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Data for Surface Composition Dynamics Relevant to Erosion Processes

Summary Report of the first Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

17 – 19 October 2007

Prepared by

R.E.H. Clark

February 2008

IAEA Nuclear Data Section, Wagramer Strasse 5, A-1400 Vienna, Austria

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Abstract

Nine experts on particle surface interaction attended the first Research Coordination Meeting (RCM) on Data for Surface Composition Dynamics Relevant to Erosion Processes, held at IAEA Headquarters on 17-19 October 2007. Participants summarized recent relevant developments related to fusion applications. Specific objectives for the CRP and a detailed work plan were formulated. Discussions, conclusions and recommendations of the RCM are briefly described in this report.

February 2008

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Introduction

The first Research Coordination Meeting (RCM) dedicated to “Data for surface composition dynamics relevant to erosion processes” was held on 17-19 October 2007 at IAEA Headquarters, Vienna. The main aims of this RCM were to review the relevant research activities of the participants, identify data needs for erosion processes, and formulate and agree an appropriate work plan for the initial phase of the Coordinated Research Project (CRP).

All nine participants are experts in the experimental study and theoretical modelling of surface composition dynamics. The list of participants is given in Appendix A. Each participant presented a summary of their on-going research activities and areas of expertise. A detailed work plan was subsequently formulated after detailed discussions of the fusion needs for atomic data describing and quantifying erosion processes induced by plasma-surface interactions.

Meeting Proceedings

A. Nichols (Section Head, Nuclear Data Section) welcomed the participants on behalf of the International Atomic Energy Agency (IAEA). Demands for good quality atomic and molecular data for fusion have significantly increased following the official establishment of the ITER project on a multinational basis. He expressed confidence that the participants would together contribute substantial new knowledge and data inputs to quantify plasma-surface interactions that induce erosion. R. Clark (Scientific Secretary) reviewed the proposed agenda, which was accepted without change (see Appendix B).

Current Research Activities

During the first two days of the RCM, the participants presented their current research activities of relevance to the quantification of surface dynamics. There was a good balance between experiment and theory in these presentations. A number of potential collaborations on specific topics were identified during the course of the subsequent discussions. All presentations were distributed electronically to the participants.

R. Doerner presented recent studies of material erosion, including the use of the PISCES-B facility to handle Be in isolation. Erosion suppression of C in a Be-seeded plasma has been observed, and this behaviour is poorly modelled by the ERO-TRIDYN code. We need to understand the dynamic formation of Be/C and Be/W surfaces created during the Be seeding of plasmas, and correlate surface composition changes to erosion behaviour. He discussed the importance of defining the precise nature of chemical bonding in plasma-created mixed material surfaces, and the need to measure erosion rates from H/D-saturated metallic surfaces. Surface morphology after high-fluence plasma exposure was discussed (for example, as a consequence of He bombardment on W surfaces). Dierner also noted the need to consider the implications of Be-W alloying for ITER.

A. Allouche described molecular dynamic (MD) studies of Be-W mixed materials. The goals of this work are to understand the first step of Be/W mixed materials formation at the highest *ab initio* level of quantum theory (including energies, barrier and structures), and derive from these data MD simulations that approximate the quantum description. He noted the close tie to experiments, particularly to the Be plasma-seeded experiments on tungsten surfaces in PISCES-B (Doerner and coworkers) and W (/Be) deposition on Be(/W) (Linsmeier *et al.*). Quantum methods are used in the calculations, and a brief description of molecular dynamics was given. Recent work has included W on Be, Be on W and H in Be - further studies are required on the following: (i) dynamics of W films deposited on a Be slab, (ii) improved definition of the atom-atom potential for Be on W, (iii) fitting of the potentials on DFT energies and forces, and (iv) determination of the structure and retention for Be/H and Be/W/H as well as inter-atomic potentials for Ar.

A.A. Haasz presented recent work at the University of Toronto on the oxidative removal of D from co-deposits obtained from DIII-D and JET divertor tiles, and D retention in W. A brief overview of the ITER project and a summary of the anticipated conditions in the divertor were presented. Haasz noted the important role erosion and hydrogen retention will play in the ITER project. The tritium inventory in ITER will be strictly limited, and is expected to be dominated by the effects of co-deposition. Some T-removal techniques are also being developed. Work continues on the thermo-oxidation of co-deposits from DIII-D and JET tiles, and the results of previous oxidation studies and their implications for ITER were presented. A new oxidation/co-deposition facility is being built to study cyclical co-deposition and oxidation of seeded specimens. Experiments on hydrogen retention in tungsten are also continuing. Work on the sequential C^+ implantation followed by D^+ bombardment has been completed, and the results were summarized.

R. Zalavutdinov reported on the erosion of soft and hard amorphous-C:H (*a-C:H*) films in neutral atomic and molecular hydrogen mixtures. A proposal to use C as a target material in ITER was presented – while carbon can withstand a high heat load, one major disadvantage is that high T retention may occur as a consequence of the co-deposition of C with hydrogen isotopes. Studies of the properties of soft and hard a-C:H films were summarized. The erosion of soft films differs from that of hard films: erosion of soft films occurs simultaneously with thermal sublimation and the subsequent re-deposition of the sublimation products in regions at lower temperatures. Magnetic fields prohibit the use of a hydrogen plasma to remove a-C:H films in ITER. Therefore, neutral flows of H/H_2 need to be produced in order to remove the hard films in remote parts of the facility. Neutral H/H_2 mixtures reduce the strongly temperature-dependent erosion rate of hard a-C:H films exponentially with distance from the atomic hydrogen source; this effect is also directly proportional to the atomic hydrogen flow towards the surface of the film. Methane is the main erosion product in neutral H/H_2 mixtures.

D. Kato reported on hydrogen trapping in metals relevant to fusion. First-principle calculations of binding energies for hydrogen atoms at mono-vacancies in Fe and W have been carried out by means of the VASP code. The Generalized Gradient Approximation (PBE type) was used for the exchange-correlation energy functional of the Kohn-Sham effective potential. Nanocavities formed in Fe-9Cr after high fluence irradiation by deuteron beams at high temperatures, and were also found in W specimens exposed to the high heat-flux of divertor plasmas at the large helical device (LHD) of the National Institute for Fusion Science (NIFS). These observations are relevant to material erosion during off-normal events in fusion devices. Hydrogen trapped at the cavities in Fe-9Cr was only desorbed at higher temperatures (800 and 1000K). The mechanisms for nucleation and growth of the cavities containing hydrogen may differ from those for He bubbles, but they remain unknown. Thermostatic theories predict that the thermal equilibrium concentration of vacancies is strongly enhanced by high concentrations of hydrogen and vacancy-hydrogen (VH) cluster formation in metals. Nucleation and growth of the cavities can be enhanced by a high concentration of hydrogen (vacancy) and VH cluster formation.

Y. Martynenko described studies of changes to W and C surfaces when exposed to high dose plasmas. Erosion processes include physical sputtering, chemical erosion, thermal shock (e.g. disruption, ELM and arcs) and neutron radiation. Material changes can include modifications to material composition, structure and phases, as well surface relief and defects. These changes may affect erosion, D and T retention and permeation, mechanical properties and particle reflection. A number of examples of surface changes in fusion-relevant materials were presented. Experiments for many of these processes can be performed on the LENTA beam discharge facility. Studies of D plasma impact on plasma-facing materials will be carried out under the IAEA contract. Available diagnostics include SEM for surface structure analysis, Auger spectroscopic analysis for surface composition studies, and the possibility of depth composition profile measurements by means of Rutherford Backscattering Spectroscopy (RBS).

P. Krstic reported on studies to determine the chemical sputtering of plasma-facing carbon surfaces. Theoretical and experimental work at Oak Ridge National Laboratory (ORNL) was described. Computer simulations based on classical molecular dynamics (MD) include efforts to model the impact of D, D_2 and D_3 (molecules in the ground state, vibrationally excited, or undergoing dissociation before impact) at impact energies from 7.5 to 30 eV/D on amorphous, deuterated carbon surfaces. Both a new code and simulation methodology have been developed and benchmarked against experimental results. Calculations were carried out for sputtering yields, reflection, dissociation and implantation probabilities, kinetic energy and angular spectra of sputtered/reflected atoms and molecules and internal energy (rovibrational) spectra of sputtered/reflected molecules. Experimental studies led by Meyer have included the sputtering of D^+, D_2^+ and D_3^+ on ATJ graphite and HOPG samples with decelerated beams from the ORNL Multicharge Ion Research Facility, a floating surface scattering chamber and absolute yield determinations by means of calibrated hydrocarbon leaks. Results have been obtained for the sputtering yields of methane and acetylene in the energy range 10 to 100 eV/D for both ATJ and HOPG, the isotope effects of H and D impact on ATJ with methane sputtering, and by analysis of surface samples by Raman spectroscopy.

K. Krieger and co-workers are investigating the surface processes of mixed materials by means of multi-species ion bombardment. Erosion and implantation processes were described, along with comparisons of the modelling codes with experimental results. The experimental facilities at IPP were described: a high current ion source is operated in conjunction with LOS-QMS, TDS and a micro-balance. Dual Ion Beam experiments incorporate *in-situ* beam analysis; UHV ARTOSS experiments have a D-ion source, C/Be evaporators, XPS, LOS-QMS and TDS capabilities; UHV XPS experiments are equipped with W/Be/C evaporators and heating (1200K). Other available analytical techniques include SEM, AFM, TEM (with ion beam cutting for sample preperation), XRD, PALS (in collaboration with TU Munich) and magnetron sputter deposition for up to three simultaneous elements. Work is in progress to study alloy formation at the W/Be interface as a function of temperature, and to develop a model of erosion/implantation/surface morphology for D/He + C → W D-retention in mixed material systems for ITER-based combinations.

K. Nordlund described work on multi-scale atomistic simulations of plasma-wall interactions. This approach can be applied over short to very long time scales on small to very large samples of material. Different techniques are needed for different regimes, including density functional theory (DFT), molecular quantum dynamics (MD) and kinetic Monte Carlo (KMC). Results for carbon were presented, including the erosion of CH molecules and the sticking of CH_x and C_2H_x molecules. There is a large difference in the depth for H and He bubble formation, and models have been applied to understand this effect. Studies of the erosion of tungsten carbide were described, and work has begun to define the potential for BeCWH. A further proposed investigation involves WC erosion under H + He/Ne/Ar/C/W co-bombardment.

D. Humbert of the IAEA discussed issues related to the sharing of data and the classification of erosion processes. Current data exchange methods are determined by internet technologies (IT), where new techniques are constantly being developed in which structured data, consistency and relationships are important features. Different databases and applications must speak the same language, and the tool of choice is eXtensible Markup Language (XML), a meta-language tool for language developments. Details of the classification of processes is an important issue in the initial development of a web search engine for AM/PSI data (DANSE). Four major sections were proposed:

heavy particle-heavy particle interactions,
electron-heavy particle interactions,
photon-particle and field-particle interactions, and
particle-matter interactions.

"Particle-matter interactions" includes both particle-surface interactions and particle penetration processes. Inputs from the CRP on the details of the classification scheme would be most welcome.

Data Needs for Fusion

Following the presentations of the various relevant research activities, the participants discussed and summarized the data requirements in order to understand and quantify erosion processes in fusion devices. A comprehensive list of specific needs was formulated that would assist considerably in the modelling of erosion, and could be addressed during the course of this CRP.

Requirements:

- phase diagram for the BeC system;
- understand the behaviour of WC under irradiation: does this material amorphise? what are the damage levels?
- ratios of sputtering yields of atomic Be to molecular BeD from deuterium saturated Be surface;
- both physical and chemical differential sputtering yields from Be_2C surfaces;
- D retention level in pre-damaged W;
- He bubble growth rates as a function of temperature in W;
- formation and migration energies of VH (D,T) clusters in W, Be, and W/Be/C compound materials;
- diffusion coefficients of hydrogen in W/Be/C compound materials, e.g. $Be_{12}W$;
- self diffusion coefficients of W, Be, C for pure materials, materials with voids and mixtures of such materials;
- oxidation of JET tiles (mixed Be C) at temperatures below 350ºC;
- 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;
- D^+ irradiation of WC at elevated temperatures, in terms of D retention and erosion products for both bulk material and films;
- MD model to assist in the interpretation of D retention in W during combined He, D irradiation;
- 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);
- sound inter-potentials for H, C, W and Be for MD simulations;
- 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;
- mutual and self diffusion coefficients of H, C, Be and W as a function of temperature - experimental data in order to verify the modelling;
- quantification of erosion products during simultaneous bombardment of W with D + C and He + C;
- experimental data on absorption, adsorption and retention of H and D by Be and mixed materials for comparison with theory;
- *ab initio* MD calculations on very large computer systems for the above processes involving Be and W;
- surface loss probabilities and sticking for different hydrocarbons on various pure and mixed surfaces;
- modelling of retention in all materials, including mixed systems.

Formulation of Agreed Work Plan

After the data needs had been identified and discussed in detail, the participants assessed the possible means of addressing the most pressing requirements. Each participant indicated areas in which they could contribute, and a work plan was proposed.

Nordlund:

- Complete a working set of BeCWH potentials.
- Simulate W and WC erosion and formation 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.
- Simulate formation of BeD molecules during D bombardment of Be in collaboration with Doerner.

Doerner:

- Measure Be/BeD erosion rates for comparisons with the simulations of Nordlund.
- 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.
- Investigate the influence of Ar added to a Be-seeded plasma to measure the effect on Be_2C surface formation and sputtering behaviour.
- Carry out specific experiments to compare total H retention in pure Be and Be/C and Be/W mixtures with simulation results of Allouche.

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.
- Carry out KMC 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 the collaborations.
- Experimental measurements of cavity size distribution and thermal desorption spectrum in collaboration with Japan and IPP (who have initiated some activities in this area).

Martynenko:

- Measure erosion and surface changes for C, W and perhaps WC under off-normal processes (disruption and ELM).
- Measure erosion of materials after changes induced by the off-normal processes.
- These measurements will take place at the MK200 facility for plasma processes: QSPA (Quasi Stationary Plasma Accelerator with shorter pulses) and MKT plasma accelerator.

Haasz:

- Continue experiments on the oxidation of DIII-D and JET specimens for co-deposition removal.
- 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.
- Perform W irradiation with simultaneous C^+-D^+, and study D retention as well as release of hydrocarbons in collaboration with IPP.
- Perform D retention studies in WC as a function of temperature, varying beam fluxes and beam energies; use laser-induced TDS to measure D retention.

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.
- 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).
- 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).

- Better quantify the interatomic potentials for C-W-Be-H in collaboration with Allouche, Nordlund and Stuart.
- 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.

<u>Other experiments (Meyer (ORNL))</u>:
- Develop the time-of-flight technique for a direct sight of sputtered molecules to lead to measurements of the energy distributions of the products.
- Perform erosion measurements on thin hydrocarbon films provided by IPP.
- Determine the D/C ratio of the surfaces using SIMS and residual gas analysis.
- Carry out Raman and Auger diagnostics of the surfaces (for example, measurements of sp^2/sp^3).
- Initiate measurements related to chemical sputtering and reflection on metal W-, Ti- and V-doped C films obtained from IPP-Garching.
- Investigate the effects of doping at impact energies of relevance to ITER, along with the influence on molecular size and isotope effects.

<u>Krieger</u>:
- Perform measurements of erosion, implantation and D retention of D + C on W, He + C on W, D + ^{13}C on ^{12}C at room and elevated temperatures in collaboration with the University of Toronto.
- Develop a model system of 2-D surface roughness (Si ridges on Si).
- Measure D-retention in ASDEX Upgrade tungsten plasma-facing components.
- Measure D-retention in deposited layers.
- 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.

<u>Allouche</u>:
- 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.
- Use these results to calculate H absorption and adsorption energies, and optimized structures for H interaction with pure Be and BeW alloys.
- Molecular dynamics:
    - obtain bond-order atomic potentials from quantum DFT and *ab initio* approaches;
    - carry out quantum and/or classical molecular dynamics simulations of the Be/W/H interaction.

<u>Zalavutdinov</u>:
- 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.
- 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.
- Measure the evolution of the surface composition of Mo during the removal of a-C:H films.

Recommendations and Conclusion

Extensive discussions during the course of the first RCM on “Data for surface composition dynamics relevant to erosion processes” have resulted in a comprehensive list of data needs for the assessment and design of fusion devices, and the formulation of an agreed work plan for the initial activities of the participants and co-workers. A number of collaborations between theorist and experimentalists were identified and specific studies were proposed for various comparisons. Definitive objectives were agreed for the Coordinated Research Project (CRP), and will be reported at the second RCM in approximately 18 months.

First IAEA Research Co-ordination Meeting on Data for Surface Composition Dynamics Relevant to Erosion Processes

17–19 October 2007, IAEA Headquarters, Vienna, Austria

Scientific Secretary: R.E.H. Clark

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Appendix 2

First IAEA Research Co-ordination Meeting on Data for Surface Composition Dynamics Relevant to Erosion Processes

17–19 October 2007, IAEA Headquarters, Vienna, Austria

Scientific Secretary: R.E.H. Clark

Meeting Agenda

Wednesday, 17 October **Meeting Room: ACV U1 U 640 0**

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

Session 1: Reports I

Chairman: D. Kato

10:00 – 10:45 A. Allouche
Combined Quantum and Molecular Dynamics Study on Mixed Materials Formation

10:45 – 11:15 *Coffee Break*

11:15 – 12:00 R. Doerner
Interaction of Beryllium Containing Plasma with ITER Materials

12:00 – 14:00 *Lunch*

Session 2: Reports II

Chairman: A. Allouche

14:00 – 14:45 A.A. Haasz

Thermo-oxidation of C-Be Mixed JET Codeposits

14:45 – 15:30 R. Zalavutdinov

Erosion of a-C:H Films under Interaction with Hydrogen Glow and Afterglow Discharge

15:30 – 16:00 *Coffee Break*

16:00 – 16:45 D. Kato
Hydrogen Trapping in Metals of Reactor Material

Thursday, 18 October

Session 3: Reports III

Chairman **A.A. Haasz**

09:30 – 10:15 Yu. Martynenko

Tungsten and Carbon Surface Change under High Dose Plasma Exposure

10:15 – 10:45 *Coffee Break*

10:45 – 11:30 P. Krstic
Computer Simulation and Beam-surface Experiments on the Plasma-surface Interactions for Fusion

11:30 – 12:15 K. Krieger

Investigation of Mixed Material Surface Processes and Multi-species Ion Bombardment

12:15 – 14:00 *Lunch*

Session 4: Reports IV

Chairman: **Yu. Martynenko**

14:00 – 14:45 K. Nordlund
Atomistic Simulations of Plasma-wall Interactions

14:45 – 15:15 *Coffee Break*

15:15 – 16:00 D. Humbert
Data Format, Classification and Transfer Issues

Friday, 19 October

Session 5: Review of Current Status

Chairman: **R. Doerner**

09:00 – 12:30 All
Comprehensive Review of Current Status, including Proposed Areas of Data Needs

12:30 – 14:00 *Lunch*

Session 6: Formulation of Work Plan for CRP

Chairman: **P. Krstic**

14:00 – 17:00 All
Formulation of Work Plan for First Two Years of CRP

17:00 – Adjourn

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