomak with Ga on the walls; otherwise, these materials are essentially uncharacterized except for lithium.

Although good for the plasma, Li metal research is at a very early stage. Li is good for the plasma, and is compatible with the operation of tokomaks - self healing and pumps He, if flowing, although droplet spattering is a potential problem. Creates no dust if kept in the liquid phase, assuming wall temperatures are higher than 200°C. Pure Li is compatible with other metals such as Mo and stainless-steel mesh structures, and is relevant to the proposed breeder blanket.

There is a need for demonstrations of Li as a divertor target. Data are required for high heat fluxes, off-normal events, pumping properties and JXB effects. Information is needed on how to introduce Li into the machine, along with wetting, insulation and materials compatibility. The impact of impurities needs to be explored (Be for example), along with temperature dependence. Embrittlement is also an unknown factor, and should be an issue of concern.

Beryllium:

Beryllium getters oxygen. As a low Z material, Be possesses good mechanical and thermal properties, and offers resistance to radiation at the operational temperatures of ITER. However, the surface morphology changes during irradiation, Be does melt, and any resulting Be dust will be problematic. Crack formation under thermal loading and plasma disruptions occurs, and mixed Be species are known to form with the proposed bulk materials of ITER.

An important requirement will be to determine the impact of energetic helium on first wall Be through careful examination of Be specimens obtained from the JET ITER-like wall experiment. Permissible levels of oxygen impurity in Be will have to be defined with respect to plasma performance. The effect of O impurities and porosity on Be erosion and H retention require quantification (e.g. co-deposition, and the effect of neutron irradiation on such properties as embrittlement). Information is also needed on H behaviour with Be mixed materials (although some retention data exist already).

Carbon/graphite:

Erosion

The existing database is reasonably comprehensive. While the processes for pure carbon are understood, mixed materials remain a significant issue. Studies are required on the effect of noble gases (argon) on structures and potential dust formation. Experiments involving transient high-power loads on Be-contaminated C are also needed.

Re-deposition/co-deposition

An extensive database exists on re-deposition - key remaining issue is transport, especially in the locations where deposition occurs.

Modelling groups would benefit substantially from interact with experimentalists. Both the erosion and thermal properties of the deposits are poorly understood, and there is a need for improved definition of the effects of impurities. Global erosion and deposition are complicated and not well understood. There is a need for diagnostic techniques such as QMB (quartz microbalance) to track where and when co-deposition occurs.

D Retention

D retention will be significant under ITER-like conditions, and modelling predictions need to be undertaken. The amount of T transported into the bulk of the facility also needs to be quantified, and will depend strongly depends on the temperature and type of CFC.

Co-deposit removal

Several techniques have been proposed and tested. Photon methods include flash lamp release and laser desorption. Plasma discharges are limited to plasma-facing components, while high pressure glow discharges have the ability to go into shadow regions (although the effectiveness to remove co-deposits diminishes with time). Other techniques include the use of nitrous oxide and ozone, but these are corrosive on various components of the machine. Inadequate oxidation data exist.

Improved knowledge of re-deposition would be beneficial in the application of photon methods, and there is the issue of plasma recovery after discharges. There is the need to test thicker layers in oxidizing conditions. Other issues include the role of impurities and the observed “leveling-off effect”. What sort of surface morphology is left after oxidative removal? Is there collateral damage? There is also a need for more information on plasma recovery after oxidation.

Tungsten:

D Retention, He and H/D irradiation

When irradiated with helium, bubbles are formed with diameters that vary from nanometers to several micrometers at fluences above 10^{24} and temperatures over 1000K. Erosion can occur due to exfoliation of these bubbles as well as dust formation. The presence of such bubbles affects the thermal conductivity, and leads to an increase of surface temperature and further bubble formation. Combined He and D irradiation leads to an increase of D retention in the near surface, and decreased retention in the bulk material. Helium appears to reduce the amount of D that diffuses into the bulk.

Deuterium irradiation of polycrystalline tungsten results in saturation of D retention at room temperature for fluences above 10^{23}. There is also evidence of flux dependence on D retention. At 500K, D retention increases with fluences up to 10^{25}, and blister formation (10-100 micrometers) at fluences above 10^{24}, but there is no evidence of blister formation at temperatures above 700 to

900K. Blisters are also observed at 10^{24} for single crystal tungsten, but these features are smaller (1-3 micrometers) even at low temperature.

The type of structure that exists in plasma-deposited W needs to be determined. Information is also required on T retention, thermal conductivity, blistering etc., and the effect of C and Be on D retention and blister formation. Both long and transient thermal cycling will affect the nature of the damage for all forms of W, and this behaviour requires quantification. There is also the need to identify the effects of neutron damage.

Participants noted the need for barriers to prevent the transport of T into the coolant, but this concern was judged to be beyond the scope of the Technical Meeting.

Possible CRPs:

High priority

Liquid metals in tokamaks

Goal: develop liquid metals as first wall component and divertor target.

Issues include heat flux limits, resilience to off-normal events, pumping efficiency, J*X*B effects, flows and the effects of impurities.

Potential Participants:

R. Majeski
G. Mazzetelli
D. Cowgill
I. Lyublinski
D. Ruzic U Ill.
Fernandez, Portugal (Mazzetelli to provide contact details)
N. Zhang, SWIP (South West Institute of Physics)
Y. Hirooka, NIFS
A. Pisarev
India (Dick to advise)

Synergistic effects of D/T, He and energy transients on the properties of ITER materials

Goals: quantify the synergistic effects on D and T retention, transport, trapping, erosion and dust formation; determine the effects of transients on structural stability, dust formation, alloy formation, melting, ablation and vapor shielding.

Potential Participants:

N. Ohno
R. Doerner
A. Haasz
V. Alimov
A. Pisarev
N. Yoshida, T. Tanabe, Kyushu
J. Roth, IPP
G. Maddaluno, ENEA
D. Cowgill
I. Kupriyanov
P. Coad
DIII (Doerner to advise)
J. Linke, FZ Jülich
Y. Ueda, Osaka
V. Safronov, Triniti
A Gervash, Efremov
China (Tony to advise)

Detritiation techniques
Goals: determine the efficiency of various techniques (photon, laser, discharge, oxidation) and applicability to ITER; quantify the spatial distribution of T co-deposits in tokamaks.

Potential Participants:

- A. Haasz
- R. Causey
- P. Coad (Glenn Counsell)
- C. Skinner
- A. Semerok [alexandre.semerok@cea.fr]
- P. Gasior [gasior@ifpilm.waw.pl]
- T. Tanabe
- L. Rivkis, Bochvar Institute
- D. Whyte, MIT
- Tritium Institute at Sarov (Alexander to advise)
- Alimov to nominate

Lower Priority

Tritium diffusion, permeation and solubility, permeation barriers
Goals: measure diffusion and permeation parameters and develop effective barriers.

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Meeting Agenda

Monday, 4 December **Meeting Room: ACV U1 U6330**

09:30 – 09:45	R.E.H. Clark	Welcoming remarks, Adoption of Agenda

Session 1: Reports on current status

Chairman: P, Coad

09:45 – 10:15	D. Cowgill	"Transient Trapping of Helium by Bubble Formation in Liquid Metals"
10:15 – 10:45	R. Majeski	"Liquid lithium wall research in CDX-U and LTX"
10:45 – 11:15	*Coffee Break*	
11:15 – 11:45	I. Lybulinski	"Lithium Capillary-Pore Systems as New Plasma Facing Material for Fusion"
11:45 – 12:15	G. Mazzitelli	"Experimental results with liquid Li as plasma facing component on FTU"
12:15 – 12:45	R. Doerner	(pending)
12:45 – 14:00	*Lunch*	

Session 2: Reports on current status II

Chairman: I. Lyublinski

14:00 – 14:30	I. Kupriyanov	"Main aspects of Be application as PFC material"
14:30 – 15:00	A.A. Pisarev	"Deuterium thermal desorption from graphites"
15:00 – 15:30	P. Coad	"Current erosion/deposition issues on JET, and plans for the ITER like Wall Experiment"
15:30 – 16:00	*Coffee Break*	
16:00 – 16:30	V. Alimov	"Deuterium retention in plasma-facing materials"
16:30 – 17:00	N. Ohno	"High Flux Helium and Hydrogen Plasma Exposure to Bulky Tungsten and Tungsten-coated Graphite"
17:00 – 17:30	A.A. Haasz	"The effect of impurities on D retention in W and D removal from C-D codeposits"

Tuesday, December 5

Session 3: Summary of current status and needs for new data

Chairman: A.A. Haasz

09:00 – 10:30	Summary of current status		
10:30 – 11:00	*Coffee Break*		

Session 3: Continued

11:00 – 12:00	Discussion of overall need for new data.		
12:00 – 13:30	*Lunch*		

Session 4: Recommendations for possible research projects

Chairman: R. Doerner

13:30 – 15:00	All participants:	Discussion of scope of possible new CRPs to fit these needs. Formulation of statement of goals of new CRPs. Formulation of list of participants for new CRPs.
15:00 – 15:30	*Coffee Break*	

Session 4: Continued

15:30 – 17:00	All participants:	Formulation of conclusions of the TM with specific recommendations for new CRPs.
17:00 –	*Adjournment of Meeting*	

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