INDC(NDS)-0609
Distr. LP,NE,SK

IAEA
International Atomic Energy Agency

INDC International Nuclear Data Committee

Improving the Database for Physical and Chemical Sputtering

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria
12–13 December 2011

Report prepared by

B. J. Braams

February 2013

IAEA Nuclear Data Section, Vienna International Centre, A-1400 Vienna, Austria

Selected INDC documents may be downloaded in electronic form from
http://www-nds.iaea.org/reports-new/indc-reports or sent as an e-mail attachment.
Requests for hardcopy or e-mail transmittal should be directed to *services@iaeand.iaea.org*
or to:
Nuclear Data Section
International Atomic Energy Agency
PO Box 100
Vienna International Centre
A-1400 Vienna
Austria

Printed by the IAEA in Austria

February 2013

INDC(NDS)- 0609
Distr. LP,NE,SK

Improving the Database for Physical and Chemical Sputtering

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

12–13 Deecember 2011

Prepared by

B.J. Braams

Abstract

Seven experts and IAEA staff convened in Vienna to review the existing database for physical and chemical sputtering of fusion wall materials and to make recommendations about priorities for further work. Recommendations were made about database needs for pure and mixed Be, C and W wall material for the processes of physical and chemical sputtering, reflection, penetration and trapping and also for effects of surface and material microstructure. The proceedings and recommendations of the meeting are summarized here.

February 2013

TABLE OF CONTENTS

1. Introduction

The meeting on "Improving the database for physical and chemical sputtering" brought together a group of researchers that have contributed in the past and continue to contribute to the database of sputtering, reflection and erosion properties for plasma-facing materials. The main objective was to assess the quality and coverage of the existing database and identify areas where the database can be improved through new experiments or modelling with relatively modest effort. The attention was focussed on the primary wall material used in fusion energy research: beryllium, carbon and tungsten in pure and in mixed form and possibly impregnated with hydrogen and helium. The processes of most interest are erosion by physical and chemical sputtering, reflection and de-trapping of hydrogen, and deposition and retention of hydrogen (tritium) in the wall material.

Section 2 provides a summary of presentations at the meeting. Section 3 reviews the discussions and conclusions. For near-term work recommendations were made on database needs for pure and mixed Be+C+W wall materials, database extension to molecular processes on surfaces and to diffusion and retention in wall materials. For the longer term recommendations were also made about issues of surface morphology and material microstructure.

2. Presentations

R. A. Forrest and B. Braams: Opening

Dr Forrest, head of the Nuclear Data Section, welcomed participants to the IAEA. He recalled the importance of properties of plasma wall interaction for the development of fusion energy and noted the objective of the Nuclear Data Section and the A+M Data Unit to provide internationally recommended data in support of nuclear energy and nuclear applications. Dr Braams (scientific secretary) extended his welcome and noted the principal tasks for this meeting: to review the existing database of sputtering, reflection and penetration data and to make recommendations about work that can be done in relatively short time to improve the database.

J.W. Davis: The IAEA database for chemical erosion, physical sputtering and radiation-enhanced sublimation: history, current status and future directions

The core of the present database at IAEA on physical and chemical sputtering is collected in volumes 7A and 7B of Atomic and Plasma-material Interaction Data for Fusion (APID). Dr Davis reviewed the work that led to this database and discussed ways to improve it. This presentation served as a guide for the further meeting.

The database in APID Vols 7A and 7B [1-2] developed out of an IAEA Coordinated Research Project (CRP) on "Plasma-Interaction Induced Erosion of Fusion Reactor Materials" that was active 1992-1997 with participants Tony Haasz (Toronto), Egon Vietzke (Jülich), Wolfgang Eckstein (Garching), Yoshi Hirooka (UCSD), Maria Guseva (Moscow), Kenji Morita (Nagoya) and Luo Zheng-Ming (Chengdu). The decision was made to compile data, particularly for the wall materials Be, C and W that were foreseen for ITER. Data on chemical sputtering are assembled in volume 7A and data on physical sputtering and radiation enhanced sublimation in volume 7B. These volumes were intended to provide a comprehensive database for use by the fusion modelling community. Data were extracted from papers and analytical or empirical fits were created for all datasets; in the reports the datasets are displayed along with the fitting equations.

All relevant published data was eligible for inclusion in the database and this poses a problem for the use of APID 7A and 7B: there is too much information. In particular for chemical erosion the database

contains competing results with large variation. It is valuable for a researcher in plasma-material interaction, but not so useful for a non-expert user of the data, and in practice plasma modellers go to specific papers for their data rather than obtain them through the IAEA database. The APID authors had considered to be more selective or to display uncertainty bands on the graphs, but decided against it. In the end the APID 7A and 7B volumes do not provide endorsed or recommended data, and it is hard to see how it could have been done.

For physical sputtering there is generally good agreement between experimental and computational results and not such large variation; in part perhaps because the work was largely done at one lab (IPP Garching; data compilation and calculations by W. Eckstein). The fitting equations are based on the physics and have some predictive capability. These data have been updated subsequent to the appearance of APID 7A and 7B and they are available as IPP lab reports (most recently 2009) and through IAEA.

APID 7A and 7B contain data for radiation-enhanced sublimation (RES) and this data appears to be very comprehensive and not in need of much new attention. There has been little new experimental work, if any, and the process is not considered so relevant in fusion. Dr Davis suggests that work on the database for RES can be focused on simplifying the presentation of the data; just a few graphs will suffice. These graphs may show the temperature dependence of RES for different incident species, the energy dependence, and the flux dependence. Mixed materials are not so important. Data that might be added are those for high temperature erosion of Be and possibly other elements.

Chemical erosion is the area that needs most work and that is most difficult. Different experimental techniques and small differences in experimental conditions may lead to very large differences in results. The fitting equations for chemical sputtering are strictly empirical fits to the data without justification in the physics. There are many complicating factors including surface treatment and the presence of small concentrations of elements other than C. The authors of APID were not selective about which data to include and this needs to be reconsidered, but it is not obvious that one should be more selective.

To summarize the situation with the database in APID 7A and 7B: it represents a large effort, especially by J. Stephens, W. Eckstein and the speaker, and it is a comprehensive data compilation that is useful for PMI researchers, but less useful for the intended audience of plasma modeller. Clearer objectives are needed for any extensions.

Dr Davis turned to discussion of future directions in the database on sputtering and erosion. New plasma experiments have extended the erosion database towards lower energies and higher fluence, which is very relevant for fusion devices and is complementary to accelerator-based measurements. It needs to be considered which aspects of these studies are suitable for inclusion in the IAEA database; e.g., particle retention and material modification.

Molecular dynamics calculations did not play any role in the creation of APID 7A and 7B, but they are becoming available for production calculations. A database of MD calculations must include details of the interaction potential, which is the critical ingredient. Perhaps such a database should be primarily addressed to the MD community and less to the plasma community.

Dynamic BCA modelling (calculating and taking into account modifications to the material) is now routinely possible and it needs to be considered how the results can be included in a database. One looks for general results related to surface roughness, timescales for compositional changes and timescales for geometric changes.

R. Doerner: Sputtering studies using the PISCES-B linear plasma facility

PISCES-B is a linear plasma device for study of plasma-wall interaction with ITER materials including beryllium both as wall material and as plasma impurity. The plasma parameters are similar to those of the ITER near-wall plasma, although not reaching the high density and flux expected in the divertor. The device is inside a sealed enclosure to prevent release of beryllium to the surroundings.

Physical sputtering is measured on PISCES-B by two techniques: weight loss measurements and near-wall spectroscopy. Weight loss measurements are preferred for low density plasma because the low density reduces prompt redeposition, whereas line emission spectroscopy works better in high density plasma. In practice the spectroscopic measurements are calibrated to weight loss measurements. This presentation covers only data based on weight loss.

There are significant variations in the measured Be sputtering yield. For particular conditions the measured yield is near 0.7% on PISCES-B, near 3.5% in BCA (TRIM) calculations by W. Eckstein and near 8% in ion beam sputtering experiments. Primarily this is attributed to effects of surface conditioning (oxidation), but there are multiple other factors that confuse the measurements. The total ion flux is accurately known on the beam experiments, but not so well on the plasma experiments. There may be molecular ions in the species mix. Redeposition needs to be accounted for. Hydrogen is absorbed on the surface and this confuses the weight loss data. The spectroscopic measurements are additionally subject to uncertainties in the atomic data, in the plasma profile data, in data on the angular distribution of sputtered material and in surface geometry effects on the loss fraction.

Chemical sputtering is primarily important for carbon, but also beryllium has chemical sputtering forming BeH and BeH_2. This is being studied at PISCES-B with support from molecular dynamics modelling by C. Björkas et al. For chemical sputtering BCA is not suitable and hopefully the MD simulations will fill the void.

Sputtering of beryllium in helium plasma has been measured on PISCES-B and for particular conditions (bias voltage -50 V) the measured rate is about a factor 10 less than predicted by W. Eckstein's TRIM calculations. Similar low yields for sputtering by helium plasma were measured for W, Al, Mo, Fe and Ti surfaces, but for graphite the measured sputtering rate is within a factor 2 of the TRIM results. There appears to be a flux dependence; at high flux density (as in PISCES) the sputtering rate is less than at low flux density.

In the presentation Dr Doerner provided further illustrations of the effects of surface oxidation, surface morphology, presence of H/D in the near-surface layer, presence of adatoms on the surface and surface temperature. Evidently it will be very difficult to incorporate all the issues related to plasma exposure in a sputtering database using conventional tabular methods. Codes are essential and in the plasma environment BCA is no longer good enough.

P. Krstic: How to define the data and database for PMI in Fusion?

Dr Krstic described some of the complexity of plasma-material interaction (PMI) for fusion and provided a perspective on the needed computational tools and data. As an interfacial problem PMI mixes plasma and materials science. Surface dynamics (changes in composition, structure and shape) is important and because so many parameters are involved these effects are very difficult to include in a database; in addition to basic data one will need a layer of codes to handle the complexity of PMI for fusion applications. The description involves multiple timescales in space (material migration) and time (surface evolution). Relevant processes include reflection, implantation, trapping and detrapping and diffusion in the material; also damage effects including vacancies, dislocations, bubbles and at

some point also transmutations; surface changes due to erosion, redeposition and codeposition and formation of very complicated structures such as tungsten "fuzz".

Molecular dynamics is needed, but it is limited by the quality of the interatomic potential that is used. When chemistry is involved it becomes necessary to employ quantum-classical MD. This can be done at present on massively parallel computers using the self-consistent charge density functional tight binding (SCC-DFTB) method developed at the Bremen Center for Computational Materials Science. Comparison of such calculations with beam surface experiments done at Oak Ridge show remarkable agreement without any fitting parameters.

In conclusion Dr Krstic presented a vision for integrated experimental and theoretical PMI research. On the experimental side this requires a facility to provide the high-dpa relevant irradiated materials for ion-surface scattering experiments and a high-flux linear plasma experiment. On the theoretical side the emphasis must be on massively parallel molecular dynamics and Monte Carlo simulations using quantum-classical potentials. PMI data must be built from the bottom up recognizing its multiscale character and starting at the shortest time and spatial scales.

K. Ohya: Modeling plasma interactions with ITER wall materials

Dr Ohya described uses of atomic, molecular and plasma-material interaction data for ITER modelling with special interest in long distance transport of Be and C through the edge plasma, tritium retention in tungsten, and hydrocarbon surface physics. The PWI codes for Dr Ohya's work include static and dynamic BCA codes (the TRIM/SDTRIMSP family) and molecular dynamics codes.

Typical choices of PWI data are summarized. For physical sputtering the yield is taken from BCA calculations (W. Eckstein's data or related work) and then a Thompson distribution is used for the energy and a cosine distribution for the angle. For chemical sputtering (methane) the Roth formula may be used or it may be input in some other form; the energy distribution is thermal and the angle distribution may be isotropic or cosine. Sticking and reflection of atomic projectiles comes from a TRIM database (BCA calculations) while for molecules it is a special input. For atomic processes in the plasma ADAS is favoured and the Janev/Reiter dataset for hydrocarbons. The molecular dynamics simulations employ empirical bond order potentials from the REBO/AIREBO family parameterized for Be-C-W systems by N. Juslin, C. Björkas, K. Nordlund et al. from Helsinki.

Specific calculations were described involving the interaction of hydrogen and hydrocarbons on carbon and beryllium deposits. The presentation of these calculations serves to illustrate the importance of plasma-material interaction data. One class of calculations is concerned with long distance transport of beryllium and carbon and of tritium codeposition with Be and C in ITER plasma for the case of the Be-C-W wall. A second class of calculations is concerned with tritium retention and desorption in tungsten targets in ITER; these calculations also address interpretation of thermal desorption measurements. A third class of calculations involve molecular dynamics to study the interaction of hydrogen with deposits of beryllium and carbon, with emphasis on the process of chemical sputtering.

K. Nordlund: A critical review of the use of classical interatomic potentials for sputtering calculations

The key part of any MD calculation is to get the forces acting between atoms. For high energy projectiles the Ziegler, Biersack and Littmark (ZBL) potential used for stopping calculations is accurate to about 5%, which is excellent by our standards. The difficulty is all in the low energy range where chemistry occurs. Dr Nordlund provided a review of philosophies for the construction of potentials for various systems. There are special potentials for highly ionic materials, but this is not relevant for fusion. For metallic systems the embedded atom method (EAM) is used as a guide for constructing

EAM-like potentials. For covalently bonded materials it is important to introduce terms that depends on bond angles. In the most widely used potentials for carbon-based materials, going back to Tersoff and Brenner, the bond order is explicitly introduced. The functional form is only one part of the problem; then there is the hard work of fitting the potential to data. Sometimes the fitted interaction potential is optimized for a particular application.

Some issues with low flux and high flux MD calculations were discussed in the presentation. Cumulative simulations are more relevant for fusion than single-impact (independent) simulations; in the cumulative simulations the material composition and structure is adjusted to match the fluence, at least in principle. Sample calculations were described in which different potentials are compared and evaluated.

For fusion applications the most relevant materials are Be, C and W and their mixtures. Potentials for these mixed materials including H (D, T) and He have been developed in Helsinki (Juslin et al., 2005, and Björkas et al., 2010). An important lesson from MD simulations and experiment is that phase separation occurs in mixed materials so that not any $Be_xC_yW_z$ composition is relevant. Most important are Be_2C, Be_2W, $Be_{12}W$, $Be_{22}W$, CW and CW_2. Recognition of this phase separation greatly simplifies the database requirements.

In the third part of his talk Dr Nordlund described the use of rate equations to simulate H and He retention in tungsten. A system of coupled reaction-diffusion equations is used to describe the density of hydrogen atoms, molecules and clusters and of vacancies and interstitials of various sizes: vacancies of size 1-10 and interstitials of size 1-5. The energetics for hydrogen and helium migration in the bulk and on the surface and for release from the surface, and thereby the transport and reaction coefficients for the H and He in the model, are based upon first-principles (DFT) calculations using the VASP code package (work carried out by K. Heinola et al.). The lattice structure of tungsten is relevant; bcc, fcc and A15 structures have been considered. The clustering and annihilation properties of the defects in the continuum model are obtained from molecular dynamics simulations using an MD potential that is based upon DFT calculation and experiments. The initial damage profile for the rate equation model is derived from MD and BCA calculations.

The outcome of the rate equation model, given an initial damage profile and the transport and reaction coefficients and an assumed incoming flux of H and He, is a profile of the concentration of H and He as a function of depth into the surface. Comparison is shown between measured and calculated deposition profiles for bombardment of tungsten by a deuterium beam and these show excellent agreement for a variety of energies of the incoming D.

R. Schneider: SDTRIMSP: sensitivity studies and new developments

SDTRIMSP -- Static and Dynamic TRansport of Ions in Matter for Sequential and Parallel Computers – is the present development of W. Eckstein's TRIM code, which is itself a variant of several codes that all carry the name TRIM (Transport of Ions in Matter) and that are based on the Binary Collision Approximation (BCA). Dr Schneider provided an overview of the code and described new physics capabilities.

The TRIM family of codes has been the workhorse for building up the database of coefficients for physical sputtering by plasma-material interaction. The code simulates a collision cascade. Initially there is a single fast incoming particle, which undergoes deterministic slowing down and uncorrelated random hard collisions. A hard collision may produce a secondary fast particle, hence the cascade. The cross section for elastic collisions is derived from a screened Coulomb potential. Continuous energy loss between collisions is derived from electronic stopping cross sections. Projectiles and knock-on atoms are followed until their energy falls below a threshold; thereby implantation profiles and erosion

rates are calculated. The principal atomic parameters that define a “TRIM” (BCA) calculation are the collision cross sections and surface binding energies.

In the dynamic version of SD-TRIM the target composition and concentration profiles evolve by proper bookkeeping of projectiles and recoils. The surface binding energy evolves as a mean value depending on composition. In general the BCA approach is quite satisfactory for high energy effects (deposition profile, physical sputtering) but it breaks down below about 10 eV as many-body and quantum mechanical effects become important.

Dr Schneider showed some sensitivity studies for SDTRIMSP calculations, varying the interaction potential between several models, varying the surface binding energy and varying numerical parameters such as the integration method and the threshold energy at which a trajectory is terminated. Within the reasonable variations the effect of changing the surface binding energy is the most pronounced. Very stable results that also agree well with experiment are obtained for sputtering and deposition calculations for high-energy (~10 keV or more) impact of Ar and Xe on Si. Further validation studies were shown in which a 2D version of the dynamic TRIM code is used to simulate etching and calculated and measured surface profiles are compared. The 2D version of SDTRIMSP was also used to simulate the development of the tungsten surface structure under bombardment by carbon at high (6 keV) energy.

The BCA approach was developed for simulation of fast particle cascades and in its original version it is not suitable for problems involving chemistry. The SDTRIMSP code now includes extensions to surface chemistry based primarily on work by Mech et al.. This and several other models for hydrocarbon surface chemistry are compared by Rai et al. [A. Rai, A. Mutzke and R. Schneider, Nucl. Instrum. Methods B, Vol. 268 (2010), 2639]. Calculations based on the Mech model for CH_4 release from hydrogen bombardment of graphite show very good agreement. In conclusion, the original TRIM code has been extended to treat time-dependent problems and surface chemistry. For many applications more complicated tools are needed (MD, Kinetic Monte Carlo, continuum models), but due to its speed the BCA approach in SDTRIMSP remains a very valuable tool for simulation of plasma-wall interaction.

B. Braams: PMI database activities at IAEA

Dr Braams provided an overview of the activities of the Atomic and Molecular Data Unit. These include the coordination of an international data centre network (DCN) and a code centre network (CCN), maintenance of databases (ALADDIN and AMBDAS), development of a new wiki-style knowledge base, a database search engine (GENIE), development of interface standards (XSAMS), and several coordinated research projects (CRP). These activities are all reflected on the unit home web page at http://www-amdis.iaea.org. As a supplement to the presentation of J.W. Davis he then supplied some more information about PMI data in ALADDIN.

At present the IAEA ALADDIN database for PMI processes contains data for the processes of reflection, physical and chemical sputtering, radiation enhanced sublimation (RES) and penetration. There are almost 4000 datasets in the database: 530 are classified as experimental, 2601 are classified as theoretical and 806 are classified as derived.

The projectile can be hydrogen (H, D, T), He, Li, Be, B, C, N, O, Ne and heavier possible impurities up to W, Hg and Bi, and molecules H_2, D_2, H_3^+, D_3^+, H_2O, OH and O_2. Many surface materials are found in the database, but the principal ones are Li, Be, B, various forms of C (graphite, CFC, amorphous C and diamond) and W.

For many combinations of projectile and surface there are data for reflection, physical sputtering and penetration. Data for chemical sputtering are provided for projectiles H, D, O, H_2, D_2, H_3^+, D_3^+ and O_2, primarily on the carbon-based materials (also on Si and two odd ones: B_4C and TiC). Data for RES are provided for projectiles H, D, He, C, O, Ar, H_3^+ and D_3^+, again primarily on the carbon-based materials.

The experimental data concerns only reflection, physical sputtering and RES; not chemical sputtering and penetration. The theoretical data concerns only reflection, physical sputtering and penetration; not chemical sputtering and RES. The derived data concerns reflection, physical sputtering and chemical sputtering. Viewed from the other side: Reflection and physical sputtering data in the database is experimental, theoretical or derived, chemical sputtering data is all derived, RES data is all experimental and penetration data is all theoretical.

A. Ito: Binary collision approximation and molecular dynamics hybrid simulation

Dr Ito began with a description of molecular dynamics (MD) simulations of chemical sputtering. There are two important processes subsumed under the name chemical sputtering: a long time process of thermal desorption and a short time process of chemical detachment. For the case of an amorphized graphite target bombarded by H the thermal desorption process produces CH_4, which is built up in the solid via $CH \rightarrow CH_2 \rightarrow CH_3 \rightarrow CH_4$. The chemical detachment process produces a variety of molecules including CH, C_2H and C_2H_2.

The studies of chemical erosion illustrate problems with MD simulations: the need to use a small time step for high energy collisions (because of the steep nature of the interaction potential at close approach) and the long calculation time in general. For high energy processes use of the binary collision approximation (BCA) is effective. The remainder of the talk is concerned with the challenge to combine the good features of BCA for high energy processes and MD for low energy. New codes AC∀T and AC∀T-MD are developed for this purpose.

AC∀T (Atomic Collisions for Any Target) is described by A. Takayama, S. Saito et al. (2011) and succeeds the ACAT (Atomic Collisions for Amorphous Target) classical BCA code by Y. Yamamura and Y. Mizino (1985). In AC∀T arbitrary structure particle positions can be treated and all particle positions are remembered for simulation of continuous injection.

The code AC∀T-MD is the most recent and ongoing development. In AC∀T-MD the BCA approach is employed for high energy trajectories and the simulation switches to a strictly local MD when the particle is sufficiently slowed down. An intermediate stage is being developed to handle the process of channelling: in this intermediate stage noteworthy particles are followed by MD, but moving in a potential energy surface generated by surrounding fixed particles.

3. Discussion and Conclusions

Database needs for single element materials

Better theoretical data, based on molecular dynamics, are needed for processes on Be and C at low energy, where chemistry is important and where the BCA calculations do not work very well. The most important processes for which these low energy data are needed are reflection and chemical sputtering, but data for penetration and trapping at low energy are also needed.

For hydrogen atoms or ions colliding with any surface MD calculations are needed to provide rates for the production of H_2. Information about production of vibrationally and rovibrationally excited H_2 is completely absent from the database.

There is new data from J. W. Davis on hydrogen retention in tungsten. However, these data show several orders of magnitude variability presumably associated with tungsten microstructure (see below); it does not look suitable for inclusion in ALADDIN at this time. There are recent calculations by C. Becquart (ENS de Chimie, Lille) of plasma material interaction with tungsten surfaces and we should see if these are suitable for inclusion in ALADDIN.

Database needs for mixed materials

The mixed materials of primary interest are Be:C:W impregnated with hydrogen and helium. The present ALADDIN database has very poor coverage of processes on mixed materials and (considering at first only the processes covered by the present database) data are needed for reflection, physical and chemical sputtering and penetration. Radiation-enhanced sublimation is less of interest; it primarily affects graphite and in present machines the surface temperature is generally not high enough to make it an important process. As the database is extended to retention and diffusion the same mixed materials are again of interest.

It is an important observation from molecular dynamics simulations (K. Nordlund) and experiment that in a generic $Be_xC_yW_z$ target phase separation tends to occur, and in fact one obtains primarily any of a small number of discrete phases. Specifically the most likely mixed phases with those components are WC, W_2C, Be_2C, Be_2W, $Be_{12}W$ and $Be_{24}W$; therefore priority must be given to those stable phases (impregnated with H and He) rather than to a general amorphous three-component mixture.

Besides Be:C:W mixtures also doped graphite is a common mixed material; however, it is considered to be a lower priority for database work. The reason for assigning it lower priority is that one hardly knows the composition of doped graphite in a tokamak environment, it varies with erosion and redeposition and one would first need to understand the evolution of the doped material.

With regard to the dependence of PMI data on the concentration of H and He in the surface it should be reviewed what is the role of the flux versus fluence. There is no mystery in the observation that an effective reflection coefficient for H impinging on any surface depends on the concentration of absorbed H. It is somewhat mysterious that the effective reflection coefficient should depend on the intensity of the bombardment. It needs to be studied in more detail what is the nature of this possible dependence on flux.

It is noted that BCA calculations can be done very quickly at this time and therefore with regard to mixed materials priority should be given to the database for high-energy impact data for reflection, sputtering and penetration; these are processes for which BCA is most suitable.

Task: Encourage use of BCA calculations to extend the current physical sputtering database to include mixed materials and compounds, focussing primarily on the stable phases of Be:C:W impregnated with H.

New experimental data on plasma-material interaction for mixed materials Be:W and Be:C is available from PISCES; we need to identify it and include it in ALADDIN if it is found suitable. This includes data for Be/C mixing, Be/W mixing, codeposition D/Be ratio and similar quantities. Some general parametric expressions are also provided. Results are available in publications from PISCES and need to be collected. We should also pay attention to experimental data from Pilot PSI and (in the future) Magnum PSI at FOM that could be suitable for ALADDIN.

Some papers are available on mixed material preferential sputtering; we need to look into this material and see what is suitable for a database.

Database extension to molecular processes on surfaces

There are a few datasets for molecular processes in ALADDIN, but in the discussions this was agreed to be the area that is most ready for improvements and additions. Molecule as projectile is the critical case for codeposition. Molecule as product is important for divertor plasma modelling.

At this time ALADDIN has no data at all for collisions of hydrocarbon molecules on surfaces, which is the critical case for codeposition. Molecular processes cannot be treated by the BCA tools that have been used for ALADDIN to date and in experiments it is not possible to resolve the outgoing molecular state (and perhaps not the incoming state either). Therefore the principal tool for upgrading the database of molecular processes on surfaces has to be molecular dynamics.

Whenever possible the data for molecular processes should be resolved with respect to the vibrational state of the molecule. This is especially important for H_2 (and isotopic variants) as the dominant molecular constituent of divertor plasma. In the case of more complicated molecules probably the more appropriate parameter is internal energy and perhaps also total angular momentum; these are classical quantities in the context of MD simulations.

The most important molecular processes (molecule in or molecule out) are associated with CH, CH_2, CH_3, CH_4 for the case of C and a-C:H surface; and H and H_2 for any surface involving a Be:C:H mixture impregnated with H.

Task: Locate existing molecular dynamics data not yet in ALADDIN on reflection, sticking and erosion involving molecular projectiles or molecular products. Possible authors: J. Marian (LLNL) and K. Nordlund; there will be others.

Database extension to diffusion and retention in materials

At present ALADDIN contains data on penetration, so on the deposition profile, but nothing on diffusion or retention in the material. This data would be highly sensitive to material microstructure and even to multiscale microstructure (grain boundaries and voids) in the case of graphite. The structure needs somehow to be parameterized and there is not a ready-made method for such parameterization.

Microstructure is important for transport and retention in any material, but the dependence is most extreme in the case of tungsten. In pure crystalline tungsten retention is very low, and in actual tokamak tungsten essentially all hydrogen is trapped in microvoids. There is variation of many orders of magnitude in data from experiments on hydrogen retention in tungsten.

The description of microstructure is difficult even if the only imperfection is microvoids; one needs then, in principle, the density of microvoids as a function of their size. In order to introduce microstructure as an independent parameter in a database one has to characterize it using only 1 or 2 parameters. Adding in temperature as another independent parameter the diffusivities and other properties are then already functions of 2-3 variables in the database.

It was remarked that the deposition profile is not too controversial. For energetic particles this is in general very well calculated by the BCA codes.

Taking for granted the microstructure and the deposition profile there remains the problem of calculating the diffusion and retention. In many cases molecular dynamics is the appropriate tool for this, but quantum effects are important for hydrogen diffusion at low temperature, especially in tungsten. Keeping that in mind, nevertheless the primary need is for MD calculations to provide diffusion coefficients and desorption rate coefficients as input for retention calculations.

Database extension to surface morphology and microstructure

In connection with the desired addition of data on diffusion and retention in actual materials it is also of interest to obtain data on actual occurring microstructure. It was remarked in the discussions that it is difficult to get experimental information over a wide range of scales; one misses either the small voids or the large voids. In the spirit of our focus on the surface and plasma surface interaction we should probably care most of all for structure on the smallest scale rather than on coarser granularity and larger voids.

The notion of an experimental database on surface morphology and microstructure reminds us of the intended database on dust particle properties that is being developed at IPP Garching as part of the CRP on "Characterization of Size, Composition and Origins of Dust in Fusion Devices". Like the dust database an experimental database on surface microstructure could be based on many images and analyses of surfaces that have been exposed to plasma, including samples taken from a tokamak after an extended campaign. On the experimental side we should check especially what has been done in this area on Tore Supra.

Dynamic BCA (SDTrimSP) and molecular dynamics can both contribute to a theoretical database of surface morphology and microstructure. SDTrimSP has been used quite extensively already to study erosion and surface morphology change due to PMI. R. Schneider can extend these calculations to mixed materials. Beyond BCA it is important, but it requires much more time, to employ molecular dynamics to study the evolution of microstructure (dislocations, microvoids) and amorphization.

Is there any useful fluence scaling for macroscopic surface morphology changes?

Discussion about data evaluation and recommendation

There is a well justified preference for validated and recommended data. We agreed that data evaluations and provision of recommended data are very important; we also agreed that it is a very difficult task. Experimental data vary widely for all processes at low energy; chemical sputtering and hydrogen trapping and migration being the most difficult. For the case of chemical sputtering results depend strongly on surface composition of the target as affected by oxidation and carbidization. Hydrogen trapping and migration depends very much on material microstructure (porosity). A precise characterization of these properties is usually not available for experimental data and without that information it is not really possible to recommend one dataset over another.

The A+M Data Unit is putting increased emphasis on data evaluation and establishment of a standard recommended library for atomic and molecular data. It was agreed that for the case of plasma-material interaction data for the present the emphasis should remain on the collection of data and on careful documentation and not on efforts to recommend unique best data.

Discussion about codes, code coupling and code comparison

In a database one provides quantities such as particle and energy reflection coefficients as a function of a limited number of parameters including the incoming particle energy. If the quantities in the database should depend on more than one or two continuous parameters to characterize the material then it becomes infeasible. One then has to forget about providing a database and instead one needs to couple a suitable coarse model for PMI to the plasma calculation.

A suitable model that can very well be coupled to a plasma code may describe hydrogen trapping and reflection through a one-dimensional model (in terms of depth into the surface) using simple transport coefficients and reaction rate coefficients. Models of this nature are used with ERO, EIRENE, DEGAS2 and other such codes to describe hydrogen in the plasma-facing materials. We should identify

such models and see what kind of parameters are used for their specification. Note in this connection the work by C. Björkas at FZJ in connection with ERO and molecular dynamics.

The calculations that underlie the present ALADDIN database on PMI are almost all based on the binary collision approximation (BCA) as implemented in the SDTrimSP (Static and Dynamic BCA, Serial and Parallel) code and earlier variants of that code. Certainly molecular dynamics (MD) is much more accessible now than it was 15 years ago and the meeting discussed the future roles of BCA and MD approaches.

It was agreed that BCA continues to be valuable for processes at high impact energy. It provides good data for deposition profiles and for material damage. Dynamic BCA is also is a suitable tool for surface evolution studies, which requires long calculations.

Molecular dynamics is essential for processes at low energy, including all chemical processes. We discussed the value of a database of MD methods, procedures and technical parameters used in PMI modelling. Issues to be noted there include temperature control and surface preparation strategy. These data are largely for internal use by MD community and they may be most suitable for the Wiki pages; it does not look like an appropriate task for the A+M Data Unit.

We discussed the interest in a code comparison project. Such comparisons have been carried out for the major codes used in fusion plasma modelling, for example comparing SOLPS and UEDGE or more specifically the neutral gas components EIRENE and DEGAS2. Code comparison efforts of that nature are best organized by the code authors and users. Alternatively a code comparison exercise could be done for some precisely specified model problems that can be treated in different ways (MD, BCA, maybe other approaches). Such an exercise would involve a larger set of codes and would involve also people from outside the fusion plasma modelling community.

Plans for future meetings

The A+M Unit will organize jointly with NFRI a meeting on data evaluation for A+M+PMI processes, to be held at NFRI in September 2012. It is expected that at that meeting A+M data will be emphasized, and the question was raised if there should be a more focussed meeting on data evaluation for PMI processes. The consensus was that it would not be a suitable topic for a large (by our standards, 20+ participants) technical meeting. We should consider primarily consultancies and small consultants meetings on a more narrowly focussed topic. An example could be to evaluate experimental data on chemical sputtering of graphite or on hydrogen retention in tungsten. In each case it has to be carefully considered if a consultants meeting can resolve differences due to varying experimental conditions.

Conclusions

The primary intended audience of our PMI databases are fusion plasma modellers who require inputs for simulation of near-wall plasma. Low-energy ions dominate the plasma-surface contact and the most important data needs are for processes of low energy ions, including chemical sputtering and molecular reflection, the latter resolved with respect to vibrational excitation of the outgoing molecule. For the case of mixed Be:C:W material the database effort must be concentrated on the few stable phases of the binary compounds: WC, W_2C, Be_2C, Be_2W, $Be_{12}W$ and $Be_{24}W$. Dynamic BCA calculations and experiments are needed to obtain sputtering and deposition profile data for these compounds for the case of continuous bombardment at relatively high energy. For the case of pure tungsten the most critical need is for study of hydrogen trapping as it depends on tungsten microstructure, but this requires development of approaches for parameterizing microstructure.

Appendix 1

List of Participants

J.W. Davis, University of Toronto, Institute for Aerospace Studies, 4925 Dufferin St., Toronto, Ontario, CANADA M3H 5T6

K. Nordlund, University of Helsinki, Institute of Physics, P.O. Box 43 (Pietari Kalmink. 2), 00014 Helsinki, FINLAND

R. Schneider, Universitätsrechenzentrum, Ernst Moritz Arndt Universität, Felix-Hausdorff-Straße 12, D-17487 Greifswald, GERMANY

A. Ito, National Institute for Fusion Science (NIFS), Department of Helical Plasma Research, 322-6 Oroshi-cho, Toki-shi 509-5292, JAPAN

K. Ohya, University of Tokushima, Institute of Technology and Science, 2-1 Minamijyosanijima-cho, Tokushima 770-8506, JAPAN

R. Doerner, University of California, San Diego, UCSD Fusion Program, Experimental Research Division, 9500 Gilman Dr., La Jolla CA 92093-0417, USA

P. Krstic, Oak Ridge National Laboratory, Physics Division, One Bethel Valley Road, Oak Ridge, TN 37831-6372, USA

IAEA:

B.J. Braams, IAEA Division of Physical and Chemical Sciences, Nuclear Data Section, P.O. Box 100, Vienna International Centre, A-1400 Vienna, AUSTRIA

H.-K. Chung, IAEA Division of Physical and Chemical Sciences, Nuclear Data Section, P.O. Box 100, Vienna International Centre, A-1400 Vienna, AUSTRIA

R.A. Forrest, IAEA Division of Physical and Chemical Sciences, Nuclear Data Section, P.O. Box 100, Vienna International Centre, A-1400 Vienna, AUSTRIA

Appendix 2

Agenda

Monday 12 December **Meeting Room: B0485**

09:30 – 09:45 *R.A. Forrest, B.J. Braams: Welcome*

Session I ***Chair: R. Schneider***

09:45 – 11:00 *J.W. Davis*: The IAEA database for chemical erosion, physical sputtering and radiation-enhanced sublimation: history, current status and future directions

11:00 – 11:15 *Break*

11:15 – 12:00 *R. Doerner*: Erosion in a wall-controlled plasma environment

12:00 – 12:45 *P. Krstic:* How to define the data and database for PMI in Fusion?

12:45 – 14:00 *Lunch*

Session II ***Chair: R. Doerner***

14:00 – 14:45 *K. Ohya*: Modeling plasma interactions with ITER wall materials

14:45 – 15:30 *K. Nordlund*: A critical review of the use of classical interatomic potentials for sputtering calculations

15:30 – 15:45 *Break*

15:45 – 16:30 *R. Schneider*: SDTRIMSP: sensitivity studies and new developments

19:30 – *Social dinner (outside VIC)*

Tuesday 13 December **Meeting Room: B0485**

Session III ***Chair: K. Nordlund***

09:00 – 09:45 *B. Braams*: PMI database activities at IAEA

09:45 – 10:15 *A. Ito*: binary collision approximation and molecular dynamics hybrid simulation

10:15 – 10:30 *Break*

10:30 – 12:30 *All*: Review of data needs, data capabilities

12:30 – 14:00 *Lunch*

Session IV ***Chair: J.W. Davis***

14:00 – 17:30 *All*: Recommendations and report

Nuclear Data Section
International Atomic Energy Agency
P.O. Box 100
A-1400 Vienna
Austria

e-mail: services@iaeand.iaea.org
fax: (43-1) 26007
telephone: (43-1) 2600-21710
Web: http://www-nds.iaea.org