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Data for Surface Composition Dynamics Relevant to Erosion Processes

Summary Report of the Second Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

11–13 March 2009

Prepared by

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April 2009

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Abstract

Nine experts on particle surface interaction attended the second Research Coordination Meeting (RCM) on Data for Surface Composition Dynamics Relevant to Erosion Processes, held at IAEA Headquarters on 11-13 March 2009. Participants summarized progress made since the first RCM. The detailed work plan from the first RCM was reviewed, progress was noted and modifications made where appropriate. Discussions, conclusions and recommendations of the RCM are briefly described in this report.

May 2009

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1. Introduction

The second Research Coordination Meeting (RCM) dedicated to "Data for surface composition dynamics relevant to erosion processes" was held on 11-13 March 2009 at IAEA Headquarters, Vienna. This meeting acted as suitable forum to present progress reports from all participants, and to review and modify the work plan from the first RCM.

The nine participants are experts in the experimental study and theoretical modelling of surface composition dynamics. Each participant gave a detailed review of the work accomplished as part of the work plan formulated at the first RCM. Although P. Krstic was unable to attend due to health problems, a progress report had been electronically prepared and provided. The list of participants is given in Appendix 1, and the agreed agenda can be found in Appendix 2.

2. Presentations and Proceedings

A.L. Nichols (Section Head, Nuclear Data Section) welcomed the participants on behalf of the International Atomic Energy Agency (IAEA). He noted that the second research coordination meeting can be crucial to the eventual success of the CRP. The initial work plan will be reviewed, progress noted and an assessment made of the effectiveness of the project. He expressed confidence that the participants had made good progress and that results from the first phase of the CRP would indicate significant advances in our understanding of erosion processes in fusion devices. R.E.H. Clark (Scientific Secretary) reviewed the proposed agenda, which was accepted without change (see Appendix 2).

Progress Reports

During the first two days of the RCM, the participants presented progress reports on their agreed work plan items. A number of very interesting results were reported and good collaborations was seen to have developed in the course of the first phase of the project. All presentations were distributed electronically to the participants, and are available on the IAEA A+M web pages. Brief abstracts can be found in Appendix 3. The detailed work plan was reviewed on the third day, progress was noted on each item and modifications made where appropriate in consideration of research findings during the first phase.

R. Zalavutdinov of the Russian Academy of Sciences reported on studies of the erosion of a-C:H films, which can form on surfaces that are not in contact with the plasma. The main aim of this work was to study the removal of films using chemically active species formed in RF and DC glow discharges with nitrous oxide and molecular hydrogen mixtures. Both the experimental apparatus for the study of the glow discharges and the properties of these soft and hard films were described. A number of experiments have been carried out to study the erosion of these films in different discharges, including RF and DC discharges with N_2O, and DC discharges using H_2/N_2O, H_2/N_2 and H_2/air mixtures. The erosion rates of the films were measured with respect to the type of discharge. Studies were also carried out on the effect of the discharges on the substrate surfaces.

Yu. Martynenko of the Kurchatov Institute (Russia) presented recent studies on changes to tungsten and carbon surfaces under high-dose plasma exposure. The initial objective of the work was to study the composition dynamics of doped tungsten and carbon at low ion energies, and compare the effects with those from high ion energies, leading on to the quantification of such behaviour at elevated temperatures corresponding to ELMs conditions in ITER. Experiments at elevated temperatures were undertaken at the LENTA facility, with nitrogen plasma rather than deuterium because recent results from ASDEX-U show that nitrogen mitigates ELMs problems. These results were summarized and discussed - changes in surface composition and microstructure were observed. Future work will include an investigation of surface composition dynamics that involves re-deposition of tungsten and carbon undergoing joint exposure to simulate divertor conditions.

J. Davis of the University of Toronto Institute for Aerospace (Canada) discussed investigations of C^+ + D^+ on tungsten, and the evolution of mixed Be/C co-deposit layers following thermo-oxidation. Carbon impurities in fusion machines will lead to the formation of mixed material layers on non-

carbon surfaces. Experiments were performed to investigate the processes of chemical erosion and radiation enhanced sublimation (RES) in the erosion of mixed C/W layers. Chemistry was found to be a very important feature of such systems. Clear evidence of RES was not observed, with some evidence that carbon may diffuse into the tungsten. Thermo-oxidation is a possible mechanism for the removal of co-deposits, but doubts remain as to the composition of the residual layers, precisely when a layer is completely removed, and what happens when co-deposits form over residual layers. Residual layers remain on the surface following the thermo-oxidation of co-deposited layers with some impurity content. The nature of the residual layer depends on the impurities, and further studies are merited to determine the cumulative effect of forming co-deposits on top of residual layers.

K. Nordlund of the University of Helsinki (Finland) presented recent work on the interatomic potential for the Be-C-H system, and simulation of WCH erosion and BeD molecule formation. Future fusion devices such as ITER will contain mixtures of such materials that will undergo complex plasma-wall interactions and molecular processes. A molecular dynamics can only be successfully used if the correct potentials are known. A table of relevant potentials was presented - nearly all required potentials have now been determined, and the remainder should be derived soon. Background information on plasma-wall simulation was presented which exhibited reasonable agreement with experiments. Work on the Be-C-H potential was described, while equivalent studies of WCH plasma-wall interactions revealed higher C sputtering yields for C-terminated surfaces, increased sputtering yields for impurity bombardments, much smaller W erosion yields than C erosion yields, amorphization of samples and blistering.

R. Doerner of the University of California at San Diego (United States of America) discussed recent plasma-material interaction studies on PISCES. There were indications that BeD undergoes physical sputtering from targets after D irradiation - the amount of BeD can be quantified and comparisons have been made with molecular dynamics calculations. Experiments involving mixed species plasmas have been carried out in order to simulate PSI conditions in fusion devices. The current application is for D/He on tungsten, but future studies will include D/He/Ar. Nanostructure growths were reported, and mixed plasma effects differ substantially from the results of pure plasmas. The presence of He impacts significantly on the growth of tungsten fuzz, blister formation and D retention. Measurements were made for tungsten-sputtered atoms from argon bombardment - sputtering yield as a function of argon-ion energy agrees well with calculations from the widely used TRIM code. However, the angular distribution is not in good agreement, and possesses a significantly different shape.

A. Allouche of CNRS/Université de Provence (France) described quantum studies on beryllium-based materials. The first principles quantum method was described, which is appropriate for small systems in stationary states. This method has been applied to the physics of hydrogen interacting on a substrate of beryllium. The calculated barrier to desorption agrees well with TDS results on Be (0001) and in constrained sites within the bulk. Two models were considered for H retention in the bulk, and variable and fixed cells. Variable cell calculations were carried out for dissolution energy, and gave two minima. Calculations for bulk modulus are in very good agreement with experimental observations, indicating that beryllium hydride can exist in different forms from amorphous to crystalline dihydride and the formation energies are comparable. Studies were undertaken on Be/W with the aim of deriving a quantum description of the first steps of Be/W alloying starting from surface reactions. Potential energy surfaces were constructed and density of states determined. A tungsten film on beryllium leads to alloy formation, while a beryllium film on tungsten leads to the formation of beryllium clusters.

D. Kato of the National Institute for Fusion Science (Japan) presented studies on hydrogen trapping and erosion of crystalline tungsten. Multiple trapping of hydrogen by mono-vacancies in crystalline tungsten has been observed by Myers. Calculations have been carried out with the VASP code which show a mono-vacancy in a tungsten crystal can trap multiple hydrogen atoms with appreciable binding energies. The stability of VH complexes in W can be described in terms of covalent bonding via hybridization of the H-1s and W-5d orbitals. An equilibrium thermo-statistic model gives enhanced vacancy concentration (hydrogen trap) in an eroded W crystal under hydrogen-rich conditions. Studies have ben carried out of D retention in Mo induce by high-flux low-energy ion implantation. The present model does not conflict with a speculative suggestion from DIONISOS experiments that new hydrogen traps may be created by super-saturated low-energy hydrogen implantation. Large

uncertainties in the transport coefficients of low-hydrogen solutions may be ascribed to the different abundances of natural traps inherent in low-solubility materials. At elevated levels of hydrogen, the vacancy concentration could strongly depend on the hydrogen concentration. Work undertaken by the group headed by Ohya was also described, and involves theory and code development for the evaluation of tritium retention and exhaust in fusion reactors.

K. Krieger of the Institut für Plasmaphysik, Garching (Germany) reported on studies of mixed-material surface dynamics. The dual beam experiment at the IPP was described, along with modelling calculations carried out with the TRIDYN code. Two regimes were observed in the co-bombardment of tungsten by deuterium and carbon which depended on the carbon concentration, and the growth of the carbon film or continuous erosion. Within the continuous tungsten erosion regime, the chemical erosion of W-C was greatest at room temperature, and decreased with increasing temperature. Over the carbon deposition regime, the chemical contribution is negligible until the build-up of carbon occurs, which then follows pure C behaviour. Roughness effects were also studied: a sample was prepared with parallel ridges in a silicon layer and bombarded with argon, and the resulting erosion rates were found to be in good agreement with SDTrimSP-2D calculations. Investigation was made on the surface processes of the Be/C/W materials of ITER. The influence of mixed material layers on fuel retention and permeation properties were also investigated.

Guang-Nan Luo of the Chinese Academy of Sciences described studies on tungsten of relevance to the EAST project, involving wall interactions with high flux plasmas. The importance of tungsten in many existing and planned fusion devices was emphasized. EAST will use a tungsten/copper divertor, which has lead to increased research on the properties of tungsten. Testing on the EAST device is at an early stage, and collaborative studies of tungsten are being carried out at JAEA and PISCES. Simulators for tokamak edge plasmas are under continuous development, and retention analyses are ongoing. Experiments are underway on plasma-wall interactions, particularly focusing on effects due to particle energy, fluence, temperature, material grade and surface effects (such as scratching). Studies will continue.

D. Humbert of the IAEA presented work on a new interface to particle surface interaction (PSI) data. PSI is much more complex than atomic data, and a number of difficulties had to be resolved in the construction of the interface. The organization of data within the database was defined, and the new interface was demonstrated. Discussions focused on methods to describe surfaces and processes accurately. The development of an XML schema for atomic, molecular and solid material data (XSAMS) was described - the interface can generate XML files on the basis of this schema.

3. Review and Modification of Work Plan

Following the presentations of the various relevant research activities, participants discussed and reviewed the list of data requirements formulated at the first RCM. Progress on each item is noted in italics.

- Phase diagram for the BeC system: *no CRP member is able to provide this information.*
- Understand the behaviour of WC under irradiation: does this material amorphise? what are the damage levels? *work is ongoing; bombardment of carbon by tungsten is also of interest (Davis to check previous results).*
- Ratios of sputtering yields of atomic Be to molecular BeD from deuterium saturated Be surface: *work is nearly complete, with further comparisons between experiments (Doerner) and MD calculations (Nordlund) to be carried out.*
- Both physical and chemical differential sputtering yields from Be_2C surfaces: *essentially completed (UCSD).*
- D-retention level in pre-damaged W: *work on cyclotron-induced damage followed by D-plasma exposure (Kurchatov) is in progress, as well as an investigation of high-energy ion-beam-induced damage (IPP Garching) and fission-neutron-induced damage (Oak Ridge National Laboratory/Idaho National Laboratory).*
- He bubble growth rates as a function of temperature in W: *work is ongoing (Toronto, UCSD, Oak Ridge National Laboratory).*

- Formation and migration energies of VH (D,T) clusters in W, Be, and W/Be/C compound materials: *work is ongoing (IPP Garching, Marseille, Helsinki, Oak Ridge National Laboratory).*
- Diffusion coefficients of hydrogen in W/Be/C compound materials, e.g. $Be_{12}W$: *work is ongoing (IPP Garching, Marseille, Helsinki).*
- Self-diffusion coefficients of W, Be, C for pure materials, materials with voids and mixtures of such materials: *work is ongoing on both modelling and experiment (IPP Garching, Marseille, Helsinki, Kyushu, Kyoto).*
- Oxidation of JET tiles (mixed Be C) at temperatures below 350ºC: *almost completed, with some questions remaining about residual layers (Toronto).*
- *Removal of Be/mixed co-deposited layers on tungsten and removal of hydrogen from such layers: identified as a new data need (UCSD, IPP (?), Toronto (?)).*
- H measurements of retention and erosion products for C^+ and D^+ implantation during simultaneous irradiation of W at elevated temperatures by means of a dual beam accelerator and LOS detection: *work is ongoing (Toronto).*
- D^+ irradiation of WC at elevated temperatures in terms of D retention and erosion products for both bulk material and films: *work is ongoing (Alimov (with IPP), Toronto).*
- MD model to assist in the interpretation of D retention in W during combined He, D irradiation: *work ongoing on theory (Helsinki, Oak Ridge National Laboratory) as well as experiments (Toronto, IPP, UCSD).*
- Measurements of reflection, sputtering, sticking, implantation and deposition of dynamically-hydrogenated (deuterated) carbon surfaces over the energy range 1 eV to 1 keV, with angular and energy distributed impacts of hydrogen, inert gases, carbon and hydrocarbons, and information on the final state (sputtered, reflected) spectra (angular, energy, rovibrational): *substantial progress has been made, work is ongoing (Oak Ridge National Laboratory).*
- Sound inter-potentials for H, C, W and Be for MD simulations: *essentially completed (Helsinki).*
- MD calculations to gain insight into the preparation of surfaces (D + C and He + C on W), and assessment of the applicability of the BCA model: *work is ongoing (Helsinki, Tokushima).*
- Quantification of erosion products during simultaneous bombardment of W with D + C and He + C: *work is ongoing (Toronto).*
- Experimental data on absorption, adsorption and retention of H and D by Be and mixed materials for comparison with theory: *work is ongoing for both modelling and experiment (Marseille, IPP, UCSD, Moscow (Alimov)).*
- *ab initio* MD calculations on very large computer systems for the above processes involving Be and W: *substantial progress has been made, and work is ongoing (Helsinki).*
- Surface loss probabilities and sticking for different hydrocarbons on various pure and mixed surfaces: *Work is ongoing (IPP, IPCE, IPC-Prague).*
- Integrated modelling of retention in all materials, including mixed systems: *work is ongoing at many locations.*
- *High fluence retention measurements in ITER PFCs: identified as a new data need - work is ongoing at many locations.*

After a review of the list of pressing data needs, each participant summarized progress on their specific work plans from the first RCM, and indicated any additional tasks to be undertaken in the next period of the CRP. Progress and new tasks are indicated by italics.

Nordlund:

- Complete a working set of BeCWH potentials: *substantial progress has been made, and the potentials will be finalized during the next work period.*
- Simulate W and WC formation and erosion under the co-bombardment of H + He/Ne/Ar/C/W, and compare with beam and plasma experiments to be performed at the University of Toronto and IPP: *work is ongoing.*

- Simulate formation of BeD molecules during D bombardment of Be in collaboration with Doerner: *completed.*
- *Comparison of interatomic potential energetics of H in Be with DFT calculations of Allouche.*
- *Study of angular dependence of W sputtering by low-E Ar, to be compared with experiments of Doerner.*
- *Study of erosion and formation of BeC mixed systems under H and plasma impurity bombardment, to be compared with experiments by other CRP partners.*

Doerner:
- Measure Be/BeD erosion rates for comparisons with the simulations of Nordlund: *essentially complete.*
- Carry out Be seeding and simultaneous CD_4 injection to create different compositions of Be/C surface, and correlate with the erosion behaviour of the surface: *work is ongoing, but difficulties have been encountered in determining the C content of the plasma.*
- Investigate the influence of Ar added to a Be-seeded plasma to measure the effect on Be_2C surface formation and sputtering behaviour: *essentially complete - Ar has virtually no effect on chemical erosion suppression.*
- Carry out specific experiments to compare total H retention in pure Be and Be/C and Be/W mixtures with simulation results of Allouche: *work is ongoing – studies with pure Be have been completed, while mixed materials remain to be finished.*
- *Removal of Be/mixed co-deposited layers on tungsten, and removal of hydrogen from such layers: ongoing work.*
- *He bubble growth rates as a function of temperature in W: work is ongoing.*
- *High fluence irradiation on different W grades in collaboration with EAST.*

Kato:
- Perform DFT and MD calculations of atomic structure and energies for VH (D, T) clusters in fusion reactor materials (W, Be and W/Be) to obtain cavity nucleation energy surfaces in (NH/D/T, NV) coordinates: *work is ongoing.*
- Carry out simulation of cavity nucleation and growth in the (NH/D/T, NV) coordinates in order to evaluate size-density distribution and hydrogen retention by the cavities for W, Be and W/Be – completion is dependent on the evolution of the proposed research and success of collaborations: *work is ongoing, with the focus on W, and Be studies will be carried out in collaboration with Marseille.*
- Experimental measurements of cavity size distribution and thermal desorption spectrum in collaboration with Japan and IPP (who initiated activities in this area): *facility for this research is no longer available for the continuation of agreed task.*
- *Calculations of transport coefficients of H, D, T in W with vacancies: collaboration with experimental input underway at Kyushu and Kyoto.*

Martynenko:
- Measure erosion and surface changes for C, W and perhaps WC under off-normal processes (disruption and ELM): *new focus of this task is on steady-state measurements.*
- Measure erosion of materials after changes induced by very high fluences: *shift in priority from first work plan - measurements will take place at the LENTA facility.*
- *Re-deposition of W and C as a function of dose temperature and ion energy.*

Haasz/Davis:
- Continue experiments on the oxidation of DIII-D and JET specimens for co-deposition removal: *essentially complete, with some surface analyses to be carried out in collaboration with VTT-Finland and JET.*
- Study cyclical oxidation and deposition of layers with impurities to determine the effect of repeated oxidation/co-deposition on the amount of D build-up in the co-deposited layers: *facility for this task under construction.*

- Perform W irradiation with simultaneous C^+-D^+, and study D retention as well as release of hydrocarbons in collaboration with IPP: *work is ongoing – LOS measurements are in progress, and initial studies indicate that the chemical reactions produce hydrocarbons; RES is also under investigation.*
- Perform D-retention studies in WC as a function of temperature, varying beam fluxes and energies, and use TDS to measure D retention: *work is ongoing.*
- *He blister formation on W; and also mixed D + He bombardment of W.*

Krstic - computer simulation:

- Investigate isotopic effects of the impact of hydrogen atoms and molecules on amorphous, hydrogenated carbons surfaces at impact energies from 1 to 30 eV, and note threshold effects: *completed - surface chemistry exhibits only a weak dependence on the mass, and sputtering yields exhibit a clear mass dependence which originates in the increased energy transfer for increasing projectile mass.*
- Simulate the effects of surface preparation, including pre-plasma exposure conditions and temperature, on sputtering and reflection yields and spectra of sputtered/reflected molecules (angular, energy, rovibrational): *essentially completed, showing significantly higher reflection and lower erosion when irradiated with a plasma possessing more randomized impact angles and energies than with a normal beam of the same particles at average plasma energy - further analyses remain to be done on the rovibrational and angular distributions of the sputtered particles.*
- Improve the hydrocarbon potentials (REBO/AIREBO) at higher energies (for example, the Ziegler-Biersack-Littmark (ZBL) potential), and the reactive barriers for complex hydrocarbons (for example, CD_3-D): *essentially completed, but more testing and comparison with experiments required for both reflection coefficients and sputtering yields.*
- *Chemical sputtering MD simulations of carbon, with improved hydrocarbon potentials and at elevated carbon temperatures.*
- Better quantification of the interatomic potentials for C-W-Be-H in collaboration with Allouche, Nordlund and Stuart: *work is ongoing.*
- Study the low-energy processes of co-deposited mixed material surfaces (C-W-Be-H), the impact of hydrogen isotopes, and isotopic and temperature effects; benchmark the results with appropriate experiments for the total and spectral yields for H isotopes, in collaboration with Haasz, Krieger, Doerner and ORNL: *work is ongoing.*
- *Particular attention will be paid to the study of tungsten at elevated temperatures of interest for DEMO (are "fuzz" nanostructures and blistering related to the H-retention? and the synergy of He and H retention) - particular attention will be paid to the development of the relevant interatomic potentials.*
- *Simulations of the PSI processes at the neutron-irradiation damaged surfaces.*

ORNL experiments - Meyer:

- Develop a time-of-flight technique for direct line-of-sight detection of sputtered species to study energy distributions of the products, and obtain insight into radical vs. stable hydrocarbon emission: *work is ongoing.*
- Perform erosion measurements on thin hydrocarbon films provided by IPP: *essentially completed.*
- Determine the D/C ratio of the surfaces using SIMS and residual gas analysis: *analyzing the transient response of beam-prepared graphite surfaces, and determining kinetic ejection cross sections for various hydrocarbon species.*
- Carry out Raman and Auger diagnostics of the surfaces (for example, measurements of sp^2/sp^3): *mostly completed - measurements of sp^2/sp^3 will have to await availability of a UV Raman system.*
- Initiate measurements related to chemical sputtering and reflection on metal W-, Ti- and V-doped C films obtained from IPP-Garching: *work is ongoing.*
- Investigate the effects of doping at impact energies of relevance to ITER, along with the influence on molecular size and isotope effects: *work is ongoing.*

- *Use the TOF technique to make chemical sputtering measurements at elevated graphite temperatures.*

Krieger:

- Perform measurements of erosion, implantation and D retention of D + C on W, He + C on W at room and elevated temperatures, in collaboration with the University of Toronto: *essentially completed - studies on D + ^{13}C on ^{12}C from the original work plan have been rated as low priority.*
- *^{3}He + D co-bombardment on W; influence of He on D retention; use of ^{3}He to allow NRA analysis of both species: dual beam facility being upgraded to decelerate beams.*
- Develop a model system of 2-D surface roughness (Si ridges on Si): *substantial progress has been made and work is ongoing, including the additional study of angular dependence.*
- Measure D-retention in tungsten plasma-facing components of ASDEX upgrade: *largely completed.*
- *Measuring D retention in W of different types, and with different pre-damage; characterization of damage sites: ongoing collaboration with EAST.*
- Measure D-retention in deposited layers (NRA and TDS): *largely completed with regard to the ASDEX-U tiles, and is ongoing for JET and PISCES; work is also planned for EAST.*
- Perform experiments on surface chemistry (characterization of chemical binding states) and D retention in W/Be, W/C, Be/C and W/Be/C mixtures, providing benchmark data for the computational models of Allouche: *experiments on binary materials are largely completed, and work is ongoing on the other tasks.*
- *Modelling material mixing at plasma-facing surfaces of tokamaks (JET) to provide benchmarking and predictions for ITER.*

Allouche:

- Calculate reaction energy, reaction barrier and optimized geometric structure of mixed material (Be/W) by means of the adiabatic approach of the quantum chemistry methods: *essentially completed.*
- Use these results to calculate H absorption and adsorption energies, and the optimized structures for H interaction with pure Be and BeW alloys: *work for pure Be has been completed, and is ongoing for BeW.*
- Molecular dynamics:
    - obtain bond-order atomic potentials from quantum DFT and *ab initio* approaches: *essentially completed, but there is the possibility of further studies in collaboration with Nordlund.*
    - carry out quantum and/or molecular dynamics simulations of the Be/W/H interaction: *work is ongoing.*
- *Diffusion of vacancies in pure Be, and the reactivity of vacancies in pure Be: in collaboration with IPP.*
- *Reactivity of BeO surface layer: in collaboration with IPP.*

Zalavutdinov:

- Measure erosion rates of soft and hard a-C:H films interacting with nitrous oxide glow and afterglow discharges in laboratory plasmas at different temperatures (soft and hard a-C:H films will be deposited on Si and Mo substrates): *completed.*
- Measure erosion rates of soft and hard a-C:H films interacting with hydrogen-admixture glow and afterglow discharge in laboratory plasmas at different temperatures in which the admixtures are N_2, N_2O and air: *substantial progress has been made concerning N_2O, and work is ongoing for N_2 and air.*
- Measure the evolution of the surface composition of Mo during the removal of a-C:H films: *work is ongoing, and will also be considered for W substrates.*

Luo:

- *Achieve W coatings with impurity content < 1 at.% and porosity < 10% on Cu alloy substrate by means of vacuum plasma spraying technique, and finish necessary R & D for manufacturing W/Cu components for use on EAST in near future.*
- *Carry out studies on the behaviour of W coatings exposed to tokamak- and laboratory-based H and He plasmas compared with other material grades - in collaboration with UCSD, GA, SNL and IPP (for exposures and subsequent analyses).*
- *Continuing efforts on MD simulations on H/He/C-W interactions in collaboration with Nordlund and Japanese researchers (Ohya) based on potential upgrade, simulation method and data analysis/comparison.*
- *Help establish linear plasma devices for PWI studies and improve data analyses of NRA in Chinese universities and institutes that show increased interest in fusion materials - in collaboration with UCSD and IPP.*

4. Recommendations and Conclusions

All participants presented progress reports detailing active research on the data needs identified at the first research coordination meeting. A significant number of fruitful collaborations have emerged, and impressive progress has been made on all items of the original work plan. Modifications have been made to this work plan on the basis of the studies undertaken and the progress achieved in addressing the agreed data needs. Very good cooperation between theoretical and experimental researchers has also been achieved.

A large amount of new data has been generated from the research conducted during the course of the ongoing CRP. These data will be incorporated into the ALADDIN database of the IAEA A+M Data Unit. Since the coordinated research project is well on the way to fulfilling the goals as set forth in the original proposal, a successful conclusion to the CRP can be anticipated in 2011.

Appendix 1

IAEA second Research Coordination Meeting on Data for Surface Composition Dynamics Relevant to Erosion Processes

11–13 March 2009, IAEA Headquarters, Vienna, Austria

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Appendix 2

IAEA second Research Coordination Meeting on Data for Surface Composition Dynamics Relevant to Erosion Processes

11–13 March 2009, IAEA Headquarters, Vienna, Austria

Agenda

Wednesday, 11 March **Meeting Room: A-07-42**

09:30 – 10:00 Opening, Adoption of Agenda, A. Nichols, R. Clark

Session 1: Reports I

Chairman: K. Nordlund

10:00 – 10:45 R. Zalavutdinov
Erosion of a-C:H Films under Interaction with N_2O and H_2/N_2O (N_2, air) Mixture Glow and Afterglow Discharge

10:45 – 11:15 *Coffee break*

11:15 – 12:00 Yu. Martynenko
Tungsten and Carbon Surface Change under High Dose Plasma Exposure

12:00 – 14:00 *Lunch*

Session 2: Reports II

Chairman: R. Zalavutdinov

14:00 – 14:45 J. Davis

1. Investigation of the C+ + D+ => W System
2. Evolution of Mixed Be/C Codeposit Layers following Thermo-oxidation

14:45 – 15:30 K. Nordlund

Interatomic Potential for the Be-C-H System and Simulation of BeD Molecule Formation

15:30 – 16:00 *Coffee break*

16:00 – 16:45 R. Doerner
Mixed Plasma Species Bombardment of Tungsten

Thursday, 12 March

Session 3: Reports III

Chairman D. Kato

09:30 – 10:15 A. Allouche
Quantum Studies on Beryllium-based Materials

10:15 – 10:45 *Coffee break*

10:45 – 11:30 D. Kato
Hydrogen Trapping and Erosion of W Crystal

11:30 – 12:15 K. Krieger
Overview on Studies of Mixed-material Surface Dynamics at IPP Garching

12:15 – 14:00 *Lunch*

Session 4: Reports IV

Chairman: R. Doerner

14:00 – 14:45 Guangnan Luo
Tungsten Project for EAST and Related PWI Studies with Exposure to High Flux Plasmas

14:45 – 15:15 *Coffee break*

15:15 – 16:00 D. Humbert
New ALADDIN Web Interface for Particle Surface Interactions: Data Structure and Data Exchange Issues

Friday, 13 March

Session 5: Review of Progress

Chairman: K. Krieger

09:00 – 12:30 All
Comprehensive Review and Summary of Progress Made

12:30 – 14:00 *Lunch*

Session 6: Update of Work Plan for CRP

Chairman: J. Davis

14:00 – 17:00 All
Update of Work Plan for CRP

17:00 – Adjourn

Appendix 3

IAEA second Research Coordination Meeting on Data for Surface Composition Dynamics Relevant to Erosion Processes

11–13 March 2009, IAEA Headquarters, Vienna, Austria

Abstracts of Presentations

Erosion of a-C:H Films Under Interaction with N_2O and H_2/N_2O (N_2, Air) Mixture Glow and Afterglow Discharge

R.Kh. Zalavutdinov, A.E. Gorodetsky, V.L. Bukhovets and A.P. Zakharov

A.N.Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Moscow, Russia

Soft and hard a-C:H films have been deposited by means of RF and DC discharge, respectively, on Si and Mo substrates at 300 K. In soft and hard a-C:H film removal experiments a stream technique has been used in which N_2O or H_2/N_2O (N_2, air) mixture moved through a cylindrical quartz tube in laminar flow with controlled inlet rate. The erosion of the films in RF and DC glow and afterglow discharge has been studied by weighing, electron probe microanalysis (EPMA) and in-situ a quadrupole mass-spectrometer (MS).

Soft film erosion experiments in N_2O RF discharge have shown that in afterglow regions the erosion rates were 16×10^{-3}, 6×10^{-3} and 3×10^{-3} nm/s at distances from plasma of 3, 11 and 17 cm, respectively. In the plasma the erosion rate, *G*, was about 2 nm/s (0.2 μg/cm^{2}s). *G* of the films was proportional to the film mass, i.e. the whole film volume was involved in oxidation.

For the hard films it was found that in N_2O DC afterglow region (11 cm from plasma) *G* increased linearly with increasing N_2O pressure (up to 24 Pa) in the temperature range 300-500 K. The H_2, H_2O, CO, and CO_2 molecules were recorded by MS. If the a-C:H film was heated in N_2O without discharge (24 Pa, 500 K) *G* was lower than 3×10^{-3} nm/s.

After film removal the oxygen content in Mo surface layers was less than 3×10^{16} at.O/cm^2 (afterglow region). The oxide thickness depended on the sample location and decreased from the cathode, through the positive column to the afterglow region. The relatively low oxide film thickness on Mo which was in contact with oxygen atoms may be explained by enhanced recombination of oxygen atoms on the metal oxide surface.

The measurements have shown that in the afterglow region *G* did not practically depend on the N_2O content in H_2 under N_2O partial pressure changing from 3 to 7 Pa and H_2 partial pressure of 40 Pa. *G* increased noticeably (from 0.02 to 0.45 nm/min) with the temperature (up to 650 K). In such medium activated by the DC glow discharge the main erosion film products were CO and CO_2.

During interaction of a-C:H films with hydrogen admixture (N_2 or air) glow discharge the cyanic acid (HCN) and ammonia (NH_3) have been found in plasmolysis products.

Tungsten and Carbon Surface Change Under High Dose Plasma Exposure

Yu.V. Martynenko, B.I. Khripunov and V.B. Petrov

Nuclear Fusion Institute, RRC "Kurchatov Institute", Moscow, Russia

Study of surface composition dynamics has been made on the LENTA linear plasma simulator. Experiments have been made on tungsten and carbon materials subjected to steady-state plasma exposure. The achieved ion doses on the surface were 10^{21} ion cm^{-2}. WL 10 tungsten containing 1% of La2O3 oxide and titanium-doped graphite RG-T were studied. The following experimental conditions were varied in these experiments: energy of ions, surface temperature, working gas. Irradiations of tungsten WL 10 were executed in deuterium plasma at low ion energies (about 20 eV) and at 200 eV for temperatures below 340 K. Graphite RG-T was exposed at 1300 K. Elevated surface temperature (about 1050K) was also characteristic of experiments on tungsten sample under nitrogen plasma impact (simulated inter-ELMs condition). Surface microstructure modification has been observed and surface composition changes were found on the materials showing influence of high dose plasma irradiations on element redistribution in the near surface layers.

1) Investigation of the $C^+ + D^+ \rightarrow W$ System
2) Evolution of Mixed Be/C Co-deposit Layers Following Thermo-oxidation

J. Davis

University of Toronto Institute for Aerospace, Canada

Measurements of chemical erosion have been made for the $C^+ + D^+ \rightarrow W$ system, showing that even under conditions where the C+ fraction in the incident flux is much smaller than that required to build up a carbon surface layer, the production of hydrocarbons still occurs. We do not, however, see convincing evidence of radiation enhanced sublimation (RES) under similar bombardment conditions with the specimen at higher temperature. The present hypothesis is that there is diffusion of carbon into the bulk so that there is insufficient carbon in the near-surface to support RES.

Codeposits from the JET tokamak containing Be/C ratios as high as 1 were tested in our thermo-oxidation facility. While the majority of the D was removed in all cases, the amount of the C/Be deposit removed appears to be dependent on the Be content of the deposit. For nearly pure C deposits, thermo-oxidation completely removes the deposits. For deposits with Be/C ~ 1, the deposit thickness after oxidation was similar to that measured prior to oxidation.

Interatomic Potential for the Be-C-H System and Simulation of BeD Molecule Formation

K. Nordlund

University of Helsinki, Finland

Central features of our potential developed for the Be-C-H system will be presented, and in particular will show that the potential correctly describes the stability of the Be_2C phase. Simulation of results of the plasma-wall interactions of H with WC and Be-based materials will be presented. The results describe phase changes in WC, blistering, and show that a significant fraction of low-energy plasma bombarded Be erodes in the form of BeD molecules, in agreement with the experiments of Doerner et al.

Mixed Plasma Species Bombardment of Tungsten

R. Doerner

University of California, San Diego, USA

The effects of mixing He with D plasma on the blister formation and D retention in W at low energy (~55±15 eV), high flux (~10^{22} $m^{-2}s^{-1}$), high fluence (≤ $4.5x10^{26}$ m^{-2}), and moderate temperature (~573 K) conditions in the linear divertor plasma simulator PISCES-A will be described. The amount of D retained in W (measured with a high resolution thermal desorption spectroscopy (TDS) system capable of distinguishing between D_2 and He) exposed to D+He mixture plasmas is found to significantly decrease compared to W exposed to pure D plasmas. Scanning electron microscopy (SEM) observations reveal the suppression of the blister formation in D+He mixture plasma exposure. W samples exposed to D only plasma are observed to form surface blisters whose size and surface density roughly correlate with the amount of D retention in the samples. These beneficial effects during mixed D+He plasma exposure are caused by nano-sized high density He bubbles created in the near-surface region of the tungsten, observed with a transmission electron microscope (TEM), acting as a diffusion barrier to D atoms.

Quantum Studies on Beryllium-based Materials

A. Allouche

CNRS / Universite de Provence, Marseille, France

Simulations and Measurements of Low-energy Particle-surface Interactions for Fusion

P.S. Krstic and F.W. Meyer

Oak Ridge National Laboratory, USA

We simulated the effects of plasma irradiation of carbon surfaces by randomization of the dynamic parameters of the impact particles in classical molecular dynamics. The surface irradiation was carried out until steady state conditions were achieved. Sputtering and reflection yields were then determined, allowing studies of the synergistic effects of various impact energies and angles. Varying hydrogen isotopes projectiles in the range 1-30 eV/nucleon we showed that the chemistry at the interface is not too sensitive to the mass of the impinging atoms, however the sputtering yields increased considerably for increasing projectile mass, presumably due to the larger energy transfer per collision. We also improved the REBO/AIREBO potentials to higher impact energies and complex hydrocarbons and developed a procedure for the development of MD potentials for mixed materials.

The total chemical sputtering yields were measured by quadrupole mass spectrometry for low energy atomic and molecular deuterium ions incident on a-C:D thin films, ATJ graphite, and HOPG. The results show excellent agreement with preliminary ellipsometry measurements of crater volumes produced in beam-exposed a-C:D thin films (collaboration with IPP Garching). Kinetic ejection and detrapping cross sections were measured for ion-beam-induced release of deuterium and hydrocarbon species from beam-prepared a-C:D thin films and ATJ graphite surfaces for incident low energy atomic and molecular D ions. In addition, measurements were attempted of D_2 and hydrocarbon concentrations in beam-prepared graphite samples, using transient analysis. Finally, SEM and Auger and Raman spectroscopic analyses of beam exposed graphite surfaces were performed.

Hydrogen Trapping and Erosion of W Crystal

D. Kato

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It is known that lattice displacements in the bulk by high-energy ion impact can become traps. Radiation damage by the high-energy ion irradiation would therefore generally enhance the hydrogen retention in the bulk. However, it has also been reported [1] that after low-energy deuteron irradiation of higher flux, level of retained D/W concentration in molybdenum was orders of magnitudes higher than one would expect from inherent or 'natural' traps in the bulk. It becomes an issue of study to investigate mechanisms of new trap creation during high-flux and low-energy ion implantation.

Tungsten as well as molybdenum has very low natural hydrogen solubility in the bulk crystal, because of its high heat of solution. However, it has been pointed out [2] that significantly lower heat of solution would be obtained by taking account of vacancy-hydrogen cluster formation; vacancy-hydrogen attractive interaction would reduce formation energies of the vacancies dressed with multiple hydrogen atoms. In this context, it may be noteworthy that several interesting phenomena observed under hydrogen-rich conditions have been explained by the superabundant vacancy formation induced by hydrogen, e.g. large volume contraction of some metals [3, 4], enhancement of inter-diffusion at the junction of two metals [5], etc. Thus, it is intriguing to investigate enhancement of the vacancy abundance by the vacancy-hydrogen cluster formation in non-occluder metals like tungsten.

Summary of my talk would be as follows:

- Mono-vacancy in W can trap multiple hydrogen atoms with appreciable binding energies. (first-principle calculations).
- Variation of binding energies along number of trapped hydrogen atoms are described in terms of zero-point vibration and symmetry of super cells.
- Stability of VH clusters in W is described in terms of covalent bonding via hybridization of H-1s and W-5d orbital.
- Equilibrium thermo-static model can describe enhanced vacancy (hydrogen trap) concentration in an eroded W crystal under hydrogen-rich conditions.
- In natural hydrogen solution, large uncertainties in transport coefficients may be ascribed to different abundance of natural traps inherent in low-solubility materials. However, in the present work we showed that at elevated hydrogen concentrations, the vacancy concentration itself could depend on the hydrogen concentration strongly.

References

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[2] Y. Fukai, Y. Kurokawa and H. Hiraoka, J. Japan Inst. Metals **61(8)**, 663 (1997).
[3] Y. Fukai and N. Okuma, Japan J. Appl. Phys. Part 2 **32**, L1256 (1993).
[4] M. Iwamoto and Y. Fukai, Mater. Trans. JIM **40**, 606 (1999).
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Overview on Studies of Mixed-material Surface Dynamics at IPP Garching

K. Krieger

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Processes of mixed-material surface evolution and corresponding material properties are investigated at several experiments at IPP Garching. The following topics will be presented and discussed:

1. Studies on co-bombardment of tungsten by D and C. Co-bombardment of tungsten by D and C leads to synergistic effects, which result in two principal dynamic regimes. One regime is characterised by continuous erosion of the tungsten surface while in the second regime one observes continuous growth of a carbon layer on the tungsten substrate. The processes involved and their influence on the boundary between these regimes will be discussed.

2. Surface processes in the formation of layers with binary and ternary ITER relevant material combinations (Be/C/W). Migration and redeposition of wall materials in fusion machines leads to formation of mixed material surface layers. At elevated temperatures carbides and/or metal alloys will form, which have a significant influence on erosion properties and fuel isotope retention. The principal processes have been identified and discussed.

3. Formation of mixed-material layers leads to significant modifications of fuel retention and fuel isotope permeation properties of the substrate materials. Results of corresponding studies for the ITER-relevant material combinations will be presented and discussed.

Tungsten Project for EAST and Related PWI Studies with Exposure to High Flux Plasmas

Guang-Nan Luo

Chinese Academy of Sciences; Institute of Plasma Physics, Hefei, China

The plasma-facing surfaces in EAST have been covered by SiC-coated C tiles bolting to heat sink since summer of 2008. With increasing the heating and driving power to the plasma in the near future, a comprehensive project of tungsten plasma-facing materials (PFM) and components (PFC) is to be launched soon. As well as engineering issues, e.g., preparation of the PFM, design of the PFC structure, and testing as PFC using high heat flux facilities and in tokamaks, the issues on plasma-wall interactions (PWI) are also being addressed in laboratory and tokamak experiments and computer simulations, like surface and bulk modification and retention of H isotopes in different tungsten materials, including polycrystalline, re-crystallized tungsten, and thick tungsten coatings prepared by vacuum plasma spraying.

New ALADDIN Web Interface for Particle Surface Interactions: Data Structure and Data Exchange Issues

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The interface for access to the PSI data has recently been upgraded to version 3.2, which is similar to the interface to the A+M collisional data. This test version is available on line at http://www-amdis.iaea.org/AL1. Searches are performed efficiently using combinations of search criteria. A filtering function allows the user to quickly find specific data from the large number of entries in the database. All requested data are displayed in the same units to the extent possible, to permit easy comparison. A unit conversion tool is available and all results can be displayed in tabular and graphical mode.

Specifications for the web interface were presented and reviewed during the last RCM. Issued recommendations on the process classification, data quantities and data structure were carefully addressed in the new ALADDIN version. Nevertheless during implementation of version 3.2 and migration of former PSI ALADDIN data, some difficulties arose.

After a short demonstration of the new interface, data structure problems and some unresolved issues will be presented.

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