INDC(NDS)-0670
Distr. LP,NE,SK

# INDC International Nuclear Data Committee

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

## Summary Report of the Second Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

18–19 August 2014

Report prepared by

Bastiaan J. Braams
Hyun-Kyung Chung

IAEA Nuclear Data Section

May 2016

**IAEA Nuclear Data Section**
**Vienna International Centre, P. O. Box 100, 1400 Vienna, Austria**

Selected INDC documents may be downloaded in electronic form from

*http://www-nds.iaea.org/publications*

or sent as an e-mail attachment.

Requests for hardcopy or e-mail transmittal should be directed to

*NDS.Contact-Point@iaea.org*

or to:

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

Produced by the IAEA in Austria

May 2016

**INDC(NDS)-0670**
**Distr. LP,NE,SK**

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

## Summary Report of the Second Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

18-19 August 2014

Report prepared by

Bastiaan J. Braams
Hyun-Kyun Chung

IAEA Nuclear Data Section

## Abstract

The Second Research Coordination Meeting of the IAEA Coordinated Research Project (CRP) on "Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials" was held 18-19 August 2014 at IAEA Headquarters in Vienna with 6 external experts and IAEA staff. Participants reviewed their work in connection with the CRP and they developed a work plan for the remainder of the project. The proceedings and conclusions of the meeting are summarized in this report.

May 2016

# TABLE OF CONTENTS

# 1. Introduction

Beryllium is foreseen as the wall material in ITER away from the regions of highest load (where tungsten will be used) and since the Fall of 2011 the JET experiment is operating with a Be-W ITER-like wall. 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 provide basic data to support analysis of measurements of plasma-material interaction on JET and to help prepare for operation of ITER. The CRP held its first Research Coordination Meeting (RCM) in September 2012 and the second RCM was held 18-19 August 2014. This report summarizes the proceedings of that 2nd RCM.

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.

Section 2 provides a summary of the presentations. Section 3 reviews the status of the CRP and Section 4 describes the work plans through the expected close of the CRP in 2016. The list of participants is in Appendix 1 and the Agenda is provided in Appendix 2. Appendix 3 contains research summaries by participants.

Most of 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. Presentations

## R. A. Forrest: Opening

Nuclear Data Section Head Dr Robin Forrest opened the meeting and welcomed the participants to Vienna. He recalled the main objective of the Second RCM to review the status of the CRP and to make plans for a coherent output at the end of the CRP about 18–24 months later.

## R. P. Doerner: Plasma interactions with beryllium surfaces; recent data from PISCES. Presentation and extended discussion

The first morning session was entirely given over to Dr Doerner for a presentation with discussion about the PISCES-B experiment and its recent results. Recall the general parameters of PISCES-B: it is a linear plasma device, steady-state operation, $n_e$ in the range $(10^{12}–10^{13})/cm^3$, $T_e$ in the range (4–40) eV; the target plate can be biased to (20–300) eV and that defines the approximate ion impact energy per unit charge. The device and surrounding equipment is in a safety enclosure. PISCES-B is qualified and extensively used for operation with beryllium as a target material and beryllium can also be injected into the plasma.

The main topic for this presentation and discussion is the erosion behaviour of beryllium in the high-flux plasma environment of PISCES. (High flux relative to beam-target interaction studies.) The erosion has been found to be less by a factor ~5 than is expected based on TRIM (W. Eckstein) calculations that match beam-target data. There can be very large changes in surface morphology in PISCES experiments (extreme roughening of the beryllium target) and this may explain some of the difference in erosion behaviour. The development of surface morphology has been studied under different plasma conditions (including argon impurity) and under different surface conditions (surface temperature).

The difference between net erosion and gross erosion, or the sticking coefficient of beryllium on the beryllium surface, was studied using cavity probe measurements. The experiment is done using a controlled source of Be. The results are complicated as apparently a redeposited beryllium surface has different sticking or erosion properties than a beryllium tile surface. The results depend on surface temperature too and this may have to do with the properties of BeD molecules. Molecular dynamics simulations are being done in an effort to understand the data better.

Aluminum is viewed as a surrogate for beryllium for laboratory studies and Dr Doerner described direct comparison studies done on PISCES between Be and Al surfaces. These experiments were coordinated with studies of erosion and deposition due to plasma interaction with Al surfaces on DIII-D. One objective of the PISCES studies was to determine the inverse photon efficiency (S/XB) factor for Al to be used for spectroscopic erosion measurements on DIII-D. As a general rule, the erosion behaviours of Al and Be are similar whereas the hydrogen retention behavior is different.

Finally Dr Doerner described studies of the response of Be-coated W to high transient heating by laser pulses (to simulate ELMs). A Be/W alloy is formed where the coating attaches to the substrate and this alloy cracks at lower energy density than pure W.

## M. Köppen: Multi-method approach towards a detailed understanding of beryllium for fusion

Since the closing down of the TEXTOR experiment the plasma physics programme (IEK-4) at the Jülich research institute is entirely devoted to study of plasma-material interaction. Dr Köppen reviewed surface experiments and methods using the X-ray photoelectron spectroscopy (XPS) device and the ARTOSS complex of diagnostics. The XPS diagnostic is used to measure composition and chemical binding states, sputter profiles and chemical depth profiles and an experiment of nitrogen implantation into clean Be was described. The principal diagnostic capabilities of ARTOSS are ion beam analysis including nuclear reaction analysis (NRA) and Rutherford backscattering spectroscopy (RBS), thermal desorption spectroscopy (TDS) and X-ray diagnostics. ARTOSS was used for the study of thermal desorption spectroscopy of D in Beryllium. In collaboration with the Helmholtz Zentrum Berlin (HZB) energy-resolved XPS (ERXPS) experiments with beryllium are being carried on the SurICat (Surface Investigation and Catalysis) photoemission end station. The beryllium source is handled in the “LAICA” preparation chamber.

Dr Köppen also described laser-based surface diagnostics and plans for the Jule-PSI and JUDITH plasma experiments. Laser-based surface analysis includes laser-induced desorption spectroscopy (LIDS), ablation spectroscopy (LIAS) and breakdown spectroscopy (LIBS). High heat flux experiment setups at JUDITH1 and JUDITH2 were also presented to assimilate transient and steady heat loads. The experimental work is intended to provide data for a coupled reaction-diffusion system (CRDS) for use with modelling codes such as ERO, SOLPS and WallDyn. The work is supported by DFT calculations.

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

Dr Borodin reviewed the 3D Monte-Carlo impurity transport and plasma-surface interaction (PSI) code ERO, a useful bridge allowing to interpret various PSI-relevant experiments and test the relevant Be data (erosion, atomic and molecular processes, etc.). Applications include several experiments at JET ILW and other devices (both tokamaks and linear devices) and ITER predictive modelling. ERO modelling provides proper extrapolation of the experimental data from the existing experiments for ITER, implementation of physical effects and their sensitivity analysis.

Most focus was on the interpretarion of the passive spectroscopy at solid shaped limiter at JET during 1) plasma density scan 2) surface temperature scan. Both scans were carried out in the limiter plasmas shifted towards the observed limiter position (inner wall, midplane). ERO simulations on Be erosion including BeD release and the respective light emission (BeI, BeII, D lines and BeD band) inside the observation chord (ERO serves like a synthetic diagnostic) are compared in detail with the experimental observations. The influence of shadowing (PFCFlux simulations of connection lengths along the surface), metastable tracking (triplet and singlet line ratios in BeI), uncertainties in the plasma parameters and MD data for BeD release were discussed. The "minimal estimate" fit for physical sputtering yield (parametric formula for called "ERO-min") assuming 50% D concentration in the surface was proved to give good results for the plasma-wetted areas. Photon emission coefficients (PEC) and other atomic data form ADAS seems to be full and accurate, whereas the data for BeD release (MD) and further decay in plasma (rates from the literature) recently included into ERO are still quite pure.

Further applications of ERO were also mentioned for instance $^{10}$Be marker migration at JET ILW main wall or rotaiting probe collector in the divertor, Be target erosion at PISCES-B and possible Be-proxy experiments at FZJ linear device PSI-2. It was demonstarated that 3D surface shape, shadowing and local changes in the plasma parameters are of great importance. For that purpose an ERO benchmark at EAST using a sample, shaped very similar to the ITER blanket module, was presented. Finally, an outlook for the new massive-parallel ERO 2.0 was given, which should provide performace adequate to the full-scale ITER simulations

## W. Jacob: Beryllium-related PSI experiments in IPP Garching

Dr Jacob described Be-related activities at IPP Garching: Ion-beam analysis station for the handling of Be-containing samples, XPS depth profiling, data analysis of Be-containing samples from high current ion source and thermal desorption spectroscopy of Be-containing samples. These activities are possible only for experiments where no significant Be amounts are mobilized as much of laboratory studies were moved from IPP to FZ Jülich in the course of the appointment of Prof. Ch. Linsmeier as director of the PSI department in FZJ. In 2013 IPP has commissioned a dedicated measurement station ("SAK Chamber") at the Tandem Accelerator. Using this device IPP has participated in the analysis of material transport issues in JET for the ILW experiments [1]. Participation in comparable analysis campaigns are foreseen for the future. SAK remains at present the only remaining dedicated device for Be-related studies. With the remaining experimental capabilities IPP will continue to collaborate with international partners on research of PSI issues for Be-mixed materials. Close collaboration exists with PISCES (UCSD, USA) and MEdC (National Institute for Laser, Plasma and Radiation Physics, MEdC, Bucharest, Romania).

## K. Nordlund: Review of MD potential development and MD simulations of plasma interactions with Be-containing fusion reactor materials

Prof Nordlund presented Molecular Dynamics (MD) simulations and kMC (kinetic Monte-Carlo) simulations applied to the rich materials science of plasma-wall interaction. He focused the problems of mechanism of He-induced fuzz formation in W and H istope interactions with Be and Be-W. The status of potentials used by MD simulations relevant to Be-C-W-H-He system and the MD formalisms (independent and cumulative simulations) were reviewed. Briefly the application to He in W by KMC simulation to model W fuzz formation was shown. Data compiled for Be sputtering by D were presented: sputtering yields of both Be total and Be in $BeD_x$ molecules, D reflection yields, D release yield and $D_2$ molecule release yield. BeW alloy formation after Be irradiation of W surfaces were investigated as well as the surface structure changes form mixed D, Be bombardment of W. It was noted that at least 2 different potentials should be tested to get some idea of reliability of MD simulations.

## S. Irle: Progress towards quantum chemical molecular dynamics simulations for hydrogen-beryllium interactions

Prof Irle described the work of the self-consistent-charge density-functional tight-binding (DFTB) method applied to perform atomic-scale, long timescale simulations of hydrogen isotope H/D/T chemical sputtering on Be surfaces. DFTB (density-functional tight-binding) is a well established approximate DFT method but there are no available Be-X parameters. Hence, corresponding Be-Be and Be-H parameters for DFTB method were developed. The electronic DFTB parameters were generated on the basis of solid state band structure fitting, and repulsive potentials were created using $Be_x$ and $(BeH_2)_y$ molecular compounds. Two different parameter sets performed well for either molecular compounds or solid state simulations, but not for both systems simultaneously. The origin of the mutually exclusiveness of these two parameter sets was discussed, and a possible solution based on an atomic coordination-number based global scaling approach for the repulsive potential was suggested.

### M. Probst (indirect): Quantum chemical and molecular dynamics simulations of plasma interaction with beryllium surfaces

Prof Probst could not attend the meeting but sent the presentation on his work on plasma interaction with Be surfaces. The presentation consisted of 5 sections: 1) molecular dynamics simulation of sputtering of $Be_nW$ (n=2, 12), 2) calculations of thermodynamics data of $BeD_n$ formation reactions, electron impact cross-section calculations of Be-species, 4) comparison of vacancy formation and C-adsorption energies between Al and Be, and 5) energy barriers for the intrusion of $BeH_x$ into graphite. Results showed that $BeD_3$ is not very stable in plasma conditions while $BeD_2$ formation gains much energy preferring such reactions. Also surface energetics of Be-Be and Be-C surface interactions were found to be stronger than Al-Al and Al-C. Surface energetics of Be-W alloys are in progress.

## 3. Status Review

### Erosion

The key data for erosion are from PISCES experiments with relevant targets of pure Be, $Be_xW$, BeO, and Be-N. The data from PISCES experiments should be extrapolated to fusion devices with complex plasma conditions such as JET or ITER. Beryllium is relevant for the outer wall of fusion experiments where conditions are rather variable due to plasma oscillations, non-Maxwellian plasma conditions, sheath potential and distribution of incident angle.

Angle distribution is a critical factor for determining the effective erosion yields on fusion experiments. While the PISCES experiment uses a bias potential that results in near-normal incidence, the erosion data from beam-surface interactions shows a significant angle dependence. Depending on angular distribution the difference can be a factor of 2-3 for PISCES data or a factor of 5-10 for fusion experiments. A theoretical angular function (Eckstein 2007 formula) has been assumed to produce an effective erosion yield. An averaged erosion yield over angle of incidence using TRIM code results in 2-3 times higher yield over that of normal incidence.

Related to the issue of angle distribution, surface roughness and surface morphology should be taken into account in erosion yield determination. It is hard to predict how surface will evolve during the plasma interaction and therefore determining impact angle on such surface is not simple. Every experiment has different surface condition and angle dependence and hence integrated yields may differ by a factor of 2-3 depending on surface conditions. Particularly, for high flux plasmas, due to H retention on the surface the sputtering is reduced and a simple angular function doesn’t reproduce experimental data. Consequently, one should rely on empirical data or MD predictions. At low temperature, morphology effects due to chemical sputtering need to be considered.

There is a strong demand for more benchmark data from well-designed experiments. It is difficult to find well characterized data to be compared with MD simulations due many unknowns. Other than PISCES data, there is a shortage of laboratory data for Be. JET data can give a confidence to PISCES data when it confirms PISCES results. However, for JET there is much larger uncertainty in the basic plasma conditions in front of the wall than for PISCES. Even PISCES data have uncertainties due to flux conditions, background neutrals and impurities. A small fraction of impurities will affect the threshold for sputtering. A benchmark experiment requires a clean surface and well-characterized ion beam conditions, and it needs to be compared with MD results.

The Jülich group is planning high quality beam erosion measurements on Be and Be alloys using XPS (X-ray photoelectron spectroscopy) in 2015. With a carefully prepared Be layer sample (without oxidation), angle, energy, and temperature dependence will be investigated in the in-situ diagnostics set-up. Already N-implantation in Be experiment has been completed and the publication is in progress.

In conclusion, PISCES and other lab experiments provide key experiments with well defined input conditions. All results should be analyzed and accumulated with a modeling tool such as ERO or CRDS to be extrapolated to plasma devices such as JET and eventually to ITER. On the other hand, JET with ILW should provide the most relevant benchmark for ITER and such a benchmark is indispensable for ITER predictive modelling. The modelling using ERO and other tools is a key bridge to interpret the JET-ILW experiments and match them with the basic data from laboratory experiments and linear devices like PISCES-B.

## Hydrogen (Tritium) Retention

Hydrogen (H,D) profile and migration has been studied in Garching, Jülich and UCSD. It is a question whether there exists calibrated model for hydrogen (H, D, T) migration. For the case of clean target tiles an available model describes H trapping and release in the absence of erosion or redeposition.

For the case of a redeposited layer, the situation is more complicated. A coupling of MD simulations and diffusion models (either KMC or Rate models) is needed to analyze experiments. Trap energies are fitted to TDS spectra, variation of rates, heating rates etc. The work by A. Allouche on trapping energies and migration barriers of Be should be noted. A variation of TMAP model has been developed to allow trap concentration changes during the annealing (work by M. Reinelt) and works well with existing data. Better ab initio potentials are needed to improve MD simulations, with good experiments for benchmark.

While H retention in Be surface layer is clearly an important issue for ITER, it is not clear that diffusion in bulk beryllium is an issue. Experiments from the 1990s indicate that H retention saturates on the surface of Be layer and effective diffusion to the bulk material is very small, especially for thick tiles. In this regard, the role of codeposits in terms of H retention and trapping seems to be important. Diffusion may be high in isolated layers, but with plasma bombardment the surface damage creates traps, which leads to the H saturation and very low migration into the bulk. Also, bubble formation on the surface may influence diffusion processes significantly. The net effect of diffusion processes will depend on the balance of all the processes including molecular and surface processes.

Chemistry in codeposited layers is of interest. A phase diagram exists for Be-W, but not for Be-C. For the Be-W case a thermally stable phase exists and it was confirmed by MD simulations. However, codeposits do not necessarily thermally stable phases and usually don't. Local transport and parameters are important for the behavior of codeposits. The nature of BeD and $BeD_2$ is of interest whether it is chemical bonding or not. Normally it is considered as solid phase unless there is a gas bubble. Also important is the H retention in the codeposited layer of Be. The net erosion rate including H trapped codeposited Be layer is of safety concern. Therefore a database is needed for codeposition, release, trapping energy in codeposited layer. A codeposited target is not easily made in PISCES, but vaccum arc may be used to produce codeposits.

## Support for diagnostics

Erosion experiments often rely on spectroscopic measurements, which require atomic and molecular data for interpretation. The practice has been to do measure clean sample lines, weight loss, and get photon emission coefficients at various conditions to obtain an empirical S/XB. First principles calculations are rarely employed and in part that is because other uncertainties than atomic and molecular processes exist for sputtering experiments. For Be case, puff experiments are used to calibrate photon emission coefficients. It is noted that S/XB based on atomic data from ADAS may be accurate, but application of the photon efficiency to sputtering measurements is not straightforward due to the dependence on local transport and the line of sight of spectroscopic measurement.

# 4. Work plans

## UCSD PISCES work plan through 2016

The PISCES-B facility will continue beryllium operations at least through 2016. The effort will focus on unresolved issues associated with plasma interaction with beryllium surfaces. The ongoing effort to develop a diagnostic capable of measuring whether any $BeD_2$ molecules are released from a beryllium sample exposed to deuterium plasma will continue. If these efforts are successful, a systematic variation of incident ion energies and surface temperature will be performed. In addition, effort to develop a diagnostic technique capable of measuring, during the plasma exposure, the amount of gas atoms retained in the implantation layer will be pursued. This will likely be a laser based diagnostic, such as LIBS.

Erosion and retention measurements on Be-W mixed materials will be completed during this period. Samples supplied by the Romanian transfer arc facility will allow controlled variations in the Be/W ratio in the samples and a series of varied composition targets will be exposed at several temperatures. The effectiveness of baking Be codeposits, as a means of tritium inventory control, will also be concluded during the final years of this CRP. Long term baking at 240C and 350C will be investigated with varying thicknesses and number of layers of codeposited material. The TMAP7 code will be used to interpret the data and to extrapolate to conditions expected in ITER.

Finally, dedicated plasma exposures will be conducted in conjunction with ERO modelers, to help resolve any outstanding issues in the benchmarking of the code.

## IPP Garching work plan

Much of the laboratory experiments were moved from IPP Garching to Forschungszentrum Jülich in connection with the appointment of Prof. Ch. Linsmeier as director of the PSI department in FZJ (see presentation of Martin Köppen).

IPP Garching will continue to participate in the analysis of material transport issues in JET for the ILW experiments. For this, IPP provides ion beam analysis of Be-containing JET samples. For this purpose a dedicated measurement station equipped with a glove box for sample handling has been commissioned in 2013.

Hydrogen isotopes retention and release in Be-containing mixed materials (Be, Be:W, Be:C, and Be:O) have been investigated. Samples have been prepared by MEdC (National Institute for Laser, Plasma and Radiation Physics, MEdC, Bucharest, Romania) and been implanted with D in IPP. D retention has been measured by ion-beam analysis and by thermal desorption spectroscopy. In addition, long term annealing experiments at ITER-relevant temperatures (240 °C and 350 °C) have been performed. Data analysis is ongoing. This work will be concluded and published. Further D implantations are not possible because the corresponding device can no longer be applied for Be related research.

IPP has collaboration with PISCES and MEdC and will continue to participate in the analysis of Be-containing samples.

## Forschungszentrum Jülich work plan

Investigation of the system Be-N.

Investigation of hydrogen retention and release behavior of Be-N.

Investigation oxidation behavior of Be-N.

Experiments on the interaction of He-ions with Be-N.

Isotope exchange in Be-based mixed materials.

Understanding $BeD_x$-formation and properties.

Investigation of different behavior of atomic and ionic hydrogen.

Time resolved physics of LIBS plasma.

Investigation of LIBS plasma physics under vacuum.

gaseous (Ar, N, He ) environments.

magnetic field.

Impact of the laser wavelength on the LIBS plasma.

Combination of two laser beams (Dual LIBS).

Ablation physics: Energy distribution (ToF), species distribution, formation of cluster, reproducibility (particles/pulse).

Modelling of the laser-material interaction.

## Forschunszentrum Jülich work plan – modelling (D. Borodin)

The ERO simulations for the spectroscopic experiments at JET with new ILW should be continued. It should include the improved modelling at the inner wall aimed at testing of the sputtering yields and $BeD_x$ molecular release data (MD, K. Nordlund’s group). Another topic is the MD decay and ionisation in plasma – further data compilation is required including the collaboration with M. Probst. New similar experiments are planned during the next JET campaign (S. Brezinsek).

ERO modelling for further JET experiments such as the spectroscopy at JET outer wall close to a Be limiter near the ICRH antenna affecting the local E-field and migration experiments with 10Be marker (effect averages through the whole campaign) should provide additional benchmark.

It is agreed to revise the old simulations of ERO for PISCES Be or even to simulate a new one fully dedicated for the benchmark of ERO and erosion dara (physical and chemical sputtering). The detailed spectroscopy, deposition at witness plate and target erosion (optimally with certain variation of the target biasing and plasma parameters) as one coherent package will be useful to determine the uncertain parameters.

As a result the ERO simulations from 2011 for the ITER first wall lifetime should be revised. Sensitivity studies and uncertainty estimates should be provided.

The simulations for ITER and JET ILW have caused dramatic code performance issues for ERO. Further implementation of physical effects or even simply a full scale use of the existing features without critical sacrifices for the experiment geometry details or simulation volume limitations is impossible without a massive parallelization ERO. This and certain other reasons have led to a decision to rewrite the code to a profoundly restructured ERO2.0. A dedicated PhD work in a strong cooperation with Jülich Supercomputing Centre is planned starting from November 2014.

Obviously, ERO databanks should be consequently extended and updated with the data from the lab experiments (FZJ and other institutions) and the simulated data (MD data for chemical sputtering from K. Nordlund, molecular reactions in plasma from M. Probst etc.).

## University of Helsinki work plans

D -> Be: Non-cumulative runs with decreasing D concentration for increasing T being run: should match JET conditions with outgassing better. Data to be published ….

Be-He potential to be made.

D chemical sputtering of Al; Al–H potential exists [Apostolos and Mishin, Phys. Rev. B 82, 144115 (2010)]

Be-O potential?? Challenge…

Repeat D on Be sputtering calculations at ??? D concentration

Validation of Be-H, Be-Be potentials.

Development of Be-He potential.

Exoplore long-time scale (MD+KMC) calculations

Some comparison with Al.

## Stephan Irle, Nagoya University work plans:

Parameterization of DFTB; band potential.

Then compare MD-DFTB with MD by Kai Nordlund + Carolina Björkas.

Hope to extend to other mix: Be-W, Be-N, Be-O.

Working on an on the fly KMC code based on work at Tohoku University; adopt to DFTB.

Transition state search.

## Appendix I: List of Participants

**Mr Kai Nordlund**, Department of Physics, University of Helsinki, P.O. Box 43, Pietari Kalmink 2, Helsinki 00014, FINLAND.

**Mr Martin Köppen**, Forschungszentrum Jülich, Leo Brandt Strasse, Jülich 52425, GERMANY.

**Mr Dmitry Borodin**, Forschungszentrum Jülich, Leo Brandt Strasse, Jülich 52425, GERMANY.

**Mr Wolfgang Jacob**, Max-Planck Institut für Plasmaphysik, 85748 Garching bei München, GERMANY.

**Mr Stephan Irle**, Nagoya University, Institute for Advanced Research, Furo-cho, Chikusa-ku, Nagoya 464-8602, JAPAN.

**Mr Russel Doerner**, University of California, UCSD Fusion Program Experimental Research Division, 9500 Gilman Dr., La Jolla CA 92093-0417, UNITED STATES OF AMERICA.

**Mr Bastiaan J. Braams**, IAEA Nuclear Data Section, Division of Physical and Chemical Sciences, P.O. Box 100, A-1400 Vienna, AUSTRIA.

**Ms Hyun-Kyung Chung**, IAEA Nuclear Data Section, Division of Physical and Chemical Sciences, P.O. Box 100, A-1400 Vienna, AUSTRIA.

**Ms Kyungmi Lim**, IAEA Nuclear Data Section, Division of Physical and Chemical Sciences, P.O. Box 100, A-1400 Vienna, AUSTRIA.

## Appendix II: Meeting Agenda

**Second Research Coordination Meeting of the Coordinated Research Project on "Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials."**

### Monday 18 August 2014, room M0E67

09:00-09:15: **R. A. Forrest**, **B. J. Braams**: Welcome.

09:15-12:00: **R. P. Doerner**: Recent data from PISCES. Presentation and extended discussion.

12:00-13:30: Lunch

13:30-14:30: **M. Köppen**: Review of erosion and hydrogen retention experiments on beryllium-containing plasma-facing materials.

14:30-15:30: **D. Borodin**: Review of models and simulations for plasma interaction with beryllium surfaces.

15:30-16:00: Break

16:00-17:00: **W. Jacob**: Beryllium-related PSI experiments in IPP Garching.

19:00-: Social dinner

### Tuesday 19 August 2014, room M0E67

09:00-10:00: **K. Nordlund**: Review of MD potential development and MD simulations of plasma interactions with Be-containing fusion reactor materials.

10:00-10:45: **S. Irle**: Progress towards quantum chemical molecular dynamics simulations for hydrogen-beryllium interactions.

10:45-11:30: **M. Probst** (indirect): Quantum chemical and molecular dynamics simulations of plasma interaction with beryllium surfaces.

11:30-12:00: **B. J. Braams**: Status review

12:00-13:30: Lunch

13:30-16:00: **All**: Review of data needs and work plan through 2016.

16:00: Close of meeting

# Appendix III: Summaries by Participants

## R. P. Doerner: Recent data from PISCES

A review of progress made in the PISCES-B device investigating interactions of plasma with Be targets was presented. In addition, recent work on the applicability of Al as a surrogate for Be as a PFM was studied, both in PISCES as well as using the DiMES manipulator in DIIID.

In PISCES, the work included investigation of the morphology that develops under different various plasma exposure conditions. The development of surface morphology has been correlated with the reduction in erosion from D, or He, plasma exposed surfaces. The reduction originates in the deposition of puttered particles on the side walls of the structures extending from the surface. Such deposition of atoms sputtered at shallow angles with respect to the surface also accounts for a decrease in the axial penetration distance of sputtered material upstream into the plasma column. During high-fluence plasma exposures, the development of surface structures has been shown to account for a reduction in the sputtering yield by roughly factors of 2 or 3. The surface eventually reaches a steady-state condition where the morphology is maintained as the surface continues to erode at some rate.

The length of structures formed on the surface scales with the incident energy of the incoming ions and appears to form by erosion of the surface. However, as the temperature of the surface is increased, the morphology becomes less and less apparent, until at 0.5 Tmelt, plasma bombardment of the surface no longer produces much in the way of structures on the surface. It is also noted that bombardment of Be surfaces with Ar does not result in the formation of surface structures. After low-temperature plasma exposures, measurements of the angle of the tips of the structures with respect to the surface normal agree favorably with calculations of the optimal sputtering angle by Yamamura [Y. Yamamura, Y. Itikawa, and N. Itoh, "Angular dependence of sputtering yields of monatomic solids," Report No. IPPJ-AM-26, 1983.]. Some indications exist from the JET-ILW experiments [H. Bergsaker et al., P02-093, submitted to JNM], that similar structures may form on plasma exposed Be surfaces in the tokamak as well.

In an attempt to understand the different relationship between net and gross erosion [R. P. Doerner, D. Nishijima and T. Schwarz-Selinger, Nucl. Fus. 52(2012)103003] that was reported during the last meeting of this CRP, the sticking coefficient of Be was measured using cavity probes. The measured values showed a sticking coefficient of 0.8 – 1, in agreement with expectations. The relationship between net and gross erosion was also measured at elevated temperature, here the typical definition of net erosion being equal to gross erosion minus the redeposited fraction was recovered.

Molecular dynamics simulations of the motion of an adatom on a Be 0001 surface, revealed that adatoms have a longer lifetime on an island on the surface than do adatoms at elevated temperature due to the Ehrlich-Schwoebel barrier [G. Ehrlich and F.G. Hudda, J. Chem. Phys. 44, 1039 (1966)]. These calculations provide some insight into a possible explanation of increased erosion of depositing ions at low temperature, compared to high temperature.

Al had been proposed as a proxy for the study of toxic Be plasma-material interactions. Measurements from both the D3D tokamak and PISCES-B, show discrepancies between spectroscopic measurements of Al erosion, compared to post mortem ion beam measurements of the erosion. The explanation seems to be that Al erodes chemically in a manner similar to Be and the spectroscopic measurements would miss this erosion channel if simply relying on the emission of Be I radiation. The conclusion was that to understand Al erosion would require a substantial investment in determining the molecular break up chains of eroded molecules and that this was unlikely to be worth continuing effort. The retention of D in Al was also investigated and was shown to be different than that of Be.

Finally, the response of Be coatings on W substrates transient heating by laser pulses was investigated in PISCES-B. The goal of the experiments was to determine the ability of Be to act as a sacrificial coating to protect the underlying W substrate. While a thick enough Be coating was shown to be able to protect the substrate, alloying of the coating with the substrate material was also detected. The W/Be alloy appeared to crack at lower energy density levels than pure W samples exposed to similar transient events. The Be formation energy density was determined to be the figure of merit for when the Be coating was thick enough to protect the substrate material.

Finally, a discussion of future work areas for the PISCES Program as part of the CRP was presented and discussed with the other members of the research project.

## W. Jacob: Beryllium-related PSI experiments in IPP Garching

For a long time IPP was engaged in Plasma-Surface-Interaction laboratory experiments using Beryllium and Be-containing materials. Much of these laboratory experiments were moved from IPP to FZ Jülich in the course of the appointment of Prof. Ch. Linsmeier as director of the PSI department in FZJ (see presentation of Martin Köppen).

In 2013 IPP has commissioned a dedicated measurement station ("SAK Chamber") at the Tandem Accelerator which is equipped with a glove box for sample handling. SAK allows ion beam analysis of Be-containing JET samples and other Be-containing samples. Using this device IPP has participated in the analysis of material transport issues in JET for the ILW experiments [1]. Participation in comparable analysis campaigns are foreseen for the future.

SAK remains at present the only remaining dedicated device for Be-related studies.

In a few other surface analysis devices experiments with Be-containing mixed materials are still possible provided the amount of mobilizable Be remains under strict safety limits. This applies to the XPS depth profiling device SAX and the TDS device TESS. The IPP high current ion source ("HSQ"), which has been use a lot for Be-related experiments in the past, had to be shut down for Be operation I the mid of 2013. With the remaining experimental capabilities IPP will continue to collaborate with international partners on research of PSI issues for Be-mixed materials. Close collaboration exists with PISCES (UCSD, USA) and MEdC (National Institute for Laser, Plasma and Radiation Physics, MEdC, Bucharest, Romania).

Hydrogen isotopes retention and release in Be-containing mixed materials (Be, Be:W, Be:C, and Be:O) have been investigated in the period from 2012 until the shut-down of HSQ in mid 2013. The main aim was an assessment of the efficiency of the tritium removal procedure currently suggested for ITER, i.e., wall baking at 513 K (240 ºC) for the main chamber walls and 623 K (350 ºC) for the divertor. The tritium retention as well as the removal efficiency by a following baking procedure will strongly depend on the composition of deposited layer and the wall temperature during the plasma operation.

Mix-materials samples have been prepared by MEDC and been implanted with D in HSQ. D retention has been measured by ion-beam analysis and by thermal desorption spectroscopy in TESS. In addition, long term annealing experiments at ITER-relevant temperatures (240 °C and 350 °C) have been performed. A part of this work has already been published [2].

In the case that D is implanted at moderate temperatures (300 to 400 K), which would correspond to the "cool divertor" scenario in ITER, a large fraction of retained D is trapped in states having a lower D binding energy and correspondingly lower release temperatures. Therefore, in this case baking can release a significant amount of retained D. On the other hand, if D is implanted at temperatures above 520 K, which would correspond to the "hot divertor" scenario in ITER, the amount of retained D will be much lower, but the retained D is predominantly trapped in the high-energy binding states. In such a case, even baking at 623 K might not efficiently remove the retained tritium. Data analysis is ongoing. This work will be concluded and published.

[1] Stepan Krat, Yu Gasparyan, A Pisarev, I Bykov, M Mayer, G de Saint Aubin, M Balden, C Lungu, A Widdowson, JET-EFDA contributors, "Erosion at the inner wall of JET during the discharge campaign 2011-2012 in comparison to previous campaigns," submitted to Journal of Nuclear Materials.

[2] K. Sugiyama, C. Porosnicu, W. Jacob, J. Roth, Th. Dürbeck, I. Jepu, and C.P. Lungu: "Study of Deuterium Retention in/Release from ITER-relevant Be-containing Mixed Material Layers Implanted at Elevated Temperatures," Journal of Nuclear Materials, 438, S1113–S1116 (2013).

doi: 10.1016/j.jnucmat.2013.01.245

## S. Irle: Progress towards quantum chemical molecular dynamics simulations for hydrogen-beryllium interactions

In order to perform atomic-scale, long timescale simulations of hydrogen isotope H/D/T chemical sputtering on Be surfaces with non equilibrium molecular dynamics (MD), we developed corresponding Be-H parameters for the self-consistent-charge density-functional tight-binding (DFTB) method.

Electronic DFTB parameters were generated on the basis of solid state bandstructure fitting, and repulsive potentials were created using Bex and (BeH2)y molecular compounds. Two different parameter sets performed well for either molecular compounds or solid state simulations, but not for both systems simultaneously. The origin of the mutually exclusiveness of these two parameter sets is discussed, and a possible solution based on an atomic coordination-number based global scaling approach for the repulsive potential is suggested.

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

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21710
Web: http://www-nds.iaea.org