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

Summary Report of the Third Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

15-17 June 2016

Report prepared by

Hyun-Kyung Chung and Bastiaan J. Braams
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May 2017

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Abstract

The Third Research Coordination Meeting of the CRP on Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials was held on 15–17 June 2016 at IAEA in Vienna with seven external participants from 4 countries (Germany, Finland, Austria and USA) and ITER Organization. Beryllium is planned to be used as the main wall material away from the regions of highest heat load on ITER and since 2011 it is used on the JET experiment and other tokamak experiments. For any plasma-facing material there are two key classes of plasma-material interaction processes: erosion, which limits the lifetime and which brings impurities into the plasma, and hydrogen (tritium) retention, which removes tritium from the reactor. The work on data of plasma and beryllium surface interactions during the period of CRP was presented and a plan for the final report of the CRP as a comprehensive paper was outlined in the three-day meeting.

May 2017

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1. Introduction

There has been a very active interest at present in the properties of beryllium as a wall material exposed to plasma in a fusion reactor environment. The planned plasma-facing materials for nuclear operation in ITER are beryllium and tungsten: beryllium for most of the vacuum vessel and tungsten for the regions of highest heat load. A "ITER-Like" Be-W vacuum vessel wall has been installed on the Joint European Torus (JET) experiment and plasma experiments on that machine resumed in August 2011.

The IAEA Coordinated Research Project (CRP) on “Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials” was initiated in 2011 in order to enhance the knowledge base on fundamental particle-material interaction processes involving beryllium in the fusion plasma environment. The scope of the beryllium CRP is data for interaction of plasma or of a particle beam with beryllium or beryllium compounds. The main processes of interest are physical and chemical sputtering by H, He and Be, trapping and reflection of hydrogen (H, D, T) on beryllium surfaces, the transport of hydrogen in beryllium and means to extract trapped tritium. The target material can be pure beryllium or it can be Be-(H, D, T, He), Be-C, Be-N, Be-O and ternary and higher mixtures. In addition to H, D, T, He and Be the most important projectiles are the common impurities C, N, O, Ne and Ar.

The first Research Coordination Meeting (RCM) was held in September 2012 and the second RCM in 18-19 August 2014. The third RCM was held on 15–17 June 2016 at IAEA headquarter in Vienna where seven experts participated from 4 countries of Germany, Finland, Austria, USA and ITER Organization: Kai Nordlund of University of Helsinki, Helsinki, Finland, Martin Köppen from Forschungszentrum Jülich, Germany, Dmitry Borodin, Forschungszentrum Jülich, Germany, Th. Schwartz-Selinger, Max-Planck Institut für Plasmaphysik, Garching bei München, Germany, Russel Doerner, University of California, La Jolla CA, USA, Michael Probst, Universität Innsbruck, Austria and Gregory De Temmerman, ITER Organization.

The Project Officer B. Braams opened the meeting by welcoming participants and giving an introduction on the meeting. Participants presented their work during the period of CRP with emphasis on recent work since the 2nd RCM. Plans for databases and the final report, a topical review paper on data on plasma and beryllium surface interactions were discussed.

Section 2 contains research summaries by participants. Section 3 summarizes a plan for database and Section 4 describes the future work plans for the final report. The list of participants is in Appendix 1 and the Agenda is provided in Appendix 2.

The presentation materials for this and other meetings of the Beryllium CRP may be found through the web page https://www-amdis.iaea.org/CRP/Beryllium/.

2. Summary Reports

Russel Doerner: Summary of PISCES Be research

An extensive over view of all the Be PMI measurements made during this CRP was presented. The presentation was divided up into four sections. The four topics were; erosion of Be in a high flux plasma environment, fuel retention in Be, D release behaviour from Be and Be/W mixed material PMI.

The erosion section documented the differences between measured physical sputtering yields and binary collision approximation calculations (i.e. TRIMSP). Various aspects were described to try to identify the source of the discrepancy. For example, measurements ruling out the possibility of the surface oxide surviving during the plasma exposure were shown. The factor of 5-10 reductions of the measurements are ultimately believed to originate from both the surface morphology that develops on the surface (resulting in a factor of 2-3 reduction) and the presence of a large amount of fuel atoms residing within the stopping range of the incoming ion flux during the high flux plasma bombardment. Chemically assisted physical sputtering of BeD molecules was also presented along with molecular dynamics predictions of the effect. The experimental data agrees well with the calculations, as well as with data that was subsequently obtained for the JET-ILW. Finally, the temperature dependent loss rate from plasma exposed surfaces was described and a model for adatom creation and sublimation from the surface was shown. While the model is only a possible theory that can describe the effect, it has not been proven to be responsible.

The second topic of fuel retention in Be exposed to energetic particle bombardment was the discussed. Fuel retention due to ion bombardment of a Be surface is known to saturate with fluence. The impact of He addition to the deuterium plasma has a small effect of reducing retention during low temperature exposure, but the effect disappears as the temperature of the exposure is raised to about 500 K. Accumulation is expected to be dominated by codeposition of D (or T) with Be. Scaling of the amount of retained D in Be codeposits was presented. The scaling describes the impact of ion energy, deposition rate and temperature on the D/Be ration measured in the codeposits.

The third topic was the release of retained D from Be surfaces. This section focused on release from Be codeposits and the validation of the TMAP7 code for describing the release. The code has been validated by varying the layer thickness, heating rate and heating duration. The ultimate goal is to determine a baking efficiency for the proposed ITER bake strategy as a means of tritium removal.

The final topic discussed was Be/W mixed materials. Measurements of erosion from, and retention in, pre-created Be/W samples with varying W fraction were described. Be is seen to be preferentially sputtered from the mixed surface, resulting in a W-enriched surface. At high Be fractions in the samples retention behaved like that expected from pure Be samples, whereas in high W fraction sample the retention resembles that of pure W. There is a smooth transition between the two extremes as the sample content varies between the two. Thin surface layers of Be_2W are observed to form when a Be-containing plasma interacts with W targets. This mixed Be/W layer is not observed to dramatically change the retention properties of the bulk W sample, but may inhibit release of the retained D during baking. Finally, transient heating events of Be coated W samples was discussed. Mixed Be/W surfaces are detected at laser energy densities sufficient to remove the Be layer and melt the W substrate underneath. The figure of merit for determining the laser energy density required for removal of the Be coating is the Be layer formation energy density which is defined to be the Be enthalpy of formation multiplied by the film density and thickness and divided by the molar mass.

Martin Köppen: Experimental Possibilities in Jülich

Three years ago in 2013 the Institute of Energy and Climate Research (IEK) – Plasma Physics introduced a new focus of its research: material research for fusion. To match the requirements for this field of research new experiments are acquired. This presentation focuses on

the current status of the experiments in 2016 and the achievements since 2014 in the beryllium related research.

Aim of the research is to understand the plasma-wall-interactions in ITER. Most of the armour material of the first wall in ITER is with approximately 700 m² beryllium. Second first wall material is tungsten. In combination with the foreseen seeding gases N_2 and Ne and the plasma contamination oxygen mixed materials will be formed. The solid state reactions at the first wall are fostered by the elevated temperatures at and by ion bombardment of the first wall.

To understand the evolution of the first wall dedicated studies on the chemistry at it are necessary. The new XPS-setup is well suited for these studies. In the last two years the system was delivered, assembled, commissioned and improved. Heart of the system is a high-resolution x-ray photoelectron spectroscope (XPS). The system is equipped with two ion guns, three evaporators and a sample heater to mimic the conditions at a first wall. The low base pressure of 1×10^{-10} hPa allows studies on atomically clean Be surfaces.

In a first, preliminary experiment the isotope exchange of H- and D-ions in a Be surface is investigated. D_2^+ and H_2^+ are implanted consecutively with a fluence of 55 $Å^{-2}$. Afterwards a TDS is recorded. In the second step of this experiment the implantation sequence is reversed, first H_2^+, then D_2^+. The species, which is implanted first, occupies always the high energy release peak. No isotope exchange is observed. The low energy release peak is in both experiments by both hydrogen isotopes. Further experiments on this topic are planned, e.g. on the influence of surface temperature and on Be_3N_2, also with regard to ammonia formation.

A collaboration with Cedric Pardanaud from the PIIM research unit at the Aix Marseille université uncovered dendrite formation on Be samples irradiated with D-fluences well over 2×10^{17} cm^{-2} in Raman and AFM spectra. Further experiments are planned to elucidate the impact of dendrite formation on H retention.

In the future experiments on the interaction of Be with the noble gases He, Ne, Ar, Kr and Xe as possible seeding gas candidates and their influence on hydrogen retention are planned. In Oct. 2016 an experimental series on the thermal stability and H retention of beryllides will start.

The second new surface science Experiment is ARTOSS, an UHV-experiment dedicated to H retention in Be. The experiment has a unique combination of accelerator-based IBA methods and standard surface methods like TDS and XPS. Finally ARTOSS has been commissioned all sources and detectors. After a short additional testing period, the Be phase should start with a comparative study on the release behaviour of the three stable beryllium tungsten alloys Be_2W, $Be_{12}W$ and $Be_{22}W$. These studies are backed by already performed DFT calculation and modelled by CRDS.

The fuel retention diagnostic set-up FREDIS combines the two methods TDS and laser induced desorption quadrupole mass spectrometry (LID-QMS). The setup has already been tested the device successful outside the hot materials lab (HML) and shown, that LID-QMS is suitable to achieve spatially resolved H-release measurements. The next step is then the relocation of the setup to the HML. In the HML the FREDIS set-up will be able to handle Be samples, and irradiated and tritium-containing samples.

JULE-PSI is linear plasma device designed for studies on Be or irradiated samples. The device is currently assembled. First plasma operation is expected for fall 2016 with a new plasma source following the PISCES-B concept. The relocation to the HML is planned for 2017. Steady-state plasma exposure with plasma flux densities of $10^{21} – 10^{23}$ $m^{-2}s^{-1}$. Transient heat

loads can be simulated by a 100 J laser with pulse length up to 20 ms. For fuel retention measurements a LID-QMS system is available.

The two electron beam facilities JUDITH 1 & 2 focus on the behaviour of Be under ITER relevant cyclic heat fluxes. While JUDITH 1 has a max. beam power of 60 kW and a max. power density of 15 GW m^{-2}, while JUDITH 2 has a higher beam power of 200 kW but a lower max. power density of 2 GW m^{-2}. Since 2014 experiments are performed on the damage mapping for transient heat load. Also the experimental simulation of heat loads induced by massive gas injections was successful. In Judith 2 experiments were performed under ITER relevant high pulse numbers. And last but not least, it was shown that transient heat loads lead to oxide segregation. In a next step the comparison between transients simulated by laser and by e-beam is planned.

In conclusion, Jülich has a broad spectrum for experiments on Be: From surface science experiments, over electron beam facilities to linear plasma devices. All experiments are now running and foreseen to be soon operational. I recommend a 4th meeting in this CRP to present the experimental results.

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

The recent progress in several studies related to the CRP scope was reported:

- JET ILW inner wall guard limiter (IWGL): Density scan in limiter plasmas confirms 'ERO-min' erosion fit, and effective yield integration procedure (preferable is the analytic solution (AS) for the angle α_{imp} and energy E_{imp} distributions of sputtering particles on impact).
- Spectroscopy at JET outer wall (OW) Be limiter in L-mode experiments with ICRH antenna influence indicate the correctness of biasing implementation in AS. 'ERO-min' allows to reproduce the observed factor 3 erosion rise by antenna toggling.
- ERO applications to the divertor areas of JET and ITER can help to get an insight into the Be migration and deposition issues. E.g. it was shown that most Be reflected at divertor plates will be redeposited at remote areas. The flux of Be into the divertor is much smaller than respective C flux in the case of C-Wall.
- PISCES-B He plasma exposure confirms the Eckstein fit based on SDTrimSP data with uncertainties with "cut-off angle" probably related to the surface morphology. The effects of plasma condition and surface biasing are perfectly reproduced.
    - Initial population of quasi-MS state in BeI was detected from the singlet to triplet line ratios and was found to be always about MS:GS=0.33.
- The new kinetic model "CRDS" (Coupled Reaction Diffusion Systems) based on DFT data is capable to reproduce some non-trivial qualitative features observed in the TDS experiments.

All this work, but the last item, was based on 3D plasma-surface interaction and local transport ERO code. To achieve this progress several issues were solved. For instance, most important deviations between ERO and spectroscopy at IWGL were eliminated by the corrected background plasma (the recently processed embedded probes data has indicated that previously used electron temperatures were too high). The modelling of PISCES-B has shown

that ‘polar cosine’ distribution should be used for the physically sputtered particles. Considerable part of the progress was related to the new AS treating in detail the very last part of the ion trajectory just before the surface impact including sheath and biasing effects. The chemically assisted Be erosion (BeD_x release) was demonstrated to contribute significantly (over 50%) to the total erosion, though its influence drops with surface temperature and energy of sputtering ions.

Both IW and OW JET experiments seem to confirm the lower limit for the $Y_{Be_{\leftarrow D}}(E_{imp}, \alpha_{imp})$ we call ‘ERO-min’ supposing the large (50%) concentration of D in the surface interaction layer. Self-sputtering $Y_{Be_{\leftarrow D}}$ should have similar accuracy. The spectroscopy in He plasma at PISCES-B show for now good agreement with pure Be surface coefficient $Y_{Be_{\leftarrow He}}$, which is not in line with D plasma benchmarks and previous PISCES-B experience with mass loss measurements. Therefore it must be confirmed by further experiments with modelling. One of uncertainties is the surface morphology and, possibly, related cut-off angle in the angular distribution on release.

All the ERO applications show the importance of 3D experiment geometry, plasma and EM-field configuration and resulting impurity transport. This necessitates including very large volumes into simulation box keeping the high level of detail regarding gaps, shadowing etc. This has motivated the development of massive-parallel ERO-2.0.

Also further plans before the final report were presented including the incorporation of the new BeD_x reaction data from M. Probst and updating the ITER life time predictions.

Thomas Schwarz-Selinger: Beryllium-related PSI Studies at IPP Garching

Since the last CRP meeting the project on D retention in and release from beryllium-related mixed material layers presented in 2014 by W. Jacob was completed and a final publication was prepared [1]. This scoping study showed that admixed impurities (W, C, O) do not lead to dramatic changes of absolute D retention. Only for the high C concentrations case total retention and the release temperature increase. Fuel removal by wall baking procedure will be limited in all cases as the wall temperature is already comparable to the baking temperature.

H/D isotope exchange experiments conducted in Pisces-B with bulk beryllium targets were presented. Isotope exchange was possible even at 330K were thermal detrapping is negligible. However, large fluences were necessary ($>10^{25} H/m^2$), probably because of re-implantation of released fuel, an effect one would have to face also in a tokamak. Isotope exchange experiments with the “high current ion beam source” (HSQ) on Be:H and Be:D codeposits or magnetron sputtered thin films showed effective exchange at two to three orders of magnitude lower fluences. More experiments would be necessary to show the applicability of isotope exchange as fuel removal method, especially H/D exchange at the same ion energy and (ITER relevant baking) temperature at which D/H was implanted initially to see quantitatively the exchange rather than the built up of a new equilibrium state. However, beryllium related studies with “HSQ” came to an end and will not be started again. New experiments along this line initiated by D. Kogut (CEA) where presented but where hampered by the lack of a well characterized low energy ion beam setup for the exchange [2].

Cavity experiments conducted at UCSD and analyzed at IPP Garching were presented. In all cases investigated (vacuum, D_2 and He atmosphere, D_2 and He plasma) a sticking probability close to unity was observed. Experiments were initially conducted to explain Be seeding experiments in PISCES that needed unexpectedly high seeding values to turn Be erosion into deposition. The sticking probability can hence be excluded as a reason for that observation.

Cavities were also exposed during the first ITER like wall campaign in remote areas of the JET divertor. They showed deposition patterns that would infer surprisingly low sticking coefficients in the range between 20 and 30%. The reason for this is unclear. Re-erosion and particle reflection can be excluded as the only reason but large carbon fractions found in these in these films might play a role. Besides these cavity experiments, results from JET wall inserts from the inner wall cladding [3] and erosion and deposition measured on special marker tiles [4] exposed during the first ITER like wall campaign were presented. They showed that the inner wall is a net erosion area and beryllium is mostly deposited at the apron (tile 0 and 1) with layer thicknesses of up to 10 micrometers. WALLDYN calculations could reproduce these experimental results quantitatively [5].

In order to quantify these ion beam analysis studies in the dedicated "SAK" setup, elastic scattering cross sections for $^{9}Be(p,p_0)^{9}Be$ and nuclear reaction cross sections for $^{9}Be(p,d_0)^{8}Be$ were measured between 400 keV and 4150 keV and for $^{9}Be(p,\alpha_0)^{6}Li$ between 400 keV and 1300 keV [6].

In terms of future studies at IPP Garching experiments involving preparation or implantation of beryllium containing films came to an end, but analysis of samples especially by ion beam methods will continue into the future for samples where no significant Be amounts are mobilized. It is further foreseen that WALLDYN modelling of JET and ITER relevant issues will be continued.

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Kai Nordlund: Setting up Kinetic Monte Carlo simulations for Be

Background

The nature of H isotope (H/D/T) interactions with Be will have an important role for the operation of ITER, or any other fusion device with Be in the first wall. Unfortunately determining these is surprisingly difficult due to several factors. First, even though Be is a metal, it does experience swuft chemical sputtering. Second, the Be surface temperature varies depending on part of the reactor and operational condition. Third, the H isotopes can build up to high concentrations in the surface layers during operation, and knowing this concentration during a plasma experiment can be very difficult.

Molecular dynamics modelling

Since the incoming ion energy, surface temperature and H isotope surface concentrations do not have unique values, we have carried out molecular dynamics (MD) simulations as a function of these three parameters. The MD modelling (parts of which are published as E. Safi, C.

Bjorkas, A. Lasa, K. Nordlund, I. Sukuba, and M. Probst, J. Nucl. Mater. 463, 805 (2015)] show that the Be sputtering yield depends indeed strongly on not only the energy (which is well known), but also the surface temperature and related quantity of D surface concentration. This was also found to affect which fraction of Be is sputtered in the form of BeD and BeD_2 molecules/radicals.

Since the D surface concentration is not certainly known in the experiments, we first used MD simulations of cumulative bombardment of Be by D to estimate the concentration. This lead to very high D concentrations in the near-surface layer, which in turn amounted to large fractions of BeD_2 molecule sputtering. It is questionable whether this is realistic. BeD_2 molecules have not been observed in experiments, but on the other hand they are difficult to detect, and DFT calculations by Probst et al (carried out within this CRP) indicate they are not very stable.

The MD simulations suffer, however, from the problem that the flux used in them is very high due to the inherent time scale limitation of MD. This essentially prevents thermal D migration or desorption, and hence could lead to exaggerated D surface concentrations, in particular overestimating the fraction of weakly bound metastable states.

Kinetic Monte Carlo modelling

To estimate the D surface concentration for realistic fluxes, we turned to Kinetic Monte Carlo (KMC) modelling. This method is well suited to simulate impurity migration, trapping and detrapping at much longer time scales than MD can do. On the other hand, it requires parameterization of the D migration, trapping and detrapping coefficients from some other method, typically density functional theory (DFT).

To enable KMC simulations of D in Be, we have parameterized the open source KMC code MMonCa from DFT data from the literature and collaborators. Using this code, we carried out a 2-stage simulation of D plasma interactions with Be. First, the KMC code was ran for desired experimental fluxes and sample temperatures for the D implantation and migration in Be. From these simulations, the D surface concentration was extracted, and an molecular dynamics simulation cell for this D concentration in Be was constructed. After the MD cell was relaxed, it was used as the substrate simulation cell for non-cumulative simulations of Be sputtering by D.

The results showed overall similar sputtering yields as the MD simulations carried out without the KMC, see Fig. 1. However, the molecular sputtering obtained from the KMC+MD scheme was quite different. In particular, the combined scheme lead to lower D concentrations right at the surface, and hence lower BeD_2 sputtering yields. Additional analysis of the differences is underway.

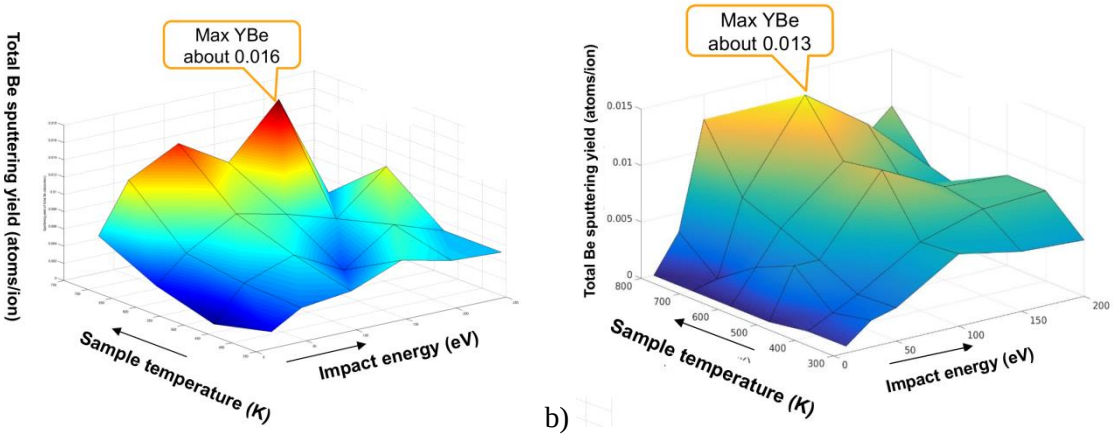

Fig. 1. Comparison of a) MD and b) KMC+MD simulations of the Be sputtering yields.

Michael Probst: Quantum chemical calculations and MD simulations for Be

1. **Electron impact ionization cross sections (EICSs)**

Following our last work on BeH_n and WH_n electron impact cross sections we studied the combined metal cross sections of Be_nW. The we want to make the EICS calculations procedure more reliable by using at least 2 independent methods (BEB and DM) and possibly more (Valence only BEB). We further worked with global geometry optimization algorithms. These works on Be_nW are finished. Electronic singlet-triplet cross section splittings and the impact of having several stable geometries were analyzed. Differences between BEB and DM calculations of up to a factor 2 (but normally considerable less) have been found Further extensions of this work are planned towards method development (optical potentials) and considerations of ionic and excited states.

2. **MD of Be-D sputtering**

The standard set-up respectively simulation protocol established by Ivan Sukuba (hcp Be surface (0001), 32x32x45(60)A^3 , ~4700 atoms for 25 and 50 eV impact energies and ~6300 atoms for 70 and 80 eV energies. 9000 impacts each) was used to look at the temperature dependence of non-cumulative sputtering on a pure Be surface. No significant temperature dependence between 420 and 720 °C was found when impact energies of D at 25, 50, 70 and 80 eV were investigated. The influence of the impact energy on the sputtering products is well established and is also found here. For example, from 25 to 80 eV the production of BeD by sputtering decreases drastically. Since the dependence of the yield mixtures seems now established from experiment and KMC, we believe that D-coverage on the surface, the presence of loosely bound adatoms or other mechanisms that simple sputtering away must be responsible for the T-dependence. Considering the fact that a temperature (kinetic energy) of about 10^4 K corresponds to 1 eV, the negligible T-dependence in our T-range is perhaps not surprising.

This work is planned to be extended by surfaces with coadsorbates and more detailed trajectory analysis.

3. **Stability of BeH molecules**

ΔG_f und ΔH_f – values (free formation energies and - enthalpies) were calculated for various neutral, cationic and anionic Be_xH_y – species. They were used to obtain $\Delta\Delta G$ – values (free energies of ***reactions***) and equilibrium constants at different temperatures for the various interconversion reactions of neutral and ionic Be_xH_y – species have been calculated. This can in turn be used to obtain the equilibrium concentrations of these molecules via the Eyring equation for rate constants: $k(T)= k_BT / h \exp(-\Delta G^{\ddagger}/RT)$

In a reaction network one can calculate all molecular concentrations at a given time if the atomic supply is known from solving a set of differential equations. One can also estimate their lifetimes if the energies of the transition states are calculated in the same way.

These quantum-thermodynamic calculations were performed by compound ab initio methods like G4 and by CCSD and QCISD. The electron-impact cross sections of the various $BeH_n^{+/-}$ molecules have also been calculated.

4. **DFT of Be_2W and $Be_{12}W$ surfaces**

Surface Binding Energies (SBE) and cohesive energies (CE) of W, Be_2W, $Be_{12}W$ and Be were calculated via plane-wave DFT. SBE calculations involved the many relevant surface sites have been treated. The results show that increasing tungsten content stabilizes the whole material (Be and W) against sputtering and that Be is removed from the surface much more

easily than W, leading in practice to preferential sputtering of only Be. We found one case where there is a large discrepancy with the analytic bond order potential. This must be further investigated and the work shall be extended to other surfaces, possibly also with codeposites.

Gregory De Temmerman: Plasma-beryllium interactions in ITER: research need

ITER will start operations with a full-tungsten divertor and a beryllium first wall. About 700m2 of beryllium will be used as plasma-facing armour in the divertor. As a licensed nuclear facility, ITER must limit the in-vessel tritium (T) retention to reduce the risks of potential release during accidents, the inventory limit being set at 1kg. Simulations and extrapolations from existing experiments indicate that T-retention in ITER will mainly be driven by co-deposition with beryllium (Be) eroded from the first wall. The ITER first wall (FW) is strongly shaped and co-deposition may occur in both magnetically shadowed areas of the wall and in the divertor (predominantly on the baffle area). A significant effort was made in the recent past to estimate the tritium retention rates in ITER. Plasma backgrounds from SOLPS and OSM were used as input for DIVIMP, and finally the WALLDYN code was used to estimate erosion/deposition balance inside the machine. Depending on the assumptions for the SOL plasma, the T inventory limit is reached after 3000-20000 400s long Q=10 discharges.

Global retention measurements will be performed by Pressure–Volume–Temperature-Composition (PVTc) and calorimetry of T absorbed on uranium beds in the T-Plant. These measurements do not, however, provide information on where the T is locally trapped. A pulsed Laser-Induced Desorption (LID) system is being designed to measure the T-retention in co-deposits forming on the inner divertor baffle. Regarding tritium removal, the baseline strategy is to perform baking of the plasma-facing components, at 240^{o}C for the FW and 350^{o}C for the divertor. Both baking and laser desorption rely on the thermal desorption of tritium from the surface, the efficiency of which remains unclear for thick (and possibly impure) co-deposits.

The TMAP code has been recently applied to estimate the efficiency of tritium removal by outgassing both for the LID case and for the case of the divertor bake. The TMAP model developed at PISCES to simulate TDS experiments on Be co-deposits was extended to the case of Be co-deposits formed in the JET divertor and analysed using ramp-and-hold TDS experiments where the samples were heated to 350C with different ramp rates and maintained at that temperature for a given duration before further heating to 1000C for complete outgassing. TMAP could well reproduce the JET TDS experiments when considering the presence of 3 trapping sites for deuterium at 0.8-0.9eV, 1.1eV and 1.4eV. This model, together with the PISCES model, was used to assess the efficiency of thermal outgassing in ITER. It was showed that for significant tritium release to occur during LID, the laser pulse duration had to be in the range of some seconds at temperatures higher than 1000K. The simulations show that this can be reached either through single long heating pulses or through cumulative shorter pulses (of equivalent total durations). Regarding the divertor bake, its efficiency appears limited for very thick co-deposits and work is ongoing to assess the frequency at which baking will be required to maintain a high efficiency while in parallel, other alternative detritiation techniques are being considered.

3. Plans for database

Traditionally a database for plasma-material interaction (PMI) data was dominated by XY data such as sputtering yields, reflection coefficients etc as a function of one or two parameters of incident beam conditions such as energy and angle. However, the PMI data needs for fusion applications are no longer limited to the kind of data sets as a variety of data sets for PMI processes becomes important. One of such examples is a database on dust particles where data sets are a collection of is an image of dust particles, size and shape information or composition and characteristics of dust particles. Participants discussed the development and scope of various databases for PMI data involving Be surfaces from this CRP.

One of the data sets that may be useful for Be surface sputtering yield is the ERO-min and ERO-max estimates based on fitting of various simulated data. The data sets can be presented in a table of impact energy, angle of impact. To calculate the sputtering yield for a given impact energy, additional fit parameters such as magnetic angles or surface temperatures are required. The data sets can be provided in a table or a code with input coefficients. It can provide the probability distribution of sputtered particles as well. A well-maintained database of ERO-min and ERO-max sputtering yields will provide the stability, history and traceability of ERO-min and ERO-max sputtering yields used for Be related modeling.

The other set that may be of interest to the community is the sputtering yields calculated by molecular dynamics (MD) and kinetic Monte Carlo (KMC) simulations on 4 dimensional data of impact energy, surface, temperature and surface element composition (e.g. hydrogen concentration on the surface). Sputtering yields will be a function of intensity of exposure as the concentration on the surface will change with hydrogen impact. Surface concentration may depend on temperature or be considered independent depending on the exposure conditions (or flux ratio of D/Be).

A set of thermal chemistry data involving Be, Be_xD_y, Be alloys may be useful, such as work functions, binding energies etc.

For hydrogen migration, kinetic or rate descriptions are widely used, however, the input data on a variety of reaction rates is not well documented. It will be useful to coordinate research groups to document and standardize the input parameters of KMC codes and Rate equation models applied to describe impurity migration or hydrogen trapping.

Data sets to model photo-emission or spectroscopic erosion measurements of atomic Be are of interest, for example, those to quantify break-up of BeH molecules by electron impact or dissociate processes.

4. Plans for final report

Participants agreed to publish a topic review paper as a final report for this CRP. Tentatively the title of the paper is (Data for) Plasma Interaction with Beryllium: *Erosion and tritium retention in beryllium-based-surface*. The contents of the paper and contributors are identified and outlined in this section.

4.1 Introduction (BJB first)

4.2 Beryllium under ITER conditions (GDT first)

- (Addressed to PMI folks that are not intimate with fusion energy research.)
- Review here the plans for Be on ITER; the geometry on JET. Mention some issues: gaps, leading edges, estimated range of power loads. Relevant impurities
- Relevant plasma conditions (steady and extreme).
- Relevant materials (Be, Be-C-W; helium).

4.3 Fundamental data for erosion, deposition, hydrogen retention, sputtering

- **Ion beam experiments (TSS first)**
    - Roth, Eckstein, Andrel (INL)
    - What beams (H, D, He, Be, C, Ne, Ar etc)
    - Experimental conditions.
    - What is measured: erosion rate, energy distribution and angular distribution of sputtered particles?
    - Issue about surface conditions (oxide layer).
    - Any beam-based experiments about redeposition, attachment?
- **Plasma experiments (RPD first)**
    - Erosion, deposition and hydrogen retention studied at PISCES.
    - Causey at Sandia, LANL; TPE experiment.
    - Range of plasma conditions.
    - Primary measurements. (Weight loss. What about energy and angle of emitted particles?)
    - Experimental information about sputtering in the form of Be, BeD, BeD2.
- **[JET experiments here or later? To be decided]**
    - If we discuss JET experiments here then we need to move the source term spectroscopy discussion up as well.
- **BCA-based modelling (KN first)**
    - Binary Collision Approximation; TRIM, SRIM and variants.
    - Work of Eckstein; review (or index) of his datasets.
    - Issues with TRIM/SRIM (surface binding energy, etc.)
    - Time-dependent BCA; other developments with BCA modelling.
    - Other BCA calculations for Be, Be-W-C compounds.
- **Molecular Dynamics modelling of erosion and deposition (KN first)**
    - Nordlund, Bjoerkas, Heilonen, etc.
    - Other MD modelling for beryllium-based materials?

- Discuss the issue of molecular sputtering; BeD and BeD2

4.4 Interlude: Data for Source Term Spectroscopy

- **Introduction, clarification of concepts (BJB first)**
  - First principles treatment requires data for plasma interactions involving H, Be, BeH, BeH_2 and their ions; maybe also BeH3+.
  - Specific lines in Be, Be+ and BeH (electronic transitions). Anything in BeH^+?
  - There are no useful measurements for BeH2 in our kind plasma environment.
- **Atomic data (BJB first)**
  - Reference to work by Aasa Larson and others, processes of BeH.
  - Enumerate what we have and what would be needed for a first principles treatment of source term spectroscopy.
- **Experimental data (RPD first; can talk with Daisuke Nishijima)**
  - Source term spectroscopy, "S/XB", calibrations on PISCES; limitations in plasma condisions. Anywhere else?
  - Nature of the experiments.
  - What say the results? How much variability?

4.5 Erosion, redeposition, retention on JET

- **Measurements (DVB first)**
  - What is available? Post-mortem tiles analysis, weight loss; also the source term spectroscopy.
- **Modelling (DVB)**
  - Primarily ERO, Walldyn?
  - What else?
- **Dust**
  - JET. Anywhere else for Be

4.6 Fundamental simulations of hydrogen in Be

- **Electronic structure (DFT) calculations for trapping and migration (MP first)**
  - Hydrogen migration, vacancy migration; evolution of microstructure.
- **Long-time scale evolution simulations (Multiple contributors)**
  - **Input data needs (KN)**

    Brief description of methods (KMC; what data are needed?
  - **Rate equations (MK will coordinate)**

Overview of approach

- Relation to TDS experiments
- Diffusion calculations, CRDS, etc.)

Cite: Coupled reaction diffusion system CRDS (Julich)

- **Kinetic Monte Carlo (KN)**

  KMC, etc., rates obtained from electronic structure calculations (DFT) of trapping energies and barriers.

  KMC, etc., rates obtained from MD simulations.

  KMC and other long-time calculations for Be-based materials; reference to the data.

4.7 Measured Data for Hydrogen Retention and Transport

- **Fundamental experiments on hydrogen trapping and hydrogen transport (MK first)**
  - Thermal Desorption Spectroscopy.
  - Data for trap energies, function of nature of vacancy. (Focus on Be, of course
  - Experimental tools for hydrogen profiling (review the qualities of NRA).
  - Gas permeation experiments? Nothing?!
  - Studies of different Be-based materials?
  - Studies involving radiation damage? Probably done in context of tritium breeding; some references will be appropriate.
- **Plasma studies including codeposition (GDT first)**
  - JET data; post mortem analysis?

4.8 Outlook, Priorities, Conclusions

5. Future work

Participants agreed that there is much open work for PMI data involving Be surfaces. Not only limited to Be, there are concerns on diffusion coefficients in different materials due to the safety risk associated with tritium contained in the waste. Related to this tritium problem, Data issues of dust containing tritium or hydrogen migration properties in metals were raised as the potential future work.

Appendix I: List of Participants

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Appendix II: Meeting Agenda

Wednesday 15 June 2016

09:30 - 09:45 B. J. Braams: Welcome and Introductions

Session I. PISCES

09:45 - 12:15 R. Doerner: Plasma interactions with beryllium surfaces

12:15 - 14:00 Lunch

Session II. Other experiments

14:00 - 15:00 G. De Temmerman: Plasma-beryllium interactions in ITER: research needs

15:00 - 16:00 T. Schwartz-Selinger: Beryllium-related PSI-studies at IPP Garching

16:00 - 16:30 Break

16:30 - 17:30 M. Köppen: Experimental possibilities in Jülich–an update

Thursday 16 June 2016

Session III. Computations

09:00 - 10:00 K. Nordlund: Combined molecular dynamics and kinetic Monte Carlo modelling to simulate D deposition and Be sputtering at realistic fluxes

10:00 - 11:00 D. Borodin: Development of models for plasma interactions with Be on the basis of dedicated experiments

11:00 - 11:30 Break

11:30 - 12:30 M. Probst: Quantum chemical calculations and MD simulations for Be

12:30 - 14:00 Lunch

Session IV. Discussion

14:00 - 16:00 All: Plans for database and final report

Friday 17 June 2016

Session V. Discussion

09:00 - 12:00 All: Plans for final report

12:00 Close of Meeting

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