INDC International Nuclear Data Committee

Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials

Summary Report of the First Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

26–28 September 2012

Prepared by

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Abstract

Nine experts in the field of plasma-wall interaction on beryllium surfaces together with IAEA staff met at IAEA Headquarters 26-28 September 2012 for the First Research Coordination Meeting of an IAEA Coordinated Research Project on data for erosion and tritium retention in beryllium plasma-facing materials. They described their on-going research, reviewed the main data needs and made plans for coordinated research during the remaining years of the project. The proceedings of the meeting are summarized in this report.

April 2013

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1. Introduction

There is very active interest at present in the properties of beryllium as a wall material exposed to plasma in fusion devices. The intended plasma-facing materials in ITER are beryllium and tungsten: beryllium for most of the vacuum vessel and tungsten for the regions of highest heat load. Since August 2011 the Joint European Torus (JET) experiment operates with an "ITER-Like" Be-W vacuum vessel wall. Beryllium has in its favour good heat conductivity, strong gettering capability, high tolerance as a plasma impurity and low nuclear activation. On the other hand beryllium is more subject to melting and erosion than other wall materials and tritium retention in beryllium is also a concern.

Because of its toxicity beryllium has generally been avoided in fusion research to-date and the database on its plasma-interaction properties is rather sparse. In present-day fusion experiments the regions most exposed to plasma are often covered with graphite or carbon-fibre composites, but because of its propensity to absorb tritium carbon is not considered suitable for use in a reactor. In ITER the radioactive environment demands remote handling anyway and the toxicity is not a particular concern. The JET experiment is also fully equipped for remote handling.

The Atomic and Molecular Data Unit of the IAEA Nuclear Data Section supports research into nuclear fusion through the provision of internationally recommended atomic, molecular, plasma-material interaction and materials properties databases. Following advice from the Subcommittee on Atomic and Molecular Data of the International Fusion Research Council (IFRC) the Unit initiated an IAEA Coordinated Research Project (CRP) on "Data for erosion and tritium retention in beryllium plasma-facing materials" to enhance the knowledge base on fundamental particle-material interaction processes involving beryllium in the fusion plasma environment. A consultancy meeting was held in May 2011 to review the status of the database on erosion and tritium retention in beryllium surfaces and the report of that meeting is available [INDC(NDS) report 0592, July 2011].

The key processes to be studied in the CRP are physical and chemical sputtering of the surface by H, He and Be, which release beryllium impurities into the plasma, trapping and reflection of hydrogen (H, D, T) in beryllium surfaces, the transport of hydrogen in beryllium and means to extract trapped tritium. It must be taken into account that the material and surface properties are highly variable as a result of interaction with impurities (most importantly C, N, O, Ne and Ar), implantation of H and He, redeposition of eroded Be and resolidification of melt layers. The CRP will emphasize data for the relevant mixed materials, especially Be-(H,D,T,He), Be-C, Be-N, Be-O and ternary and higher mixtures, and data for the principal plasma impurities as projectiles. The most important projectiles are therefore H, D, T, He, Be, C, N, O, Ne and Ar. The CRP brings together experimentalists and computational theorists that are engaged in studies of plasma-material interaction with beryllium and related mixed materials and of hydrogen migration in solid beryllium.

The first research coordination meeting of the new CRP was held 26–28 September 2012 at IAEA in Vienna and the present report is the output of that meeting. At the time of the meeting there are 6 groups officially represented in the CRP. They are the plasma-wall interaction group at IPP Garching (the Be-related activities of Ch. Linsmeier's group are now located at IEK-4, FZ Jülich), the PISCES team at UCSD, modellers at IEK-4 Jülich, the molecular dynamics group of K. Nordlund at University of Helsinki, the Quantum Chemistry group of S. Irle at Nagoya University and the Institute of Ion Physics and Applied Physics at the University of Innsbruck. ITER and JET are not officially a part of the CRP but they were also represented at the meeting, and in addition we had a contribution from the Nu-Fuse project at the University of Edinburgh. The presentations are summarized in Section 2 and the discussion and conclusions are summarized in Section 3. The list of participants is in Appendix A and the meeting agenda is given in Appendix B.

2. Presentations

M. Venkatesh, R. A. Forrest, B. J. Braams: Opening

The meeting was opened by Dr R. A. Forrest, head of the Nuclear Data Section, on behalf of Dr M. Venkatesh, Director of the Division of Physical and Chemical Sciences, who had a scheduling conflict

and visited later to say welcome. Both recalled the intense interest in properties of beryllium in fusion devices due to the recent re-start of JET with a beryllium main wall and the prospect of operation of ITER likewise with beryllium. Dr B. J. Braams, scientific officer for this CRP, noted that the general objective of CRPs in the Nuclear Data Section is to develop, evaluate and recommend best data for a particular class of processes that are important for some field of nuclear applications. The principal desired output of the present CRP is a data library that will be used in plasma modelling to support the operation of JET and the preparations for ITER.

The participants then introduced themselves and the meeting agenda was adopted.

Ch. Linsmeier: Fundamental aspects of beryllium compound formation and erosion and hydrogen retention in beryllium

Dr Linsmeier gave a wide-ranging presentation on processes involving beryllium walls with special emphasis on surface reactions and relevant chemistry and based on work done in the plasma edge and wall division at IPP Garching with theory support from Aix-Marseille University (A. Allouche). The objective of the research is to develop data for a comprehensive description of physical and chemical processes in the near-surface layer due to interaction with the plasma and ultimately to include these surface reactions in a global integrated model for plasma-wall interaction.

The reference design for ITER still has carbon in the wall for the non-nuclear phase. A list of relevant compounds for the wall chemistry therefore includes Be, W, C, Be_2C, W_2C, WC, Be_2W, $Be_{12}W$, BeO and WO_3 plus adsorbed oxygen. (Consideration of oxygen is essential for making sense of laboratory experiments and for the influence of plasma impurities due to oxidized surfaces, unavoidable air or water leaks in large-scale fusion devices.) Properties vary with temperature, they vary between original and redeposited surfaces and they may vary due to surface layers.

At IPP Garching surface material properties are studied using primarily X-ray photoelectron spectroscopy (XPS) and accelerator-based techniques. By means of XPS sputter depth and (using a synchrotron light source) chemical depth profiles can be studied; also XPS is sensitive to the chemical binding state of the material. Accelerator-based techniques are primarily used for hydrogen isotope profile analysis.

Dr Linsmeier provided an overview of a chemical modelling approach to the description of plasma-wall interaction with beryllium, including a list of species to be considered and a list of the principal reactions. He then described studies of individual reactions.

Studies were described of the Be-C compound, focussing on thermally induced reactions in the surface. The principal mixed phase is Be_2C and this is formed at an interface already with deposition of Be on C at room temperature. At higher temperature annealing takes place beyond the interface. The formation and destruction depends on temperature; for Be on pyrolytic graphite the formation of Be_2C by annealing starts at 720 K and the loss of Be_2C starts at 1170 K; for Be on HOPG formation of Be_2C by annealing starts at 870 K and the loss of Be_2C starts at 1270 K.

Formation of Be-W alloys was studied using ion beam analysis; the alloy formation starts at 1070 K. For the case of deposition of Be on W the final phase is $Be_{12}W$ and this is stable up to its melting temperature close to 2000 K. The beryllium penetrates into W by diffusion and the interaction is diffusion-limited. At lower beryllium concentration the stable phase is Be_2W.

Processes induced by energetic ions were studied for C^+ on Be and CO^+ on Be. Penetration depth is studied using Rutherford backscattering spectrometry (RBS) for a 5 keV beam of C^+. Also the relation between fluence and deposition is measured; it appears to be slightly sub-linear. The mixed material evolves through various stages as a function of fluence; first a sub-surface Be_2C mixture is formed and at higher fluence a surface layer of pure C. The CO^+ beam creates a ternary system and besides Be, C and CO-containing compounds, and Be_2C also a stable phase of BeO is formed. The composition profile depends on fluence. At high fluence there is a transition from an interaction dominated by deposition to one that is dominated by erosion.

With a view towards N_2 seeding to produce a radiating mantle N implantation in Be is studied using beam implantation (e.g. N_2^+ at 3 keV) and analysing the depth profile by XPS and RBS. The most

important stable phase is Be_3N_2, which has a melting point around 2500 K. The results look favourable for nitrogen seeding: no chemical erosion is observed and there is no increased hydrogen retention.

Oxygen implantation in Be_2W and also in pure W was studied using an O^+ beam (energy 0.5 keV or 1 keV). The deposition profile is analysed using XPS. BeO, WO_2 and WO_3 are formed, but BeO is the most stable compound. Some of the complexities of the XPS analysis of this ternary compound were described.

Dr Linsmeier described in more detail the comprehensive modelling of surface evolution in a chemical network. A complete description requires consideration of diffusion, chemical reactions and collision-induced reactions associated with energetic particles. For use as an ingredient in plasma modelling a simpler description is wanted and this is found in a "reaction front" description using rate equations. Some examples of this and related models and of their benchmarking were shown.

The final part of the presentation was concerned with hydrogen isotope retention. A system of coupled reaction diffusion equations is developed for single crystal beryllium and then adapted for polycrystalline beryllium using a model for transport associated with grain boundaries. The model describes the reactions of transport of hydrogen coupled to monovacancies and self-interstitials. Anisotropy of the crystal is important and is taken into account. Parameters for these calculations are derived in part from measurements and in part from DFT calculations at Marseille.

S. Lisgo: Beryllium erosion and tritium retention in ITER

Dr Lisgo provided an overview of the ITER project and device and described the modeling that is carried out at ITER on the effects of plasma interaction with the beryllium wall. The main wall of the ITER vacuum vessel will have beryllium tiles facing the plasma, mounted on stainless steel. Tungsten and CFC are used in the divertor, but in the nuclear phase carbon is not permitted and it is now being considered to eliminate the CFC also from the non-nuclear phase. Tungsten has an extremely low solubility for tritium and the main concern for tritium retention is beryllium. There is ongoing effort to predict the level of tritium retention in beryllium. For modelling primarily the 2-dimensional LIM and DIVIMP codes are used; these provide predictions for local erosion and redeposition and thereby for wall lifetime and beryllium migration. The WALLDYN code is used to simulate material evolution. Experimental benchmarking on JET (ITER-Like Wall) and also on EAST (using He proxy) is important. The JET ILW experiments are modelled using the same tools as are used for ITER.

The numerical data sets used for ITER modelling were noted. Sputter yields for D on Be and for Be on Be are obtained from W. Eckstein's calculations [report IPP 9/132 (2002)], sometimes multiplied by 2 to account in an approximate way for surface roughness. Beryllium molecular effects (chemical sputtering) is not included yet, but MD calculations are underway to refine the sputter yields. It is noted that experimental data from PISCES (as reported at this meeting by R. Doerner) suggests a much higher sputter rate for redeposited material than for the original surface.

The present calculations use a local 2D geometry and they will need to be superseded by fully 3D, time-dependent simulations that include the wall shape. More accurate specification of the boundary plasma conditions is also needed. At present there are still large uncertainties in the estimates of both the wall lifetime and the tritium inventory requiring further model refinements, improved rate data and experimental benchmarking.

R. Doerner: Plasma interactions with beryllium surfaces at PISCES

Dr Doerner described the research being carried out on the PISCES-B divertor plasma simulator at UCSD. This work is done in collaboration with MIT and ORNL in the Plasma-Surface Interaction Science Center. PISCES-B is contained in a safety enclosure to prevent release of beryllium dust. A beryllium oven in the device allows the introduction of a controlled amount of Be impurity ions into the plasma. There is an in-situ surface analysis station so that samples can be analysed before exposure to atmosphere. The studies on PISCES-B are focussed on tritium retention, ways to remove trapped tritium, beryllium erosion, migration and redeposition.

Ion beam studies and plasma exposure studies for D on Be show that retention saturates at approximately 1e21 D/m^2. Retention does not saturate for the case of Be codeposits and in codeposits the D/Be level depends on the deposition (redeposition) conditions. The tritium accumulation in ITER will be dominated by codeposition of T with eroded Be and options are needed to control the inventory. Possibilities are to use transient thermal loads (rapid heating of the surface during controlled plasma termination) or bulk bake-out of the plasma-facing components. Laser flash heating experiments were done using thermal desorption spectroscopy (TDS) to measure the amount of D removed during the flash. These experiments were discouraging as very little D is released; much less than would be expected from a diffusion model.

Release of D was studied further in experiments using a magnetron sputter coater to produce uniform and reproducible Be co-deposit samples. The coater is operated in 80% Ar and 20% D$_2$ gas. Codeposit layers of 1 μm thickness were created at different surface temperatures. The TMAP7 code (developed at INEEL) was used to model the deuterium diffusion and release; this code uses data on solubility and diffusivity of D and D$_2$ in Be, W and BeO. There is good agreement between the TMAP results and the TDS measurements for the samples produced in the coater. The TMAP7 calculations also confirm the low release rates observed during the short time scale, flash heating of codeposits created in PISCES-B.

Sputter yields vary greatly between PISCES-B, code calculations and other experiments and the sputter yields on PISCES-B are at the lower end of the range of variation. The low sputter yield on PISCES-B is attributed to surface morphology and to the implanted D. During exposure on PISCES-B the surface develops a fine hair-like structure on a μm scale and the sputter yield is observed to go down with increased fluence. The effect of implanted D has been studied in molecular dynamics (MD) simulations by C. Björkas et al. and they show a reduction in Be sputtering by a factor 2-4. However, the MD computations are sensitive to the precise interatomic potential and to models for surface binding energy and there is not a unique result.

The sputtering behaviour was also studied by using beryllium seeding and finding the level of seeding at which erosion is balanced by redeposition according to mass loss measurements. These experiments showed a much higher erosion rate of plasma-deposited beryllium than was expected. Possible explanations are that the actual beryllium sticking fraction on redeposited layers is lower than thought or that the erosion rate of redeposited layers is higher than that of the original surface.

In the end the beryllium experiments on PISCES-B raise many questions that this CRP should seek to resolve. Complications due to impurities in the Be surface; retention due to implantation vs. codeposition; quantifying the amount of D/T atoms in the surface during plasma exposure and the impact on erosion; need for MD potentials for a gas saturated surface; quantifying surface morphology change on erosion; different erosion and sticking fractions for Be deposits vs. original Be surface.

As an appendix to his presentation Dr Doerner showed some experimental results from Sandia Laboratories on the atomic-scale structure of adsorbed hydrogen in beryllium, following a presentation by R. D. Kolasinski at the hydrogen workshop in Schloss Ringberg, 2012 (satellite of PSI). Low energy ion scattering (LEIS) and direct recoil spectroscopy (DRS) are used to examine how hydrogen binds to the Be(0001) surface; it is found that hydrogen atoms reside symmetrically between 3 Be atoms and this is consistent with predictions of DFT calculations by Stumpf and Feibelman and more recently by A. Allouche.

J. P. Coad: Experience with beryllium at JET

Dr Coad provided an overview of beryllium evaporation, beryllium limiter and beryllium divertor experiments on JET since 1989 and leading to the present ITER-Like Wall (ILW) campaign. JET was designed for tritium operation and it is fully equipped for remote handling making it the only operating tokamak on which experiments with beryllium can be safely carried out. Beryllium evaporation was done during almost every week of operation 1989–2009 and JET has beryllium limiters 1990–1992 and beryllium in the divertor during 1995. Since the re-start of operation in 2011 JET has a beryllium main wall and tungsten divertor, as is intended for ITER in the nuclear phase. On JET this is called the ITER-Like Wall (ILW). Throughout the years there have been studies of the erosion and migration of

beryllium throughout the vacuum vessel. It may be recalled that JET started as a limiter machine, but erosion (C) and melting (Be) limited the power handling and since 1994 JET is a divertor machine. The Mk-I divertor in 1994–1995 had carbon tiles in 1994 and switched to castellated beryllium blocks in 1995. In the subsequent Mk-IIA and Mk-IIGB divertors there were no beryllium tiles, but beryllium evaporation and transport experiments continued.

The data obtained from JET in the period 1989–2009 and again since 2011 shows the erosion and material migration over the course of a campaign. Erosion is measured using special marker tiles that have a Ni or Mo interlayer. With the ILW campaign hydrogen (deuterium) retention is of high interest and it appears that long term retention has decreased by almost a factor 10 since the previous campaign where carbon-based materials were used. Future studies during the ILW phase will continue to address erosion, redeposition and material transport and H, D, T and He retention in co-deposits. Other topics for study: damage and tritium retention in bulk Be and W, alloying between deposited Be and W tiles, carbidisation of the W-coated CFC tiles, phase transformations and other material property changes in the tungsten tiles, and melt damage.

D. Borodin: Development of models for plasma interactions with Be on the basis of dedicated experiments

Dr Borodin described work carried out at Forschungszentrum Jülich on plasma interaction with beryllium. The ERO code is the main simulation tool and it has been applied to experiments on PISCES-B and on JET. ERO simulates plasma-wall interaction and the 3D local transport of material through the plasma. It simulates the content evolution of the plasma-exposed surfaces, being able to take into account certain material mixing and chemistry effects. For this purpose ERO uses pre-calculated data from the SDTrim.SP ("TriDyn") and MolDyn codes; a directly coupled ERO-SDTrim.SP version is also available. In application to ITER ERO is used to provide estimates for tritium retention, divertor targets and main wall erosion and the penetration of impurities into the plasma. ERO may use plasma parameters from a B2-Eirene or Edge2D calculations as well as empirical data (e.g. for PISCES-B). Calculations were shown for predicted erosion of the beryllium wall (determining blanket modules lifetime) in ITER due to sputtering by D and self-sputtering.

The important and most time-consuming part of ERO simulations is model and data improvent by simulation of various experiments at existing devices, which can be used for benchmarking. Dr Borodin described examples of ERO application to JET ITER-like wall (ILW) and PISCES-B and discussed some of the uncertainties in the basic data for ERO calculations. For physical sputtering there is a factor of about 4 between the "ERO-Max" sputtering rates for D on pure Be (based on MD and SDTrim.SP calculations) and the "ERO-Min" sputtering rates based on SDTrim.SP for the case of a 50% Be and 50% D target. The empirical data from various experiments scatter even stronger. Dependence on angle of incidence creates further uncertainty, which complicated the interpretation of most experiments. Sometimes it is useful to separate various effects, e.g. additional erosion experiments were carried out on PISCES-B using pure He plasma so that chemical sputtering does not occur. Be spectroscopy target weight loss and deposition at "witness plates" provide then a extensive benchmark material for ERO erosion simulation for PISCES-B. For these studies it is necessary to track also metastable state population in Be atoms (affecting ratios of triplet and singlet lines). A database is being built up and tested to describe correctly chemical sputtering of BeD. MD calculations by C.Björkas are used and (in consultation with R. Janev) data are acquired for processes of BeD in plasma, vibrationally resolved. These simulations are carried out for PISCES-B and scheduled for the JET ITER-like Wall, where BeD light is also observed. Another example of ERO application was the simulation of JET ILW solid Be limiter erosion (observed spectroscopically) during a plasma parameter scan. This experiment is obviously very relevant for the ITER wall in the context of the 3D geometry, plasma configuration etc.

Beyond the ERO modelling Dr Borodin described new and planned experiments at Jülich relevant to beryllium. Jülich has the PSI-2 linear plasma device and is planning to build JULE-PSI, a linear experiment in a hot cell similar to what is done for PISCES-B at UCSD. JULE-PSI is intended for all wall materials including beryllium and is also meant to handle low quantities of tritium. In the meantime a proxy is used for Be studies. ITPA has recommended Al as a proxy for Be but Dr Borodin

recommends to consider Mg as a possible alternative because Mg has similar oxygen getter properties as Be, a similar (hexagonal) lattice structure, and mostly because atomic structure (Be 2s2, Mg 3s2) is very similar. From the spectroscopic point of view Al is quite different from Be, moreover the availability of necessary atomic data for Mg is better (ADAS). Laser techniques (desorption, ablation and breakdown spectroscopy: LIDS, LIAS and LIBS) are used to study the surface composition of wall material; these systems were used on TEXTOR and are now being developed for PSI-2, JULE-PSI and ITER. Still, until JULE-PSI goes online a Be proxy has to be used.

K. Nordlund: Molecular dynamics simulations of plasma interaction with beryllium-based fusion reactor materials

Dr Nordlund started his presentation with an overview of the materials science of plasma-wall interactions and of possible simulation approaches. Already for the case of impact by a single ion there is a wide range of important effects that may be produced: sputtering and cratering, production of vacancies, interstitials, dislocation loops and 3D extended defects, implantation of the impurity or adsorption on the surface, and amorphization of crystal structure. For prolonged irradiation also surface roughening or ripple formation and the formation of bubbles, blisters and voids inside the material are important. An extreme case of surface change is the formation of surface "fuzz" as happens under He bombardment of a W surface. These processes are simulated by DFT ab initio calculations at the shortest time and space scale, also by binary collision approximation (BCA) codes, molecular dynamics, kinetic Monte Carlo (KMC), discrete dislocation dynamics, "rate equations" and (at the longest time and spatial scale) constitutive equations. The work in the group at Helsinki revolves around classical molecular dynamics but including DFT to construct potentials, BCA calculations for high energy processes and KMC as a follow-up to MD simulations.

The key part of any MD simulation is to obtain the forces between atoms and this requires numerical fitting of interatomic potentials. For mixed systems the work at Helsinki most often employs Tersoff-like (a.k.a. Brenner-like or bond-order) potentials. The construction and optimization of these potentials is hard work. For C-H-O systems the potentials go back to Brenner's original work. Much work was done for the full Be-C-W-H system at Helsinki as reported for BeCWH in [Björkas et al., J. Phys.: Condens. Matter 21 (2009) 445002] and for BeW in [Björkas et al., J. Phys.: Condens. Matter 22 (2010) 352206]; also work by Guang-Hong Lu (Beijing) and by Ahlgren (Helsinki) is noted. These potentials are designed with the aim to describe correctly all crucial phases of the material and Dr Nordlund showed tests of the potentials on the phase diagram for pure Be, BeC, Be_2C and BeW and also tests on the behaviour of the potentials for small molecules.

Calculations have been carried out for sputtering of (initially pure) beryllium by D and of self-sputtering of Be. These calculations are compared with experimental data from PISCES-B at UCSD. Chemical sputtering, producing BeD molecules is shown to be an important contributor. When calculations are started with a random mixture of Be-C then phase separation is seen, forming Be, C and Be_2C; therefore the detailed simulations should concentrate on these preferred phases. When W is also present then the important phases are Be, C, W, Be_2C, Be_2W, $Be_{12}W$, $Be_{24}W$, WC and W_2C. Proper ternary phases are not seen. At the present time the MD calculations are extremely useful for obtaining qualitative understanding, but getting quantitative agreement and predictive capacity remains challenging due to uncertainties in the potentials.

S. Irle: Towards accurate approximate density functional theory potentials for beryllium-plasma interactions

Dr Irle presented work towards density functional tight binding (DFTB) molecular dynamics simulations of plasma interaction with beryllium-based surfaces. DFTB is classified as a semi-empirical density functional theory (DFT) method. The DFTB equations have the structure of DFT equations but using a simplified Hamiltonian. The standard Hamiltonian of electronic structure theory is expressed in terms of one- through four-centre integrals and in the traditional DFTB approach only one- and two-centre terms are kept. The number of basis functions is also reduced to the minimum and various other approximations are made. Within that framework the coefficients that define the Hamiltonian (the one- and two-centre integrals in the traditional orbital-based view) are fitted to the

results of proper DFT (or other ab initio) periodic and/or molecular model calculations. This fitting has to be done for each pair of elements. In any subsequent calculation the Hamiltonian and overlap matrices are quickly obtained by interpolation based on pre-computed values. The resulting matrices are often very sparse, permitting calculations on large systems. The energy gradient (force) that is needed in MD simulations can be calculated analytically. Dr Irle showed examples of DFTB/MD calculations on problems involving carbon in the form of graphene, nanotubes and fullerenes.

The critical first issue for simulations of plasma interaction with beryllium surfaces is to fit the DFTB parameters for the relevant element pairs. This has been done for H-C-N-O and selected other systems, but the work is just starting for beryllium-based materials. The highest priority is parameterization for Be-Be and Be-H, followed by Be-C, Be-O and Be-W for fusion applications. The specific DFTB formalism in the present work is the self-consistent charge (SCC) DFTB following [Elstner et al., Phys. Rev. B 58, 7260 (1998)]. Several kinds of reference data are employed for the parameterization. Data for crystal band structure are obtained by plane-wave DFT calculations using the Vienna Atomic Structure Package, VASP, and the Projector Augmented Wave (PAW) method and data for small molecular clusters are obtained by DFT calculations using the B3LYP functional and the cc-pVTZ basis. The fitting is done using a particle swarm optimization (PSO) technique. Calculations for many different one- and two-element crystals have shown that the parameters optimized for one crystal structure generally transfer well to other structures.

Dr Irle showed examples of band structures calculated using DFT and fitted using SCC-DFTB for beryllium: the pure Be HCP lattice and also lattices for BeO, BeC and WBe. Also comparisons were shown between binding energies for the Be-H system in various beryllium hydride molecules and molecular chains calculated using B3LYP and fitted by SCC-DFTB. These are initial results; the parameterization of the Be-X systems for SCC-DFTB is ongoing work. Beyond the parameterization the objective is to employ DFTB/MD for chemical sputtering simulations to be compared with classical potential simulations and to carry out energy calculations and structure optimization for amorphous Be-based systems.

M. Probst: Quantum chemical and molecular dynamics simulations of plasma interaction with pure and hydrogenated beryllium surfaces

Dr Probst described work relevant to beryllium surfaces carried out in the computational chemistry group in the Institute of Ion Physics and Applied Physics at Innsbruck. The group has projects in quantum chemistry, molecular dynamics simulation of materials and data analysis and visualization. Fusion relevant MD simulations have been carried out for graphite surfaces; these studies include a comparison of projectiles H, He and Be and also investigation of the difference between atomic and molecular (e.g. BeH, BeH_2) projectiles. The energy barriers for penetration through graphene were evaluated for various projectiles and in the case of molecules assuming either adiabatic (minimum energy), in-plane or ultrafast penetration.

Electron-impact ionization cross section (EICS) calculations were carried out for various beryllium hydrides using the Deutsch-Märk (DM) and the Binary-Encounter-Bethe (BEB) formalisms; this work is done with R. K. Janev (Jülich), K. Becker (NYU) and others and was recently published [Eur. Phys. J. D 67: 2 (2013)]. The results were compared with calculations using the CCC and RMPS methods.

Electronic structure calculations for beryllium hydride clusters are carried out to support development of interaction potentials; this is done in collaboration with Profs Jan Urban and Pavel Mach at Comenius University and others. Molecular dynamics simulations are carried out by Prof Ivan Sukuba of Comenius University on sputtering of beryllium by deuterium. The analytical bond-order potential of Björkas and Nordlund (2009) is used. These calculations are cumulative over time, so the beryllium is eroding and hydrogen is deposited.

D. Hepburn: Materials science in the Nu-FuSE project: nuclear fusion simulations at exascale

Dr Hepburn described work by the group of Prof Graeme Ackland at Edinburgh on high-performance computing for the study of fusion reactor materials. This work is part of the Nu-FUSE project, Nuclear Fusion Simulations at Exascale, supported by G8. The present studies are primarily concerned with the

behaviour of austenitic Fe-Cr-Ni steel alloys in a fusion environment. An essential part is the microstructural evolution of these materials under irradiation. Ab initio calculations are done using the VASP code, which is based on DFT and a plane wave basis. These calculations provide formation energies for vacancies and interstitials, binding energies for clusters of vacancies and interstitials and barriers to migration. Impurities He, C and N are considered.

One study described in some detail in the talk concerned austenite (pure gamma phase Fe) and dilute Fe-Cr-Ni austenitic alloy [Phys. Rev. B 85, 174111 (2012)]. Vacancy formation energies, vacancy cluster binding energies and Fe self-interstitial energies in austenite were calculated for different geometries of the defect; also calculations were done for solubility, binding and clustering of dilute Ni and Cr in austenite and for the interaction between Ni and Cr and point defects. Vacancy-mediated tracer diffusion coefficients for Fe, Ni and Cr were obtained. The calculations lead to a detailed kinetic transport model for defects and impurities in the material. Further work is concerned with impurities He, C and N in austenite and Ni and with transition metal solute in austenite. In these studies too the calculations are aimed at binding energies, interaction energies and barriers to migration for the various solutes and defects. The present studies are for alloys in the dilute limit, but it is intended to follow up with study of concentrated alloys.

H.-K. Chung: Databases and knowledge base for plasma-matter interaction for fusion

Dr Chung reviewed the databases and related projects maintained by the atomic and molecular data unit. The numerical database ALADDIN and the bibliographical database AMBDAS each cover atomic, molecular and plasma-material interaction data for fusion. GENIE is a search engine to access multiple databases outside the IAEA through a common query interface. Recently the unit started a wiki-based Knowledge Base for data and other information that is not so well captured in the more structured ALADDIN and AMBDAS. The broad aim of a CRP such as the present one on beryllium is to extend these databases, especially with numerical data that are recognized to be authoritative. Data sets of interest will include sputtering yields, reflection coefficients, penetration profiles and transport properties and at a more fundamental level also interaction potential energy surfaces, surface binding energies, and other data to support modelling. Data can be in the form of tables (traditional ALADDIN), but also less structured numerical data, images, and perhaps movies. A challenge for this CRP is to agree, if it is possible, on standard data to support kinetic Monte Carlo models of plasma-material interaction with beryllium.

3. Discussion and Conclusions

General remarks

The two critical issues for beryllium as plasma facing material and for this CRP are erosion and tritium retention. There is considerable uncertainty in rates for both processes, and within the CRP we assign about equal priority to the two issues.

Erosion issues

Measurements of erosion rates vary by a factor between 5 and 10 for similar projectile energies between exposure of a target by plasma in PISCES and exposure of a beryllium target to an accelerator beam. The plasma temperature in PISCES is below ~ 10 eV but the ions are accelerated by a bias voltage of 100 eV - 200 eV. Therefore the particle bombardment in PISCES is similar to that by a beam, but the intensity of exposure is much higher in PISCES than in accelerator experiments.

The differences in measured (inferred) sputtering yields are attributed mainly to three factors, but this is only qualitative. The three factors are (1) presence of absorbed hydrogen (H/D/T) or other gas in the beryllium target; (2) differences in surface morphology; and (3) possible presence of an oxide surface layer. In some experiments (high exposure, eroding regime) there will not be an oxide layer.

For study of erosion probably the most important issue is to understand the influence of hydrogen concentration in the target. There are two sides to this. (1a) How does the sputtering yield depend on hydrogen concentration near the surface? (1b) How does the hydrogen concentration depend on

exposure conditions? It is understood that under high exposure the target is over-saturated with hydrogen; this is known from hydrogen inventory balance in experiments. However, direct measurements of hydrogen concentration in the target during plasma exposure are not available. These measurements might be supplied by the experiment of N. Ohno at Nagoya: a linear plasma device equipped with an MeV ion beam for depth profile measurements in the material. However, the Nagoya experiment cannot handle beryllium, so a surrogate or surrogates must be used.

Erosion rates are found to be different between eroding target material and redeposited layers. It is plausible that this difference is largely due to different hydrogen concentrations in the two systems; this is not known experimentally.

The issue (2) of differences in surface morphology has likewise 2 sides. (2a) How does sputtering yield depend on surface morphology? (2b) How does surface morphology depend on plasma exposure? For surface roughness on the scale larger than about 10-100 nm there is a straightforward aspect to (2a): a sputtered or reflected particle may strike the surface again after straight-line motion. From the point of view of macroscopic modelling this makes sputtering and reflection into possibly a compound process, but it is straightforward and one does not need a new database for it. Surface roughness on a scale of 10 nm or less would need explicit treatment in the sputtering and reflection data, but we don't know if this kind of roughness is at all a concern. Does a beryllium surface acquire a nanoscale fuzz-like structure?

Specific data needs for erosion

We need data for sputtering (and reflection, penetration, self-sputtering, etc.) for targets impregnated with a variable concentration of H/D/T. The most important targets are pure beryllium and the stable binary phases Be_2C, Be_2W, $Be_{12}W$, BeO and Be_3N_2. As always the data must be in a form suitable for particle simulation; so function of energy and angle for incoming and outgoing particles, and resolving the state of the outgoing atom or molecule (BeH and BeH_2). We expect that these data will be obtained by all available computational means: DFTB-MD, regular MD, and BCA simulations.

We need computational studies of hydrogen concentration as a function of exposure conditions, for the same targets as above. These computational studies are explicitly time-dependent, so much more difficult than the study of sputtering and other processes as a function of surface condition. The appropriate tools are probably time-dependent BCA (SD.TRIM.SP), classical MD, and MD or BCA coupled to rate equations. This is not routine work; the suitable approaches need to be developed and compared. We note that these studies overlap to some extent with studies of hydrogen (tritium) migration in beryllium. (They overlap very much if rate equations are used.)

We need new experimental studies of hydrogen concentration in the surface layer as a function of exposure conditions. Relevant experiments can perhaps be done by N. Ohno at Nagoya (linear device and MeV ion beam for real-time profile analysis) but the beryllium must then be replaced by a substitute material, probably aluminium.

We need a better understanding of the development of surface morphology due to plasma exposure. This is a topic for experimental and modelling studies. Data are available from PISCES and will become available from JET. Possible modelling includes time-dependent BCA and also MD.

Tritium retention issues and data needs

Tritium retention can only be understood in connection with an understanding of the nature of vacancies and other defects. Ab initio (DFT) and/or MD calculations can be used to provide data for rate equations, which are the basis for long-time transport calculations. The rate equations are basically a system of reaction diffusion equations.)

The possibility was discussed to create a database, to be hosted at IAEA, of relevant rate equation model coefficients for Be-based material. It is agreed that this will be valuable and a start can be made with data from Ch. Linsmeier for low density of H/D/T in material. One needs to agree on a common language to describe defects. Different researchers will probably agree on what is a vacancy or an interstitial, but it will need more work to agree on a common description of dislocations.

In connection with the work at Nagoya and Helsinki on DFTB simulations it is of interest to create a database of DFTB parameters for beryllium and the related mixed materials including H/D/T and He. For this kind of database there is an agreed SKL format that has been developed at Bremen.

Workplan

Ch. Linsmeier: Note: on 2013-03-01 Dr Linsmeier took up a new position as co-Director of the Institute for Energy and Climate Research, which includes fusion energy research, at the Jülich Research Centre. Specific experimental equipment relevant for the work on beryllium and Be-related compounds is transferred from IPP to FZ Jülich and the respective activities will be continued at FZ Jülich. There will be a delay in the experimental activities, however, due to the transfer of the experimental devices.

1. Study of formation and erosion of mixed Be-based materials. Calculations based on data from A. Allouche for Be-X-H will be compared with experiments. Erosion yields of beryllium by nitrogen impact will be measured. Depth resolved XPS measurements will focus on ternary systems. It is planned to use DFT-based calculations (A. Allouche) to substitute for surface binding energy in TRIM calculations.

2. Hydrogen retention and release. Experiments will be done using mixed bombardment (deuterium and some other ion) in order to separate the D retention and release issues from the defect production mechanism. Also D retention and release mechanisms will be studied for Be-based layers (thin layers; diffusion barrier). The D can be implanted within or beyond the layer. Interpret this by CRDS.

3. Study the interactions of nitrogen with Be-W alloys together with O and C impurities. DFT calculations have been carried out by A. Allouche, but the results require experimental verification. Quartz microbalance experiments on erosion of Be and Be compounds by N ions are planned in a collaboration with TU Wien.

4. Extend existing models (WallDyn) by integrating the determined parameters for various wall processes. Apply these models in simulations of JET and ITER.

S. Lisgo: Generally the role of the small physics team at ITER is to support work by others, either directly or through ITPA. For example, the physics team will generate and provide standard plasma conditions for ITER modelling and, in connection with the ITER-Like Wall campaign, also standard plasma conditions for JET modelling. These include a detailed geometry specification.

R. A. Doerner: The PISCES team plans to continue their intensive study of beryllium surfaces exposed to plasma. More studies will be done of the development of surface morphology by plasma exposure. Studies will be done with aluminium surfaces in order to test if and when Al is a good surrogate for Be; this is joint work with IEK-4 at Jülich. The comparison between Al and Be will consider erosion and retention broadly. Also in connection with work at Jülich PISCES will continue to provide experimental data for benchmarking by ERO. The behaviour of tungsten surfaces exposed to Be-containing plasma will be studied jointly with Ch. Linsmeier (IPP Garching). Tungsten surfaces will be exposed on PISCES to be analysed at Garching using their ion beam analysis facilities.

Cavity probes will be used in an effort to distinguish between reflection and re-erosion. These studies will be compared with similar work that is done on JET in order to understand better the difference in behaviour between original beryllium tiles and redeposited beryllium layers.

J. P. Coad: The VTT Research Centre in Finland will contribute primarily to the post-mortem analysis of beryllium tiles exposed in JET. They will characterize changes in the beryllium surface structure after plasma exposure. TDS experiments will be used to study deuterium and impurity profiles in exposed beryllium tiles and in beryllium redeposits on tungsten. The group at VTT also plans to study the global migration of beryllium and general balance of erosion and redeposition; these studies involve the WALLDYN code.

D. Borodin: The modelling work at Jülich will involve ERO benchmarking of surface and atomic and molecular data using data from JET, PISCES-B and new Jülich devices that operate with a beryllium substitute. Further simulations for various ITER wall components are scheduled extrapolating the

obtained knowledge for ITER and predict wall erosion rates, determining the life time, and tritium retention. A model will be developed for pre-calculation and accounting of the impinging energy and angle distribution of plasma and impurity species striking the surface in the context of 3D wall geometry and plasma configuration. In a separate effort involving also the spectroscopy team at Jülich data will be developed for the interpretation of spectroscopic signals as measurements of erosion. The new linear devices and various laser techniques will be further developed and employed for the experiments with Be proxy.

K. Nordlund: There are many further molecular dynamics studies to be carried out for plasma interaction with beryllium. One project is to simulate beryllium-tungsten alloy formation at temperatures and energies matching experiments by Ch. Linsmeier. Effects of uncertainties in the MD potentials need to be explored further and calculations for sputtering of beryllium by D impact will be carried out using DFTB parameters developed by S. Irle. In order to understand better the effect of deuterium surface concentration and the variation of sputtering rates with flux density the effect of energy mix in the D impacting on Be (high energy ions plus low-energy neutrals) will be studied. Also the sputtering yield will be analysed as function of surface D concentration.

S. Irle: The first priority is to continue to develop and test the SCC-DFTB parameterization for the case of partially or fully amorphous Be-X systems (X = H/D/T, He, Be, C, N, O, W). Sample geometries will be generated using classical MD simulations and then DFT single-point calculations of energies and band structure will provide data for optimizing and validating the DFTB parameters. This work will be done in collaboration with H. A. Witek (National Chiao Tung University, Taiwan), and M. Elstner (Karlsruhe Institute of Technology, Germany).

Beyond the parameterization it is planned to employ DFTB/MD for chemical sputtering simulations to be compared with classical potential simulations as done by K. Nordlund's group and to carry out energy calculations and structure optimization for amorphous Be-based systems including H/D/T. The specific studies will be oriented towards the general objective to study and understand tritium retention in Be-based surfaces.

M. Probst: Quantum-chemical (DFT) structure calculations are planned to clarify the differences in surface structure and sputtering between a beryllium surface and an aluminium surrogate. Also similarities and differences between action of O and N on beryllium will be studied by DFT structure calculations. In a separate effort involving electronic structure calculations data for gas phase BeH, BeH_2 and isotopic variants will be obtained and the production of hydrides on the wall will be investigated.

D. Hepburn: It should be noted that the Nu-Fuse project at Edinburgh is not presently devoted to beryllium; they are a guest at this meeting. However, there are clear opportunities for future work within Nu-Fuse. In particular the Edinburg group can do large scale DFT calculations (following upon work by A. Allouche at Marseille) to clarify vacancy and hydrogen migration in beryllium and develop models for kinetic Monte Carlo calculations.

Conclusions

At the end of the first research coordination meeting it is clear that there is much work to be done to improve the understanding of erosion and tritium retention in beryllium and its relevant compounds. On the experimental side the PISCES device carries a heavy load as really the only device for laboratory studies of fusion relevant plasma exposure of beryllium. Of course, JET provides highly relevant data as well, but the data from JET tend to be integrated over a campaign of exposure and so the experimental conditions are not nearly as clean on JET as they are on PISCES. There will not be another experimental facility in the next few years that will work with beryllium and so the experimental work can only be broadened by relying on Al surrogate (and/or perhaps Mg); but then the differences between beryllium and the surrogate need themselves to be better understood. The start of operation of the linear plasma device JULE-PSI at FZ Jülich, which will be located in a controlled area for PWI studies of neutron-irradiated (and therefore activated) materials is planned for end of 2015. In this linear plasma device and the associated experimental equipment (e.g. laser and thermal desorption facilities), also beryllium-based materials will be investigated.

On the computational side there needs to be further integration between all approaches, from large-scale ab initio calculations through DFT and MD studies to BCA calculations and kinetic Monte Carlo, and at each stage using the more accurate calculations to calibrate DFTB parameters, MD interaction potentials, surface binding energies or KMC transport coefficients. These parameters and coefficients serve to connect the work of different groups. They should be carefully specified and it would be valuable to organize them into a database to the extent that it is possible.

List of Participants

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Agenda

Wednesday 26 September   **Meeting Room: F0814**

09:30 – 09:50   **Meera Venkatesh, Bas Braams:** Welcome, introductions, adoption of the agenda

Session I   *Chair: Paul Coad*

09:50 – 10:40   **Christian Linsmeier:** Fundamental aspects of beryllium compound formation and erosion and hydrogen retention in beryllium

10:40 – 11:00   *Coffee*

11:00 – 11:50   **Steve Lisgo:** Beryllium erosion and tritium retention in ITER

11:50 – 12:40   **Russ Doerner:** Beryllium measurements at PISCES

12:40 – 14:00   *Lunch*

Session II   *Chair: Stephan Irle*

14:00 – 14:50   **Paul Coad:** Experience with beryllium at JET

14:50 – 15:40   **Dmitry Borodin:** Development of models for plasma interactions with Be on the basis of dedicated experiments

15:40 – 16:00   *Coffee*

16:00 – 16:50   **Kai Nordlund:** Molecular dynamics simulations of plasma interaction with beryllium-based fusion reactor materials

16:50 – 17:30   **All:** Discussion; review of experiments and their modelling

19:00 –   *Social dinner (outside VIC)*

Thursday 27 September   **Meeting Room: F0814**

Session III   *Chair: Christian Linsmeier*

09:00 – 09:50   **Stephan Irle:** Towards accurate approximate density functional theory potentials for beryllium-plasma interactions

09:50 – 10:40   **Michael Probst:** Quantum chemical and molecular dynamics simulations of plasma interaction with pure and hydrogenated beryllium surfaces

10:40 – 11:10   *Coffee*

11:10 – 11:40	**Derek Hepburn:** Materials science in the Nu-FuSe project: nuclear fusion simulations at exascale
11:40 – 12:30	Discussion
12:30 – 14:00	*Lunch*

Session IV	***Chair: Kai Nordlund***
14:00 – 14:30	**Hyun Chung:** Plasma-material interaction data in ALADDIN
14:30 – 17:00	**All:** Organization of a database for PMI with beryllium surfaces

Friday 28 September   **Meeting Room: F0814**

09:00 – 12:00	**All:** Work Plan
12:00 – 13:30	*Lunch*
13:30 – 15:30	**All:** Report
15:30 –	*Close of Meeting*