2014 Joint ICTP-IAEA Conference on Models and Data for Plasma-Material Interaction in Fusion Devices

Book of Abstracts

Contents

Schedule

Monday 03 November 2014

08:30 - 09:00 Ave Lusenti: Registration in the Main Lobby, Leonardo da Vinci Building

09:00 - 09:15 Sandro Scandolo, Bas Braams, Hyun-Kyung Chung: Welcome.

09:15 - 10:00 Christian Linsmeier, FZ Jülich, Germany: Hydrogen isotope retention and release in beryllium: The full picture from experiment and ab initio calculations. (Lecture)

10:00 - 10:45 Break; registration continues.

10:45 - 11:30 Kai Nordlund, University of Helsinki, Finland: Multiscale modelling of hydrogen and helium in tungsten. (Lecture.)

11:30 - 11:55 Jean Paul Allain, UIUC, Illinois, USA: Challenges and strategies to experimental validation of multi-scale nuclear fusion PMI computational modeling.

11:55 - 12:20 Manoj Warrier, BARC, Autonagar, Visakhapatnam, India: Statistical study of defects caused by primary knock-on atoms in fcc and bcc metals using molecular dynamics simulations.

12:20 - 14:00 Lunch

14:00 - 14:25 Dorothy Duffy, UCL, London, United Kingdom: Modelling the electronic excitation induced structural dynamics of tungsten.

14:25 - 14:50 Duc Nguyen-Manh, CCFE, Abingdon, United Kingdom: Trapping of He clusters by inert-gas impurities in refractory bcc transition metals: systematic first-principles predictions and experimental validations.

14:50 - 15:15 Takuji Oda, SNU, Seoul, Korea: Development of a potential model for tritium behavior in tungsten.

15:15 - 16:15 Break

16:15 - 16:40 Paul Erhart, Chalmers UT, Gothenburg, Sweden: Atomistic models for tungsten based alloys.

16:40 - 17:05 Mihai-Cosmin Marinica, CEA, Gif-sur-Yvette, France: Energy landscape of radiation-induced point defects in body centered cubic metals.

17:05 - 17:30 Stephan Irle, Nagoya University, Japan: Parameterization of approximate density functional theory and its application to the simulation of plasma-wall interactions in fusion devices.

18:00 - 20:00 Welcome reception

Tuesday 04 November 2014

08:30 - 08:55 Brian Wirth, UT, Knoxville, USA: Helium gas clustering dynamics in tungsten exposed to helium plasmas.

08:55 - 09:20 Maria Ganchenkova, MEPhI, Moscow, Russia: Calculation of defects and hydrogen in tungsten: fundamental parameters and methodological aspects.

09:20 - 09:45 Alfredo Caro, LANL, Los Alamos, USA: The capillarity equation at the nanoscale: size effects on gas bubbles in metals.

09:45 - 10:45 Break

10:45 - 11:10 Predrag Krstic, SUNY, Stony Brook, USA: The atomistic phenomena at the plasma-surface interfaces.

11:10 - 11:35 Robert Harrison, SUNY and BNL, Brookhaven, USA: Techniques in uncertainty quantification and initial application to plasma-material interfaces.

11:35 - 12:00 Poster authors: Minitalks to introduce the posters.

12:00 - 14:00 Lunch

14:00 - 16:00 Poster Session. See below. Posters will remain up Wed-Thu.

16:00 - 16:30 Break

16:30 - 17:30 Robert Harrison, SUNY and BNL, Brookhaven, USA: Institute Colloquium: Seeking a sustainable model for scientific simulation.

Wednesday 05 November 2014

08:30 - 08:55 Charlotte Becquart, University of Lille, France: Modelling the growth of He bubbles and trap mutation in tungsten.

08:55 - 09:20 Yves Ferro, Aix-Marseille University, France: H trapping and migration in W: A DFT investigation that includes temperature dependency.

09:20 - 09:45 Daiji Kato, NIFS, Toki-City, Japan: Multiple hydrogen trapping by vacancies: its impact on defect dynamics and hydrogen retention in tungsten.

09:45 - 10:45 Break

10:45 - 11:10 Gábor Csányi, University of Cambridge, UK: Constructing interatomic potentials from first principles using machine learning: the example of tungsten.

11:10 - 11:35 Hong-Bo Zhou, Beihang University, Beijing, China: Electrophobic interaction: the leading mechanism for helium self-trapping in metals.

11:35 - 12:00 Miroslav Urban, Slovak University of Technology in Bratislava, Slovak Republic: Many-body decomposition of the interaction energy in lowest beryllium clusters Be[3-8].

12:00 - 14:00 Lunch

14:00 - 14:25 Alexander Barashev, ORNL, Oak Ridge, TN, USA: Helium interaction with tungsten surfaces and subsequent evolution from atomistic simulations.

14:25 - 15:45 Discussion Session I on electronic structure computations and the development of MD potentials. Questions:

- 1a: What is the role of electronic excited states and how can effects of electronic excitation be included in the models and data?

- 1b: Are we satisfied with present strategies for the development of MD potentials from electronic structure calculations?

15:45 - Free time

Thursday 06 November 2014

08:30 - 08:55 Tomoaki Suzudo, JAEA, Tokai-mura, Japan: Migration of rhenium and osmium in tungsten.

08:55 - 09:20 Vladimir Borodin, RNC "Kurchatov Institute" and MEPhI, Moscow, Russia: Primary defect production in displacement cascades in beryllium.

09:20 - 09:45 Zeke Insepov, Nazarbayev University, Kazakhstan and Purdue University, USA: Multiscale modeling approach for defect behavior in irradiated metals of interest for fusion.

09:45 - 10:45 Break

10:45 - 11:10 Mike Demkowicz, MIT, Cambridge, USA: Design of composite materials for outgassing of implanted He.

11:10 - 11:35 Luis Sandoval, LANL, Los Alamos, NM, USA: Growth of helium bubbles in tungsten under realistic rates.

11:35 - 12:00 Jaime Marian, University of California, Los Angeles, CA, USA: Calculating the release fraction of W tendrils into the plasma using polymeric reptation theory.

12:00 - 12:15 Ahmed Hassanein, Purdue University, USA: Effect of thermal and collisional processes on the performance of plasma-facing components in mixed materials environment. (Presented by Zeke Insepov.)

12:00 - 14:00 Lunch

14:00 - 15:15 Discussion Session II on long-time evolution calculations and the development of KMC rates. Questions:

- 2a: What is the role of nuclear quantum effects and how can these effects be included in the models and data?

- 2b: Is it desirable and feasible to develop standard definitions for the objects in KMC models?

15:15 - Free time

Friday 07 November 2014

08:30 - 08:55 Zhongshi Yang, CAS-IPP, Hefei, China: Present status of plasma-surface interaction investigations for EAST and CFETR.

08:55 - 09:20 Armin Manhard, IPP Garching, Germany: Comparison of a quantitative diffusion-trap model with experiments on D uptake in damaged W.

09:20 - 09:45 NN: TBA.

09:45 - 10:45 Break

10:45 - 11:00 (C) Evgeny Marenkov, MEPhI, Moscow, Russian Federation: On hydrogen transport in solids with traps: influence of broad-band energy distribution and multiple trapping.

11:00 - 11:15 (C) Sabina Markelj, Josef Stefan Institute, Ljubljana, Slovenia: In situ study of isotope exchange mechanism in self-ion damaged tungsten.

11:15 - 11:30 (C) Régis Bisson, Aix-Marseille Université, Marseille, France: Bridging model and real systems with laboratory experiments: dynamic retention of deuterium in tungsten.

11:30 - 11:45 (C) Maria Rutigliano, CNR-IMIP, Bari, Italy: Hydrogen atom recombination on tungsten at high temperature: a combined experimental and theoretical work.

11:45 - 12:00 (C) Petrica Cristian Lungu, INFLPR, Magurele, jud Ilfov, Romania: Periodic structures formation on beryllium, carbon, tungsten films mixed films by TW laser irradiation.

12:00 - 14:00 Lunch

14:00 - 15:15 Discussion Session III on uncertainties in comprehensive modelling for present and future experiments. Questions:

- 3a: What are the most important model uncertainties for calculation of damage in fusion wall materials (primarily tungsten and steel) by neutrons and fast particles?

- 3b: What are the most important model uncertainties for calculation of hydrogen trapping and transport in fusion wall materials?

- 3c: What are some priorities for experimental information to help assess errors and uncertainties in models?

15:15 - 16:30 Any remaining business.

Poster Session (Tuesday afternoon)

(P) Agraj Abhishek, Institute for Plasma Research, Gandhinagar, India: Helium diffusion across grain boundary in ferrous-chromium alloy: a first principle molecular dynamics study.

(P) Rebecca Alexander, SRMP, CEA Saclay, France: Ab initio based modelling of the energetics of nanometric interstitial clusters in Fe and W.

(P) Bas Braams, IAEA, Vienna, Austria: Considerations on electronic excited states and the development of MD models and potentials.

(P) Ivan Cernusák, Comenius University, Bratislava, Slovak Republic: Molecular properties of neutral and charged CsH species in the context of the heating and current drive systems.

(P) Charu Lata Dube, Institute for Plasma Research, Gandhinagar, India: Positron annihilation lifetime measurement and X-ray analysis on energetic heavy ion beam irradiated polycrystalline tungsten.

(P) Jerome Guterl, University of California, San Diego, CA, USA: Effects of hydrogen surface processes on hydrogen retention in plasma facing components.

(P) Etienne Hodille, CEA Cadarache, France: Macroscopic rate equations modeling of trapping and retrapping of hydrogen isotopes in W materials.

(P) Juri Igitkhanov, Karlsruhe Institute of Technology, Germany: Impact of transient events on DEMO PFC.

(P) Peter Klaver, DIFFER, The Netherlands: Atomistic simulations using molecular dynamics and lattice kinetic Monte Carlo of tungsten surface under helium ion irradiation.

(P) Bérengère Marie Lüthi, SRMP, CEA Saclay, France: Ab initio modeling of the dislocation-carbon interaction in ferritic steels.

(P) Dmitry Matveev, FZJ, Jülich, Germany: Reaction-diffusion based modelling of hydrogen retention in Be and W.

(P) Martin de Jesus Nieto-Perez, Instituto Politécnico Nacional CICATA Querétaro, Mexico: Software engineering strategies for fast development and growth of fusion modeling tools.

(P) Jussi Polvi, University of Helsinki, Finland: Development of interatomic potential for W-N-H system.

(P) Jack Wells, ORNL, Oak Ridge, TN, USA: Retention of deuterium and helium in monocrystal of tungsten.

(Additional posters from invited speakers:)

(P) J. S. Wrobel, D. Nguyen-Manh, M. Yu. Lavrentiev, M. Ganchenkova and S. L. Dudarev: First-principles and Monte-Carlo modelling of phase stability and point defects in ternary Fe-Cr-Ni alloys.

(P) T. Suzudo and M. Yamaguchi: He embrittlement at grain boundary of bcc transition metals: Systematic study.

(P) S. Bukkuru, M. Warrier and M. C. Valsakumar: Molecular Dynamics study of interstitial diffusion in fcc and bcc metals.

Multiscale modelling of H and He in W

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In this talk, we will overview our work on using binary collision approximation (BCA), density-functional theory (DFT), classical molecular dynamics (MD), kinetic Monte Carlo (KMC), and rate equation (RE) modelling of how H and He escaping from a fusion plasma interacts with W. We will first present a brief overview of the simulation tools used, and in particular discuss our interatomic potential development approach.

We will then present results on several timely aspects of H and He interactions with W. We will show how DFT, MD and KMC simulations were used to explain why H and He bubble formation depths are very different in W [1,2,3]. We will further describe a systematic collection of BCA, MD, DFT data for describing the migration, trapping and detrapping energies of H in W, and how this data was used in a RE model to reproduce experimental data of D depth profiles before and after annealing. Analysis of the results show that a single monovacancy in W can hold about 5 H atoms [4,5]. We will finally present how a combination of MD and an entirely new KMC model has been used to study formation of W fuzz formation during high-fluence He irradiation, and in particular explain the origin of the experimentally observed sqrt(time) dependence for W fuzz formation [6,7].

[1] K. O. E. Henriksson, K. Nordlund, A. Krasheninnikov, and J. Keinonen, *Differences in hydrogen and helium cluster formation*, Appl. Phys. Lett. 87, 163113 (2005)

[2] K. O. E. Henriksson, K. Nordlund, and J. Keinonen, *Molecular dynamics simulations of helium cluster formation in tungsten*, Nucl. Instr. Meth. Phys. Res. B. 244, 377 (2006).

[3] K. O. E. Henriksson, K. Nordlund, A. Krasheninnikov, and J. Keinonen, *The depths of hydrogen and helium bubbles in tungsten - a comparison*, Fusion Science & Technology 50, 43 (2006)

[4] K. Heinola, T. Ahlgren, K. Nordlund, and J. Keinonen, *Hydrogen interaction with point defects in tungsten*,, Phys. Rev. B **82**, 094102 (2010)

[5] T. Ahlgren, K. Heinola, K. Vörtler, J. Keinonen, *Simulation of irradiation induced deuterium trapping in tungsten*, J. Nucl. Mater.427, 152 (2012)

[6] A. Lasa, K. O. E. Henriksson, and K. Nordlund, *MD simulations of onset of tungsten fuzz formation under helium irradiation*, Nucl. Instr. Meth. Phys. Res. B 303, 156 (2013).

[7] A. Lasa, S. K. Tähtinen, and K. Nordlund, *Loop punching and bubble rupture causing surface roughening - a model for W fuzz growth*, EPL 105, 25002 (2014)

Statistical study of defects caused by primary knock-on atoms in fcc and bcc metals using molecular dynamics simulations

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Damage of materials due to neutron irradiation occurs via energetic cascades caused by energetic primary knock-on atoms (PKA) created by the energetic neutron as it passes through the material. These cascades result in creation of Frenkel Pairs (interstitials and vacancies). The interstitials and

vacancies diffuse and recombine to (I) nullify the damage when an interstitial recombines with a vacancy, (II) form interstitial clusters when two or more interstitials recombine, and (III) form vacancy clusters when several vacancies come together. We report on molecular Dynamics (MD) simulations carried out in fcc (Cu) and bcc (FeCr) metals using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [1] to study:

1. Statistical variations in the number of Frenkel Pairs produced by energetic PKA directed in 1000 random directions. It is seen that at least 100 random directions have to be explored for the variance in the number of Frenkel pairs produced to become steady [2].
2. In-situ processing during MD simulations to find in-cascade cluster sizes and other parameters which are useful inputs for Kinetic Monte Carlo (KMC) / Dynamic Monte Carlo (DMC) studies. In-situ processing saves I/O of several tera-bytes when exploring 1000 random directions and shows no difference in run-time because the extra run-time processing is offset by the time saved in I/O.
3. Interstitialcy mechanism of interstitial diffusion, wherein an interstitial displaces a lattice atom thereby making the lattice atom an interstitial, in Cu, W and Fe. It is seen that the time-scale for *interstitialcy diffusion* is of the order of a few tens of pico-secs in these metals. This can contribute to further diffusive-recombinations of the Frenkel Pairs. Analysis of the diffusion process from a point of view of providing inputs to KMC/DMC will be discussed.

[1] S. J. PLIMPTON, *Fast Parallel Algorithms for Short-Range Molecular Dynamics*, J. Comput. Phys., 117 (1995) 1; http://dx.doi.org/10.1006/jcph.1995.1039.

[2] M. Warrier and M. C. Valsakumar, *Study of MD collision cascades in 1000 random directions in crystal Fe90Cr10 in the energy range 0.1 to 5 keV*, Fusion Science and Technology, 65, #2, (2014) 229-234.

Modelling the electronic excitation induced structural dynamics of tungsten

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Tungsten is the leading candidate material for application for the plasma facing wall and divertor in DEMO and future fusion reactors. Here we employ a combination of *ab initio* and empirical simulations to investigate the influence of electronic excitation on the structural response of tungsten to irradiation. We use the high electronic temperature implementation of density functional theory (HTDFT)[1] to investigate phonon dispersion and non-thermal forces in electronically excited tungsten. We observe soft transverse modes in the phonon spectra of bcc tungsten at elevated electronic temperatures (between 10000K and 15000 K) and we find that both fcc and hcp tungsten become dynamically stable at high (> 15000 K) electronic temperatures. Such observations raise the possibility of non-thermal solid to solid phase transitions occurring under conditions of strong electronic excitation.[2]

We have used HTDFT to derive a set of electronic temperature dependent interatomic potentials for tungsten, based on the Finnis Sinclair model.[3] Such potentials include the effects of the change in interatomic interactions associated with the redistribution of the electron density following electronic excitation. They can be employed in two-temperature molecular dynamics (2T-MD) simulations where the electronic energy is coupled to molecular dynamics (MD) and the time evolution of the electronic temperature is calculated by a finite difference solution of the heat diffusion equation.[4] We use the 2T-MD model with the electronic temperature dependent potentials to model the response of a tungsten thin film to laser irradiation. We find that the bcc tungsten film transforms to fcc on the

femto-second timescale, prior to transfer of energy from the electronic to ionic systems by electron phonon coupling which subsequently causes the film to melt.

1. N. D. Mermin, "Thermal properties of inhomogeneous electron gas" Phys. Rev. 137, A1441 (1965)

2. Y. Giret, S. L. Daraszewicz, D. M. Duffy, A. L. Shluger, and K. Tanimura, "Nonthermal solid-to-solid phase transitions in tungsten", Phys. Rev. B 90, 094103 (2014)

3. S. T. Murphy, Y. Giret, S. L. Daraszewicz, A. L. Shluger and D. M. Duffy "Modelling solid-to-solid phase transitions in W thin films under laser irradiation" manuscript in preparation

4. D.M.Duffy and A.M. Rutherford, "Including the effects of electronic stopping and electron-ion interactions in radiation damage simulations" J. Phys: Cond. Matt. 19, 016207 (2007)

Trapping of He clusters by inert-gas impurities in refractory bcc transition metals: systematic first-principles predictions and experimental validation

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Recently, systematic quantum-mechanical calculations of radiation defects in tungsten and iron-based alloys play important role in understanding generic materials-related problems foreseen with operation of future fusion-power plants [1-5]. In this talk, properties of point defects resulting from the incorporation of inert-gas atoms in bcc transition metals (TMs) are investigated systematically using first-principles density functional theory (DFT) calculations. For the TMs in group 6B (Cr, Mo, W) of periodic table and Fe, the most stable configuration for the interstitial neon, argon, krypton and xenon atoms is predicted in the tetrahedral site, similarly to what was found earlier for helium in all bcc TMs, whereas for the TMs in group 5B (V, Nb, Ta) the octahedral configuration is the most energetically favourable one. The calculated formation energies for single inert-gas atoms at interstitial sites are systematically larger for Ne, Ar, Kr and Xe than for the case of He and this trend can be simply understood by a strong local distortion with respect to their atomic size. However, a deeper analysis their substitutional formation energies demonstrates that vacancy-impurity interaction is more likely to be related to the covalent character of bonding between inert-gas atoms and bcc TMs. There is a remarkable variation exhibited by the binding energy between inert-gas impurity and vacancy going from He to Ne, Ar, Kr, Xe. The origin of this trend is explained by electronic structure calculations showing that *p*-orbitals play an important part in the formation of chemical bonds between a vacancy and an atom of any of the four inert-gas elements in comparison with helium, where the latter contains only $1s^2$ electrons in the outer shell. The binding energies of a helium atom trapped by five different defects (He-v, Ne-v, Ar-v, Kr-v, Xe-v, where v denotes a vacancy) are all in excellent agreement with experimental data derived from thermal desorption spectroscopy (TDS) for bcc-W. Attachment of He clusters to inert gas impurity atom in all bcc TMs is analysed as a function of the number of successive helium atoms trapped in that created by the prior inert-gas heavy ion bombardment with several discrete binding energies measured within the TDS experiments [6]. The present DFT data base can be used to explain the swelling and variation of the Young modulus due to inert-gas ion implantation in plasma facing materials for fusion device applications [7].

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the *Euratom research and training programme* 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

[1] D. Nguyen-Manh, A.P. Horsfield, S.L. Dudarev, Phys. Rev. B, 73 (2006) 020101

[2] D. Nguyen-Manh, V. Vitek, A.P. Horsfield, Prog. Mater. Sci., 52 (2007) 255

[3] D. Nguyen-Manh, M.Yu. Lavrentiev, S.L. Dudarev, C.R. Phys., 9 (2008) 379

[4] M. Mrovec, D. Nguyen-Manh et al., Phys. Rev. Lett., 106 (2011) 246402

[5] D. Nguyen-Manh et al., J. Mater. Sci., 47 (2012) 7385.

[6] D. Nguyen-Manh, S.L. Dudarev, NIMB (2014), http://arxiv.org/abs/1408.0630

[7] F. Hofmann, D. Nguyen-Manh et al., Acta Mater. (2014), http://arxiv.org/abs/1407.6051

Development of a potential model for tritium behavior in tungsten

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Tritium accumulation in plasma facing components such as tungsten is considered as an important fusion engineering issue, because (1) it affects the feasibility and economy of tritium fuel cycle and (2) the accumulation amount is vital information to make a plasma operation scenario that meets a radiation-safety regulation limit of tritium. Therefore, experimental data on the tritium accumulation has been largely acquired in the last decade. In order to predict the tritium accumulation in a fusion environment using those experimental data, it is needed to fill gaps between fusion reactor conditions and experimental conditions in tritium flux, neutron flux and fluence, etc, based on detailed understanding of the tritium behavior in damaged tungsten. Computational simulations in an atomic scale are expected to contribute to revealing the tritium behavior.

Among several available computational methodologies, classical molecular dynamics (MD) method has an advantage in an atomic scale resolution with a relatively low computational cost. MD can deal with millions of atoms, and thus can simulate complex defects, such as ones composed by multiple vacancies and multiple tritium atoms. The low computational cost is realized by describing interatomic interactions with simplified model functions, so-called potential model. Due to this simplification, however, the accuracy of simulation results depends on the quality of potential model. For tungsten-tritium systems, two potential models [1, 2] have been widely utilized in MD simulations. However, their descriptions of tritium-vacancy interaction are not necessarily satisfactory, which motivates us to develop a new potential model.

Thus, our group try to develop a new tungsten-hydrogen potential model which can adequately reproduce a great number of ab-initio calculation results on energy and force in IAEA-CRP activity. The model function is composed by multiple basis functions [3] and their coefficients are uniquely determined by solving linear simultaneous equations. In this presentation, first, formulas to represent two-body inteaction model and embedd-atom model (EAM) will be introduced. The validity and limitation of the methodology will be discussed with results of validation test on magnesium oxide, where error convergences to the number of reference ab-initio calulation data and to the number of involved basis functions are analyzed and then the effect of EAM term on reduction of the errors will be shown. Then, our plan on which tungsten-hydrogen systems are considered in reference ab-initio calculations will be explained. Finally, the quality of a potential models which were preliminary constructed for tungsten and tungsten-hydrogen systems with available ab-initio data will be is presented

[1] N. Juslin et al., J. Appl. Phys. **98**, 123520 (2005),

[2]X.C. Li et al., J. Nucl. Mater. **408**, 12 (2011).

[3] C. M. Handley and J. Behler, Eur. Phys. J. B **87**, 152 (2014).

Atomistic modelling of tungsten based alloys

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Tungsten alloys are considered for structural applications in fusion reactors, especially for armor materials at the divertor and first wall. This interest is motivated by promising physical properties such as high melting point, low coefficient of thermal expansion, high thermal conductivity and high sputtering resistance. In this context we investigate the thermodynamic and mechanical properties of tungsten based alloys on the basis of atomic scale simulations using both density functional theory calculations and empirical potential methods.

Here, we will first report on the properties of intrinsic and extrinsic (Ti, V, Zr, Nb, Hf, Ta, Re) defects in tungsten, which were considered with the eventual objective to address the potential of dilute W-based alloys in lowering the brittle-to-ductile transition temperature (BDTT). Ti, V, Nb, Hf and Ta substitutional defects are found to have negative formation energies whence these elements tend to form solid solutions with tungsten. By contrast positive formation energies for Zr and Re indicate that there is a thermodynamic driving force for segregation in alloys based on these two elements.

Interstitials generally have large formation energy due to large strain fields associated with the defect core. For Zr, Nb, Hf, Ta and W interstitials, <111> crowdions are the most stable interstitial configurations while for Ti, V and Re, <110> as well as "bridge" configurations show the lowest formation energies. Most interestingly negative values of binding energy for Ti, V and Re in both interstitial configurations indicate that these impurities trap interstitials. Under irradiation conditions interstitial defects will be produced that under normal conditions can readily recombine thanks to the large mobility of <111> type interstitials. In the presence of the aforementioned alloying elements, this process will be impeded, whence a faster defect accumulation rate is to be expected.

To explore this effect further we specifically investigate the W-Ti system. It is shown that the system exhibits a strongly asymmetric phase diagram with a large solubility for Ti in BCC-W. Ti-W mixed interstitials are found to have a strong attractive interaction, suggesting a pronounced tendency for interstitial clustering. These results are discussed in the context of the application of in particular W-Ti alloys for structural elements in neutron rich environments.

Energy landscape of point defects in body-centered-cubic metals.

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Progress in fusion and advanced fission power generation technology depends critically on the development of new high temperature materials. In metal alloys, including tungsten alloys, microstructural evolution occurring under irradiation is strongly dependent on the diffusion properties of point defects, such as interstitial atoms and vacancies, and also on the properties of extended defects, such as dislocations and surfaces. The mobilities of self-interstitial atoms and their clusters in metals, especially body-centered cubic (BCC) metals, are one of the main issues in multiscale models for the prediction of the microstructure evolution that these materials undergo under irradiation. Moreover, the morphology adopted by these defect clusters is a fundamental question with obvious practical consequences on the materials properties, since it controls also the dislocation obstacle strength and hence the strengthening of the materials and dimensional changes like swelling or growth

for anisotropic materials. We investigate the energy landscape of defects in BCC metals by the means of the ab initio methods as well as the empirical potentials developed from electronic structure calculations.

For vacancy clusters there is a competition between planar loops and voids, and also stacking fault tetrahedra in face-centered cubic metals. On the other hand, the observation of clusters of self-interstitial atoms in metals by transmission electron microscopy (TEM) techniques reveals only nanometer size planar loops. In BCC metals these loops have a ½<111> Burgers vector, except in iron at high temperatures where it is <100>. Recently, we have proposed a three dimensional periodic structure for self-interstitial clusters in BCC metals, as opposed to the conventional two dimensional loop morphology [1]. The underlying crystal structure corresponds to the C15 Laves phase. The new three dimensional structures generalize previous observations [1, 2].Using Density Functional Theory (DFT) calculations on typical configurations, we demonstrate that in $\alpha $--iron these C15 aggregates are highly stable and immobile and that they exhibit large antiferromagnetic moments. These clusters form directly in displacement cascades and they can grow by capturing self-interstitials. This new morphology of self-interstitial clusters thus constitutes an important element to account for when predicting the microstructural evolution of iron base materials under irradiation.

The mechanism of voids formation implies firstly the formation of smaller clusters as di-vacancy. Di-vacancy in tungsten, as in all BCC metals of the group VI B, has an unusual energy landscape. In tungsten, the first nearest neighbour is slightly repulsive or attractive depending of DFT calculations or exchange-correlation functional while the second nearest neighbour configuration is strongly repulsive [3]. The same tendency is observed for all elements of VI B group and is not the case for V B metals and iron for which the most stable configuration of di-vacancy is the second nearest neighbour configuration. However, in experiments, in the high temperature limit vacancy clusters are directly observed in tungsten [4]. Moreover, this work provides input data for kinetic models for microstructural evolution. The formation/migration free energies of mono- and di-vacancies / interstitials are computed using calculations. The vibrational part of the free energy is computed in the frame transition state theory (TST) using harmonic approximation. The anharmonic part is evaluated by the recently developed method based on adiabatic reweighting algorithm for computing the free energy along an external parameter from adaptive molecular dynamics simulations [5]. The electronic entropy contribution to the free energy is also taken into account. The defect binding free energies and defect diffusion coefficients deduced from these calculations can be used to perform simulations of isochronal resistivity recovery experiments. We show that the temperature deeply impact the energy landscape of di-vacancy at higher temperature and can even change the relative stability of various configurations.

Using the ab-initio data we have developed empirical interatomic potentials to study ½<111> screw dislocations in bcc iron and tungsten. The potentials use the Embedded-Atom-Method formalism and are fitted to a mixed database, containing various experimentally measured properties and ab initio formation energies of defects, as well as ab initio inter-atomic forces computed for random liquid congurations. The availability of data on atomic force fields proves critical for the development of the new potentials. In agreement with predictions from ab initio calculations, the new potentials correctly reproduce the non-degenerate core structure of the screw dislocation, with a {110} glide plane and a single hump Peierls potential, without intermediate metastable configuration.

[1] M.-C. Marinica et al. , Phys. Rev. Lett. 108, 025501 (2012), D. Terentyev et al,. Phys. Rev. Lett. 14, 145503 (2008), M.-C Marinica et al., Phys. Rev. B 83, 094119 (2011).

[2] D. J. Bacon et al., J. Nucl. Mater. 276, 1 (2000);

[3] A. Satta, F. Willaime, and S. de Gironcoli, Phys. Rev. B, 57, 11184, (1998) ; L. Ventelon, F. Willaime, C.-C. Fu, M. Heran, and I. Ginoux, J. Nucl. Mater., 425, 16, (2012). ; M. Muzyk, D. Nguyen-Manh, K. J. Kurzyd\lowski, N. L. Baluc, and S. L. Dudarev, Phys. Rev. B, 84, 104115, (2011).

[4] K-D. Rascha, R. W. Siegelab and H. Schultz, Phil. Mag. A, 41, 91 (1979) ; J. Y. Park, H. C. W. Huang, R. W. Siegel, and R. W. Balluffi, Philos. Mag. A 48, 397 (1983).

[5] L. Cao, G. Stoltz, T. Lelièvre, M.-C. Marinica, and M. Athènes, J. Chem. Phys, 140, 104108, (2014).

Helium Gas Clustering Dynamics in Tungsten Exposed to Helium Plasmas

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The plasma facing components, first wall and blanket systems of future tokamak-based fusion power plants arguably represent the single greatest materials engineering challenge of all time. Indeed, the United States National Academy of Engineering has recently ranked the quest for fusion as one of the top grand challenges for engineering in the 21st Century. These challenges are even more pronounced by the lack of experimental testing facilities that replicate the extreme operating environment involving simultaneous high heat and particle fluxes, large time varying stresses, corrosive chemical environments, and large fluxes of 14-MeV peaked fusion neutrons. Fortunately, recent innovations in computational modeling techniques, increasingly powerful high performance and massively parallel computing platforms, and improved analytical experimental characterization tools provide the means to develop self-consistent, experimentally validated models of materials performance and degradation in the fusion energy environment. This presentation will describe the challenges associated with modeling the performance of plasma facing component and structural materials in a fusion materials environment, the opportunities to utilize high performance computing and then focus on recent progress to investigate the dramatic surface evolution of tungsten exposed to low-energy He plasmas. More specifically, multiscale modeling results will be presented to identify the mechanisms of tungsten surface morphology changes when exposed to 100 eV He plasma conditions as a function of temperature and initial tungsten microstructure. The results demonstrate that during the bubble formation process, He clusters create self-interstitial defect clusters in W by a trap mutation process, followed by the migration of these defects to the surface that leads to the formation of layers of adatom islands on the tungsten surface. As the helium clusters grow into nanometer sized bubbles, their proximity to the surface and extremely high gas pressures leads them to rupture the surface thus enabling helium release. Helium bubble bursting induces additional surface damage and tungsten mass loss, which varies depending on the nature of the surface. However, these computational results also clearly identify the importance of rate effects associated with the implantation flux (plasma current) on the quantity of retained helium and the gas bubble populations, and the impact of this rate effect will be discussed in relation to ITER operation and beyond.

Calculation of defects and hydrogen in tungsten: fundamental parameters and methodological aspects

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A significant deterioration of tungsten mechanical properties as a result of radiation damage and the accumulation of high concentrations of hydrogen is among the most important problems that are to be solved in order to enable tungsten application in future fusion facilities. The understanding of the defect microstructure development in irradiated tungsten is impossible without knowing the fundamental parameters of primary radiation defects and implanted impurities (first of all - hydrogen). These characteristics include the formation energies of point defects, the solution energies of impurities, defect migration barriers and the energies of interaction between defects. The commonly accepted numerical approach for calculating the parameters of point defects in solids is the density functional theory. However, numerous published DFT studies of point defects in tungsten tend to give

remarkably different predictions even for the simplest point defects (for example - for the vacancy formation energy). A possible reason for this situation could be the use of inappropriate or insufficient computational parameters that do not ensure the convergence of calculations results.

This reports describes the results of a detailed systematic study of the influence of the exchange-correlation functional selection, the supercell size, and the technical computational parameters (the cutoff energy and the density of *k*-point mesh in the first Brillouin zone) on the predicted energies of vacancy and interstitial defects, as well as hydrogen atoms in tungsten. We formulate the minimum requirements to the choice of computational parameters that ensure acceptable accuracy of point defect energies. It is shown that calculations in tungsten are very demanding to the choice of parameters, which is more severe than for many other structural and functional materials for fusion reactors and is not satisfied in many already published papers dealing with point defects in tungsten.

The capillarity equation at the nanoscale: size effects on gas bubbles in metals.

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Gas bubbles in materials are relevant in several technological applications. A usual way to estimate the amount of gas in a bubble is to assume equilibrium, i. e. the gas pressure P satisfy the Young-Laplace capillarity equation $P=2\gamma/R$, with γ the surface energy of the host material, R the bubble radius, and the relation between P and density extracted form an equation of state (EOS) for He. In this work we show that at the nanoscale this picture is no longer correct

Both the P-density relation and the capillarity pressure need to be modified to describe nanoscale gas bubbles embedded in metals, scale at which the width of the interface region cannot be neglected. We focus in particular on the case of He in Fe.

In contrast to the common assumption that pressure inside a gas or fluid bubble is constant, we bring the concept of Tolman's length from the field of colloidal particles that provides a curvature dependence for the interface energy that becomes relevant at the nano scale. Pressure and density can no longer be defined as global quantities determined by an EOS, but they become functions of position because the bubble develops a core-shell structure. To highlight the origin of this effect we solve the bubble problem first using continuum mechanics and then using empirical potentials to find a quantitative measure of this effect.

The fact that the pressure becomes a function of position calls for a new equation of state for He at the nanoscale that accounts for these interface effects (see A. Caro et al. Appl. Phys. Lett. 103, 213115 (2013). We derive an expression to predict pressure, and from it density and the amount of He in nanoscale bubbles. We find that conditions for equilibrium are found for values of pressure or density at variance by a factor of 2 compared to the traditional way of using the capillarity equation and a bulk He EOS.

The atomistic phenomena at the plasma-surface interfaces

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Plasma-Material Interface (PMI) is one of the largest technical challenges to the advancement of thermonuclear magnetic fusion energy due to the wall erosion lifetime, thermo-mechanical and neutron damage of the reactor containment walls exposed to the fusion plasma.

Our basic hypothesis is that much of understanding on the fundamental phenomena and much information on the interactions at the plasma-material interface can be obtained by the atomistic approach, i.e. at the time scale of sub-fs to 10 ns and at the spatial scale up to few tens of nm. We have tested this hypothesis so far on several plasma-material interfaces, amorphous carbon irradiated by hydrogen plasma, lithiated and oxidized carbon irradiated by hydrogen plasma, tungsten surface irradiated by the self-atoms and deuterium, all well integrated and in agreement with experimental validation.

How to build a theoretical approach integrated with experiment? It is worth noting that, for example, a flux of 10^{25} particles/m^2s at the hot gas-material interface means that, statistically, one particle is impinging on a surface of 10 nm^2 every 10 ns. This gives to the system enough time to evolve freely from the external influx of energy and particles, still staying far from equilibrium. With an impact particle energy of 100 eV this would result in heat flux of ~160 MW/m^2. However, a typical chemistry-based process, like is chemical sputtering, at impact energies $\leq$100 eV, fully evolves at the interface for less than 50 ps, implying that each impact is independent, uncorrelated, and discrete. However, each impact changes the surface, functionalizing it for the subsequent collision, i.e. building a dynamic surface with memory, and depositing energy.

By cumulative irradiation of both pre-damaged and virgin surfaces of monocrystal tungsten by deuterium atoms of impact energy of few tens of eV, we simulate by classical molecular dynamics (CMD) the creation of a deuterium "protective layer", discussing also the competing diffusive outgoing flux. The depth and width of the layer depend on the deuterium impact energy and the diffusion rate of deuterium in tungsten, the latter being influenced by the tungsten temperature and damage. Found simulation results resonate with the recent DIFFER experimental results.

It has been known that defects in tungsten, in particular at the grain boundaries and in vacancies, are preferable sites for deuterium and helium retention. We study by CMD the dynamics of the defects creation, in particular their number saturation as function of fluence. We also study the cumulative retention of deuterium at impact energies below 100 eV as functions of tungsten temperature at models of the dislocation boundaries. We obtain a strong preference of the retention of the impact particles at the boundaries at high temperature of 1000K.

The recent unexpected finding concerning carbon wall conditioning by lithium in NSTX and in a number of other fusion machines, was resolved by quantum-classical atomistic computer simulations, showing that the presence of oxygen in the surface plays the key role in the increased uptake chemistry and suppression of erosion, while lithium is decisive factor in achieving high concentrations of oxygen.

This work was supported in part by the Institute of Advanced Computational Science at SUNY Stony Brook, and by the LDRD programs of Princeton Physics National Laboratory and of Oak Ridge National Laboratory.

Modelling self trapping and trap mutation in tungsten using DFT and Molecular Dynamics with an empirical potential based on DFT

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Being virtually insoluble in metals, but very mobile, He atoms can be trapped, associate with vacancies, forming platelets and bubbles. He atoms have been shown to contribute to swelling, cause intergranular embrittlement and produce roughening and blistering at metal surfaces. Being repelled by the metal atoms, they form stable clusters, which are also mobile. This tendency to form clusters is so strong that when too many He atoms are aggregated together it can be less costly to relieve the strain created by the interstitial elements by the ejection of one or more matrix atoms leading to the formation of one or more Frenkel Pairs (FP), i.e. vacancies and Self Interstitial Atoms (SIAs). When no vacancy is initially present, the He cluster will be trapped by the vacancy it created, in a self-trapping (ST) event; whereas when one or more vacancies are already associated with the He cluster, the same mechanism is referred to as trap mutation (TM) or loop punching, if more than one SIA is created.

The metal studied in this work is tungsten, candidate for the divertor and currently under heavy investigations experimentally and theoretically. We have investigated the thermodynamics and kinetics of ST and TM using Density Functional Theory (DFT) calculations and Molecular Dynamics with a recently developed potential for W-He adjusted on DFT calculations.

The stability of helium-vacancy clusters (He_nV_m) as well as pure interstitial helium clusters in tungsten results from a competitive process between thermal emission of vacancies, self interstitial atoms and helium atoms, depending on the helium-to-vacancy ratio in mixed clusters or helium number in pure interstitial helium clusters and will be presented in this work. We investigated in particular the ground state configurations as well as the activation barriers of self trapping and trap mutation, i.e. the emission of one SIA along with the creation of one vacancy from a vacancy-helium or pure helium object.

H trapping and migration in W: A DFT investigation that includes temperature dependency

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In this talk, the plasma wall interaction is focused on the hydrogen-tungsten system that we investigate by mean of Density Functional Theory (DFT). Because DFT is limited to small models of about one hundred atoms at zero temperature, this work is complemented by a statistical approach with the aim to yield temperature dependent data that can be directly compared with macro-scale thermodynamic and kinetic experimental data.

It follows that DFT data are included in a statistical model based on transition state theory and thermodynamic. Such model allows revising the solubility and diffusivity of hydrogen in tungsten. The discrepancy between the experimental diffusion coefficient from Frauenfelder *et al*[1] and other DFT results[2] is understood and two diffusion regimes are proposed depending on the temperature.

The trapping of multiple hydrogen atoms in tungsten vacancies is also investigated. The hydrogen population in vacancies and the vacancy concentration in tungsten are shown to depend on the temperature. Using a crude kinetic model, TDS spectra are simulated, which despite the simplicity of the model exhibit a reasonably good agreement with experimental results recorded on single crystalline samples[3,4].

1. R. Frauenfelder, J. Vac. Sci. Technol., 6 (1969) 388

2. K. Heinola, T. Ahlgren J. Apll. Phys., 107 (2010) 113531

3. O. V. Ogorodnikova, T. Schwarz-Selinger, K. Sugiyama, T. Dürbeck and W. Jacob, Phys. Scr. T138 (2009) 014053

4. M. Poon, A.A. Haasz, J.W. Davis, Journal of Nuclear Materials 374 (2008) 390.

Multiple hydrogen trapping by vacancies: Its impact on defect dynamics and hydrogen retention in tungsten

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Tungsten is the prime candidate plasma-facing materials at ITER and DEMO, which would be exposed to high-flux divertor plasmas as well as neutron. Since super-saturation of hydrogen is predicted in the tungsten divertor surfaces, its influence on hydrogen trapping by defects and defect dynamics is an issue.

In this talk, we present studies on 1) multiply hydrogen trapping in a mono-vacancy investigated from first-principles using density functional theories (DFT) and a statistical thermodynamics [1-3], 2) hydrogen trapping effects on di-vacancy formation in tungsten [1,4], 3) transition state theory analysis on thermal desorption of hydrogen atoms in a mono-vacancy [2,5], and 4) carbon impurity interstitial diffusion enhanced by super-saturated hydrogen atoms in tungsten [6].

[1] D. Kato et al., *"Super-saturated hydrogen effects on radiation damages in tungsten under high-flux divertor plasma irradiation"*, IAEA Fusion Energy Conference (St. Petersburg, Russia, 13-18 Oct. 2014) MPT/P7-36.

[2] N. Fernandez et al., *"H trapping and de-trapping in tungsten based materials (W, $Be_{12}W$): modelling TPD spectra from DFT only"*, The 21st International Conference on Plasma Surface Interactions in Controlled Fusion Devices (Kanazawa, Japan, 26-30 May 2014) P1-013.

[3] D. Kato et al., J. Plasma Fusion Res. Ser. 8 (2009) 404.

[4] D. Kato et al., J. Nucl. Mater. 417 (2011) 1115.

[5] D. Kato et al., *"Multiple hydrogen trapping and thermal release at vacancies in high-fluence hydrogen plasma-tungsten materials interaction"*, The 5th International Symposium of Advanced Energy Science (Uji Campus, Kyoto Univ., Japan, 30 Sept. - 1 Oct. 2014) ZE26A-8.

[6] D. Kato et al., Plasma and Fusion Research: Regular Article, Vol. 6 (2011) 2405062 (4pp).

Constructing interatomic potentials from first principles using machine learning: the example of tungsten

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This talk will report on our recent progress with generating force fields (interatomic potentials) with first principles accuracy using machine learning, specifically Gaussian process regression. The three key ingredients are: a representation, an interpolation scheme, and a protocol for generating data. A lot of progress was made on the first two in our group and others in the last few years, and now we are turning our attention to the much less well defined problem of what needs to be in a database of first principles calculations in order to recover specific materials properties using the interpolated potential. The first illustration will be on tungsten and if time allows on water (in cluster, liquid and ice forms).

Electrophobic Interaction: the Leading Mechanism for Helium Self-trapping in Metals

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Helium (He) is a typical impurity in metals. The solubility of He in metals is extremely low, yet it can lead to significant changes in microstructure and mechanical properties, such as the high temperature He embrittlement at extremely low concentration. Helium is produced from (n, α) transmutation reactions in both fission and fusion. It is well known that He atoms are energetically favorable clustering with each other, producing point defects, and further resulting in radiation damage and mechanical property degradation of metals. The self-trapping of He should be responsible for the effects of He on the properties of metals. However, the physical intrinsic mechanism for He self-trapping is still unclear.

Taking tungsten (W) as an example, we have investigated the He-He interaction in metals using a first-principles method. The stability of He in metals is directly associated with the He-He interaction. We found a single He prefers to occupy the tetrahedral interstitial site in comparison with the octahedral interstitial site in W. To further shed light on the physical mechanism underlying the stability of He in W, it is helpful to decompose the solution energies into two contributions, including the *mechanical contribution* (the deformation energy induced by the embedded He atom) and the *electronic contribution* (the electronic effect). Interestingly, it is found that the mechanical contribution dominates in the relative stability of He, while the electronic contribution plays a key role in the poor solubility of He in W. Furthermore, the electronic contribution will decrease linearly with decreasing of electron density. The binding energy between He atoms is calculated to be 1.03 eV with the equilibrium distance of 1.50 Å in W, suggesting the strong attractive interaction of He. We further investigate the energies and the atomic configuration in order to explore the origin of the He-He attractive interaction in W. Our first-principles calculations suggest that the electronic contribution of two congregate He atoms is much lower than that of two isolated He atoms, but the mechanical contribution shows a contrary tendency. This can be attributed to that the deformation of W induced by two congregate He atoms is larger than that of two isolated He atoms, leading to the more significant decrease of electron density at the He most stable site. Further, we show that there is an electrophobic interaction between He atoms dissolved in an electron gas, in analogy with hydrophobic interaction between salutes in water, which drives He to cluster. The electrophobic interaction provides the leading mechanism responsible for the experimentally observed phenomenon of He self-trapping in metals.

Many-body decomposition of the interaction energy in lowest beryllium clusters Be_{3-8}.

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We present the decomposition of interaction energies in beryllium clusters, Be_m, m=3─8, into a series of all possible non-identical m-particle non-additivities up to m=8. We analyse the role of the electron correlation and compare non-additivities resulting from DFT and MP2 energies with reference aug-cc-pVTZ CCSD(T) and CASPT2 calculations. Dominating non-additivity term is the four--body contribution (1,2). Five- and six-body terms are still quite large in Be_5 and Be_6 clusters but the total interaction energy in Be_6 is not significantly affected thanks to their cancellation. Clearly, non-additivities in Be clusters must be considered in constructing the interatomic potentials for investigations of the beryllium solid state. Any model based on pair and even three particle interactions is useless. Pair interactions are far from being dominating in the decomposition of the interaction energy into m─body terms since they represent weak dispersion forces, while the bonding character in higher clusters is more covalent. Binding energies increase with the size of the cluster, being higher than 1 eV per atom in Be_6 . In CCSD(T) calculations of Be clusters we checked highest CC excitation amplitudes as indicators of possible effects of quasidegeneracy.

We have also considered $B_xC_yN_z$ species as a coverage for plasma facing materials. Using the VASP package with the DFT-D3BJ method we performed pilot calculations on the thermal stability and the band gaps of h-$C_m(BN)_n$ systems. The calculations indicate that thanks to a variety of possible BCN based species some of them may fulfill requirements for using in the fusion reactor as an alternative to existing materials.

Acknowledgements: The support of EURATOM (FU07-CT-2006-0044) and the Slovak Research and Development Agency, (APVV-0059-10) is gratefully acknowledged.

(1) P. N. Ascik, J. J. Wilke, A. C. Simmonett, Y. Yamaguchi, H. F. Schaefer III, J. Chem. Phys. 134 (2011) 074110

(2) M. Šulka, M. Pitoňák, I. Černušák, M. Urban, P. Neogrády, Chem. Phys. Lett. **573**, 8 – 14 (2013).

Helium interaction with tungsten surfaces and subsequent evolution from atomistic simulations

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The results of a computational study of helium-vacancy clusters in tungsten are reported. A recently developed atomistic kinetic Monte Carlo method employing empirical interatomic potentials was used to investigate the behavior of clusters composed of three interstitial-helium atoms near {111}, {110} and {100} free surfaces. Multiple configurations were examined and the local energy landscape was characterized to determine cluster mobility and the potential for interactions with the surface. The clusters were found to be highly mobile if far from the surface, but were attracted and bound to the surface when within a distance of a few lattice parameters. When near the surface, the clusters were

transformed into an immobile configuration due to the creation of a Frenkel pair; the vacancy was incorporated into what became a He_3-vacancy complex. The corresponding interstitial migrated to and became an adatom on the free surface. This mechanism of cluster immobilization and adatom formation may provide a significant source of helium retention in and surface degradation in tungsten divertors. Clearly, the ejection of one adatom to the surface does not result in significant reconstruction of the surface. However, the cumulative effect of many such events should be studied to understand its potential as a unit process that may contribute to fuzz formation. These helium-vacancy clusters may also provide significant trapping sites for tritium and increase tritium retention. It should be noted that there are some differences between these results and molecular dynamics simulations reported recently by Hu et al. (Surf. Sci. 626, 2014, pp. 21-25); these indicate that atomic vibrations may play a stronger role in the energy landscape near free surfaces, leading to the Monte Carlo model somewhat underestimating the interaction between He clusters and free surfaces.

Migration of rhenium and osmium in tungsten

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We report a series of *ab initio* studies based upon density functional theory for the behavior of rhenium and osmium atoms in body-centered-cubic tungsten crystal. Contrary to the fast one-dimensional migration of self-interstitial atoms, interstitials of these solute elements in tungsten have three-dimensional motion because they form a mixed dumbbell having a low rotation energy barrier. The migration of these solute elements strongly influences the effects of radiation upon the materials, and our results suggest that the low rotation energy barrier leading to three-dimensional migration is a property that is key to the explanation of the radiation effects experimentally observed in tungsten-rhenium and tungsten-osmium alloys.

Primary defect production in displacement cascades in beryllium

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Beryllium is an important part of the future fusion reactor blanket. The degradation of beryllium properties in severe radiation environment is caused by the accumulation of microstructural defects (dislocations, voids, gas bubbles) that arise as a result of radiation damage accumulation. The creation of primary damage mostly occurs in collision cascades initiated by fast neutrons escaping the hot plasma. In contrast to other reactor structural and functional materials, little is known about cascade damage in beryllium.

Here we report the results of a systematic investigation of collision cascades in beryllium. Applying Molecular Dynamics (MD) at 600 K, we demonstrate that cascades in Be are remarkably different from cascades in more heavy metals. For example, the collective mode of damage production in Be is manifested in the low and relatively narrow recoil energy range of 0.5-3 keV. Recoils of higher energies are easily transported in the matrix, creating along the trajectory multiple subcascades from secondary recoils in the above-mentioned energy range. The efficiency of point defect survival after the cascade ballistic stage is less than 25%, as compared to NRT standard, while the created damage

consists of individual vacancies and interstitials, with a marginal admixture of di- and tri- vacancies. Finally, we demonstrate (both by MD and first-principles simulations) that self-interstitials are highly mobile in Be and cause strong in-cascade recombination that remarkably decreases the number of defects escaping the cascade region and contributing to the development of secondary damage.

Design of composite materials for outgassing of implanted He

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We demonstrate the computational design of solid-state interfaces patterned to achieve templated precipitation of implanted helium (He). By combining multiscale modelling with designer experiments, we show that at fcc-bcc interfaces, He initially precipitates into a quasi-periodic array of stable, sub-nanometer platelet-shaped clusters. This behavior is due to the spatial heterogeneity of interface energy: He wets high energy, "heliophilic" regions while avoiding low energy, "heliophobic" ones. At semicoherent interfaces, the heliophilic regions are located at misfit dislocation intersections (MDIs).

We then develop a set of criteria that MDI distributions must satisfy to promote the precipitation of He into stable linear channels, rather than isolated precipitates, and identify several candidate heterophase interfaces whose MDI distributions satisfy these criteria. Such channels are pathways for the removal of He through outgassing and may be used to mitigate He-induced damage in future structural materials in nuclear energy applications. Our design ensures robustness by providing solution envelopes, rather than discrete optimal solutions, and incorporates synthesis as a constraint.

This material is based upon work supported as part of the Center for Materials at Irradiation and Mechanical Extremes, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number 2008LANL1026. Support for interface design was provided though the Laboratory Directed Research and Development program at Los Alamos National Laboratory under Project No. 20130118DR, under DOE Contract DE-AC52-06NA253

Growth of helium bubbles in tungsten under realistic rates

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The growth process of helium bubbles in tungsten is investigated using molecular dynamics and parallel replica dynamics for growth rates spanning six orders of magnitude (10^{12}–$2\times10^{6}\,\mathrm{He\,s^{-1}}$). Our results show clear differences in the evolution of bubbles as a function of the growth rate, a consequence of competing kinetics at the atomic scale. Fast and slow growth regimes are defined relative to typical diffusion hopping times of tungsten interstitials around the helium bubble. For a given number of helium atoms, slow (realistic) growth rates allow the diffusion of interstitials around the bubble. Due to the extended nature of the associated crowdions and their elastic interaction with the surface, this diffusion process favours the biased growth of the bubble towards the surface. In contrast, at fast growth rates interstitials do not have sufficient time to diffuse around the bubble. This leads to a more isotropic growth and allows the bubbles to grow larger before they burst, increasing the damage on the surface. Our results demonstrate the importance of capturing the correct relative rates of competing atomic-scale kinetic processes in describing larger scale phenomenon and have implications for the growth of fuzz, a detrimental phenomenon observed in plasma-irradiated tungsten.

Present status of plasma-surface interaction investigations for EAST and CFETR

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The Experimental Advanced Superconducting Tokamak (EAST) is the world's first fully superconducting magnetic confinement facility with ITER-like magnetic field configurations and heating schemes. Before 2014 EAST campaign, the upper divertor of EAST has been upgraded with W/Cu PFCs, with ITER-like W monoblocks for the divertor targets for heat fluxes up to 10MW.m−2, flat type W/Cu PFCs for the divertor dome and baffles for lower heat loads of 4~5MW.m−2. The Materials and Plasma Evaluation System (MAPES) project, which is located at the midplane outboard H port of EAST, aims to provide a comprehensive and flexible experiment platform for Plasma-Materials Interactions (PMI) research and the test of big engineering components in real tokamak environments. During 2014 campaign, several PMI diagnostics have been installed to observe PMI processes at the MAPES samples. A Langmuir probe array embedded in samples and a dedicated optical emission spectroscopy system provide information on local background plasma and impurity. The temperature profile on the sample surface can be monitored by infrared camera at M sector and embedded thermocouples. The CCD camera at D mid-plane port can be used to observe the exposure processes on the sample surface in real time.

To promote the development of the fusion energy for ultimate use in China, design activities of the Chinese Fusion Engineering Test Reactor (CFETR) have commenced. CFETR will be an important facility to bridge from ITER to DEMO, which is a necessary step toward the fusion power plant. The main objectives of CFETR are steady-state operation, full cycle of fusion power and T fuel. It relies on the existing ITER physical and technical bases and will be complementary to ITER. Due to the moderate fusion power (~200MW) production in the first phase, similar technical approaches for EAST will be used in the first operational phase of CFETR. Full W-PFCs with an ITER-like divertor configuration could be used in the first phase. New concepts and technologies will be required in the second phase with an expected fusion power of up to 1GW. Therefore, advanced divertor configurations such as snowflake and super-x are alternative concepts and experiments with snowflake divertor operations on EAST are foreseen.

Comparison of a quantitative diffusion-trapping model with experiments on D uptake in damaged W

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Uptake of deuterium into defect rich tungsten was studied experimentally as a function of temperature and D fluence as a test case to compare quantitatively with modelling. First recrystallized W samples are implanted with 20 MeV W^{6+} ions. This creates a damaged layer of about 2.5 µm thickness. Subsequently, these samples are exposed to low-temperature deuterium plasmas to decorate the defects created by W^{6+} irradiation. In order to avoid further modification of the samples during plasma exposure due to impinging ions with sufficient energy to create displacements, the exposure is typically performed at floating potential. Under these conditions, the impinging ions are predominantly D_3^+ with a kinetic energy of 15 eV, respectively 5 eV/D. The ion flux is about $6x10^{19}$ D/m²s under these "gentle" loading conditions. The experimental procedure furthermore consists of depth profiling of the retained D by nuclear reaction analysis (NRA), as well as the

quantification of the total D amount and the investigation of D binding energies by temperature programmed desorption (TPD).

These experiments are an ideal benchmarking case for a diffusion-trapping code TESSIM[1]. They provide comparatively large and easily measurable deuterium inventories in a well-defined volume (i.e., the damaged layer). Furthermore, the samples do not change their trap density profiles during plasma exposure. For our benchmark, calculated D depth profiles after implantation as well as TPD spectra are quantitatively compared to experimental results. We try to minimise the number of free parameters in the model, with the goal being self-consistent and predictive. Our test case is based on samples irradiated with 20 MeV W^{6+} to a fluence of $8x10^{17}$ W/m^2, which corresponds to about 0.5 dpa. The modelled data set includes a set of samples exposed to plasma under identical conditions and degassed with different heating rates in order to elucidate binding energies and pre-exponential factors by the joint comparison of all simulated and measured TPD spectra. Using these parameters, we examined the dependence of the D inventory in damaged W samples as a function of fluence and temperature. To assess and determine parameters which are uncertain at very low hydrogen energies and affect the effective incoming hydrogen flux, i.e., reflection yield, stopping range and possible surface processes, we repeated the same experiments at a moderate sample bias of -100 V, which corresponds to 38 eV/D at an ion flux of $9x10^{19}$ D/m^2s, for further validation.

In our contribution, we present the details of the model and its underlying assumptions, and demonstrate that the model accurately predicts the fluence dependence of D depth profiles in damaged W under floating and biased plasma exposure conditions without any parameter adjustments. We also discuss shortcomings concerning the description of the temperature dependence of D retention in damaged W. Based on a parameter sensitivity study, we show how only one additional parameter can remedy the observed discrepancy of model and experiment. In the case presented here, it is necessary to vary the effective incident ion flux with the sample temperature. We also discuss possible physical explanations for the apparent temperature dependence of the effective ion flux.

1. K. Schmid et al., J. Nucl. Mater. 426 (2012) 247–253 .

On hydrogen transport in solids with traps: influence of broad-band energy distribution and multiple trapping

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Tritium retention in the first wall materials is one of the key issues in the performance of future fusion reactors. Therefore, calculation of hydrogen trapping and transport in fusion wall materials is of particular importance. However, now understanding of underlying physical processes is far from complete. There are experimental phenomena, which are still to be explained, and theoretical predictions, which have not been confirmed or disproved experimentally yet. For example, recent measurements on tokamaks JET and DIII-D showed asymptotic dependence of hydrogen outgassing flux, $\sim 1/t^{0.7}$, instead of expected from classical diffusion $\sim 1/t^{0.5}$. Also, many DFT calculations show that one tungsten vacancy can trap up to 6 hydrogen atoms with different binding energies. This possibility is not usually accounted for in calculations of hydrogen transport, and it is not clear whether it has or not a sufficient influence on the experimental observations.

In the present work we address both of these issues. It was already shown [1,2] that introducing of the broadband distribution of traps over binding energies with hydrogen can explain “anomalous” outgassing flux, mentioned above. Although extension of well-known rate equations, describing hydrogen diffusion in presence of traps, for this case is straightforward, their solution runs into sufficient difficulties. A computer code able to deal with these problems was developed. Modelling of

thermodesorption spectra (TDS), performed with the code, demonstrated that the role of additional trap cites can be sufficient in describing experimental results [3].

The model for H transport with multiple trapping was developed. The main equations of the model are a further development of the rate equations for diffusion in presence of traps. These equations are intrinsically nonlinear and their solution in the general case can be obtained by numerical calculations. However, several limiting cases when analytical solution is possible were considered. Analysis of these simple situations gives a general understanding of effect of multiple trapping on H transport. In order to investigate possible influence of multiple trapping on TDS, numerical solution was done.

References

1. S.I. Krasheninnikov, E.D. Marenkov, R.D. Smirnov, A.A. Pisarev. Physica Scripta, 2014, V. 2014, T159, P. 014060

2. S.I. Krasheninnikov, E.D. Marenkov, Physics Letters A, V. 378, I. 21, P. 1526–1530

3. R.D. Smirnov, S.I. Krasheninnikov, J. Guterl, M.J. Baldwin, R.P. Doerner, Contrib. Plasma Phys., 2014, V. 54, P. 610-614.

In situ study of isotope exchange mechanism in self-ion damaged tungsten

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Fuel retention in wall materials is an important issue due to safety limitation of total tritium amount in ITER and future fusion devices. Tungsten is the material which is due to its favourable properties of low hydrogen solubility, high melting point and low sputtering yield used in the present and future fusion devices. However, due to the high energy neutrons produced in the fusion reaction, the material will be damaged creating traps in the material which could lead to large amount of retained fuel. In order to study retention in such materials the neutron-damage was simulated by bombardment of tungsten by high energy 20 MeV W ions in the present experiment.

Up to now the hydrogen isotope retention in undamaged and damaged W was studied by *ex-situ* measurements, mainly by nuclear reaction analysis (NRA) and thermal desorption spectroscopy. In order to study the dynamics of deuterium retention we have investigated interaction of atomic deuterium with damaged tungsten by *in-situ* NRA employing nuclear reaction $D(^3He,p)\alpha$ [1]. With the same set-up the isotope exchange in damaged W was studied. Here, the sample was first exposed to deuterium atoms at 590 K to fluence of 4.5×10^{23} D/m^2, which was enough to almost completely saturate the damaged layer. After this the sample was exposed to hydrogen atoms with H flux of 5.55×10^{18} H/m^2. In order to see the effect of deuterium desorption due to the elevated temperature, the sample was between the two isotope exposures for one night (20 h) left at 590 K in vacuum, which resulted in D decrease for 27 % in the damaged layer. After the H atom exposure the D concentration in the damaged layer decreased in almost the same time (22h) for another 40 % from the initial concentration, which is a clear indication that isotope exchange took place. After 100 h of H exposure, fluence 2×10^{24} H/m^2, almost complete D removal was achieved, leaving 2 % of deuterium in the damaged layer. The isotope exchange was also studied at 500 K but in that case D was removed only in the near surface layers up to 1 μm.

[1] S. Markelj, O. V. Ogorodnikova, P. Pelicon, T. Schwarz-Selinger, P. Vavpetič, I. Čadež. Phys. Scr. T159 (2014) 014047.

This work was supported and carried out within the framework of the European Fusion Development Agreement and EUROfusion Consortium. Research Project was part of the CRP carried out under the sponsorship of the IAEA. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

Bridging model and real systems with laboratory experiments: dynamic retention of deuterium in tungsten

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In this contribution we will present our laboratory experimental approach, which has been especially developed to ease the comparison with DFT calculations and other modeling methods. Not only we want to quantify accurately e.g. deuterium dynamic retention but we also strive to understand the chemical and physical origin of deuterium and tungsten interactions. To this end, we have built an apparatus allowing preparation of tungsten samples, ionic implantation of deuterium with various fluxes and quantification of deuterium retention, everything being performed *in-situ* in ultrahigh vacuum. For precise quantification of deuterium retention, a state-of-the-art differentially pumped Temperature Programmed Desorption (TPD aka TDS) system has been designed allowing sub-monolayer sensitivity i.e. once the implantation depth is taken into account we are able to study fuel retention down to very low deuterium atomic densities (10^{-5} and below). This sensitivity eases the comparison with theoretical methods and will help to decipher surface effects in retention/release processes in model materials such as low defect density poly- and single crystals.

As an example of the power of this experimental approach, the study of the dynamic retention of deuterium in a model tungsten material will be presented. Dynamic retention is a process where release of retained fuel can be delayed from a tokamak plasma discharge, i.e. during reactor down-time, and can account for large portion of the fuel inventory [1].

With our new *all-in-situ* apparatus, we first measured deuterium retention for low fluences in the 10^{17} D/m^2 to 10^{21} D/m^2 range, extending the available literature explored range to nine orders of magnitude. Second, we demonstrate that the release of deuterium from tungsten occurs at room temperature and accounts for more than two thirds of the loss of implanted fuels on timescales typically of hours and days. Third, the evolution of TPD spectra as a function of waiting time in vacuum at 300 K strongly suggest that several binding energies are associated with deuterium retention in low defect density tungsten, *even when a single TPD desorption peak is measured with TPD*. These laboratory observations can be well explained by Density Functional Theory (DFT) calculation that models the trapping of several deuterium atoms on a single tungsten vacancy.

[1] Loarer *et al.*, Nucl. Fusion 47, (2007) 1112

Hydrogen atom recombination on tungsten at high temperature: a combined experimental and theoretical work

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The realization of future fusion reactors has revealed the need of new data on hydrogen recombination on several kinds of materials at high temperature level. In the literature, one can found only data at low temperature for different materials (silica, stainless steel, some pure metals and carbon). Today tungsten appears one of the most promising materials with respect to graphite and beryllium as plasma-facing material to use in magnetic fusion energy devices, both on the divertor and first-wall in tokamaks. Therefore it seems necessary to perform measurement of the recombination coefficient of atomic hydrogen at higher temperature levels. For this reason, in the last years, a large interest both experimental and theoretical was focused on this material and its interaction with hydrogen and its isotopes [1, 2].

In this contribution, we propose a joint experimental and theoretical investigation on hydrogen atoms interaction with a W(110) surface following a previous study we have performed on atomic oxygen interaction on quartz [3].

The experimental part is performed using the MESOX experimental set-up to evaluate the recombination coefficient of atomic hydrogen, based on the measurement of the relative concentration profiles $H\beta/H_2$ or $H\alpha$/He by optical emission spectroscopy [4, 5]. Experimental results obtained for the recombination coefficient of hydrogen atoms (γ_H) are obtained for tungsten from 700 to 1350 K.

These latter are compared with the results obtained in Molecular Dynamics (MD) simulations based on the semi-classical collisional method [6] for the recombination reaction between an atom adsorbed on the surface and an atom impinging from the gas phase. The simulation was done for the W(110) surface at two temperatures of 700 and 1000 K, for normal incidence of H atom hitting the surface and for collisional energies in the range 0.05-6 eV. The effect of adsorption site on the reaction dynamics was also evaluated.

A fairly good agreement between the experimental and calculated data was obtained.

[1] M. Rutigliano and M. Cacciatore 2011 Phys. Chem. Chem. Phys. 13 7475-7484

[2] S. Markelj and I. Čadež 2011 J. Chem. Phys. 134 124707

[3] L. Bedra, M. Rutigliano, M. Balat-Pichelin, M. Cacciatore 2006 Langmuir 22 7208-7216

[4] M. Balat-Pichelin, J.M. Badie, R. Berjoan, P. Boubert 2003 Chem. Phys. 291 181-194

[5] J. W. Coburn and M. Chen 1980 J. Appl. Phys. 51 3134-3136

[6] G. D. Billing 2000 Dynamics of Molecule Surface Interactions John Wiley & Sons, New-York

Periodic structures formation on beryllium, carbon, tungsten films mixed films by TW laser irradiation.

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Fusion devices based on thermonuclear reaction are intensely studied nowadays. A problem in study is the material composition of the first wall of the reaction chamber, erosion, deposition and fuel

retention of the mixed layers produced during device operation. The high energy fluxes usually found in the tokamak reactor (10-100 MW/m^2) are simulated worldwide using ion and electron beams, hot plasmas and laser irradiation.

270 nm and 400 nm widths periodic structures were formed on surfaces made of Be-C, Be-W and C-W mixtures immersed in air and deuterium after irradiation by ultrashort high-power laser pulses with λ=800nm which were focused directly or at 0.3 mm above the samples surfaces. The periodic structures were organized into small patches of 1 to 2 microns in size.

The 200-500 nm thin films of Be-W, Be-C and C-W mixed layers were prepared by thermionic vacuum arc (TVA) method. The interaction occurs with single or multiple terawatt laser beam pulses as well as under the interaction with the plasma produced by laser irradiation in a gaseous environment. The high power terawatt laser system (TEWALAS) has 20-30 x 10^{-15} s pulse duration, 400-450 mJ pulse energy, 10 Hz repetition rate. Features not observed with longer (nanosecond) laser pulses were revealed on the irradiated surfaces. Periodic structures were observed to depend on the number of pulses and the buffer gas. The coatings were characterized before and after laser irradiation by: Scanning electron microscopy (SEM), Atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy

While higher laser fluency could lead to the nano-diamond crystals formation in the carbon containing mixtures, at values between 0.2-0.5 mJ/cm2, i.e. around the carbon ablation threshold could still produce an increase of the sp3 bonds percentage at the expenses of the sp2 bonds. Only a decrease of oxygen content could be noticed by in depth XPS investigations for Be and W containing deposits, while a weak cumulative effect through the increase of the sp3 percent could be assumed for the carbon containing samples (direct) irradiation.

Funding by the Romanian National Authority for Scientific Research, UEFISCDI, through project number PN-II-ID-PCE-2011-3-0522 and RO-CERN Programme, project number: ELI-NP: E/03 is acknowledged.

Helium Atom Diffusion and Bubble Formation in Iron-Chromium Alloy: A First Principle Molecular Dynamics Study

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Helium in metals have a very low solubility leading to formation of either helium clusters or complexes with vacancies/interstitial. Clusters and complexes then diffuse and coalesce to form helium bubbles of nano - metric size or more. These bubbles are one of the reason for material to fail in brittle manner. We have done atomistic simulation of single helium and its cluster in Fe – 10%Cr alloy, the results of which will be passed to higher scale simulation such as, Monte Carlo and Rate Kinetic Model. The work is divided in two parts. Firstly, we discuss the diffusion of single helium in bi-crystals of six different orientation in tilt configuration and two different orientation in twist configuration. In this part, all the bi-crystals are initially annealed and then relaxed to obtain the final structure. Helium atoms are then inserted in Grain Boundary region to study the diffusion behavior in the temperature range of 700 K – 1000 K. Each system is simulated upto 10 ns. Secondly, we perform simulations on helium cluster with more than a thousand helium atoms at 800 K and 0.1 K. Then we determine the volumetric and radius relation of helium cluster with varying number of helium atoms. A brief summary of our observations are given below:

1. Migration energy of Helium in GB region is found to be ~ 0.3 - 0.7 eV [1] (depend upon orientation) an order of magnitude higher than in bulk. The obtained values are comparable with literature which is 0.28 eV & 0.34 eV for two different orientations [2]. The cage

distance is found to be in the range of 1 – 2.5 Å depending upon configuration which is of the order of lattice constant of host matrix (2.87 Å).

2. For a helium bubble containing 5500 helium atoms corresponding to 5.4 nm diameter, width of surface atom is found to be 0.9 nm. At 800 K, potential energy of bulk atoms in bubble is ~ 0.15 eV and surface atoms is 0.25 eV (~ 0.1 eV higher than bulk atoms). Per atom potential energy variation of helium atom with increasing cluster size is also obtained. On an average, helium in cluster with diameter more than 3.5 nm has per atom potential energy less than 0.15 eV. After a certain cluster size, dislocations are found to emit inside the material, detail of which will be discussed in presentation. The obtained results will be utilized in Rate Kinetic Model to obtain helium cluster distribution in ferritic steels [3].

References:

1. A. Abhishek, M. Warrier, R. Ganesh, Molecular Dynamics Simulation of Helium atom Diffusion in Iron-Chromium Bicrystal Grain, *Submitted in Trans IIM*.

2. X. He, D. Terentyev, Y. Lin, W. Yang, *J. Nucl. Mater.*, 442:S660-S666 (2013)

3. X. Hu, D. Xu, T. S. Byun, B. D. Wirth, Modelling Simul. Mater. Sci. Eng., 22:065002 (2014)

Ab initio based modelling of the energetics of nanometric interstitial clusters in Fe and W

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The crystalline defects produced under irradiation aggregate in clusters play an important role in the microstructural evolution of materials. Large time-space scale simulations for radiation embrittlement of fusion materials, based on radiation-induced defect and dislocation microstructure, generated by ions and/or neutrons, require valuable inputs for the growth of point-defect clusters. The dislocation loops at nanometric size are too small to be characterized by the experiment or too big to be investigated by a reliable energetic model as ab-initio. Empirical potentials give a good basis for self-interstitial clusters but the reliability of these potentials is continuously revised with the last advances in the field of ab-initio electronic structure calculations [1-4]. In this presentation we propose the development of an energetic model in Fe and W which is able to predict the relative stability of large self-interstitials clusters up to nanometric-size directly from ab initio calculations performed on small clusters. We will give particular attention to the relative stability of the traditional dislocation loops with <100> and ½<111> orientations in W as well as the C15 clusters, recently predicted by the DFT in Fe [5]. The theoretical findings will be compared with recent experiments.

[1] C. C. Fu, F. Willaime, and P. Odrejon, «Stability and mobility of mono- and diinterstitials in α-Fe», *Phys. Rev. Lett.*, **92**,175503, (2004).

[2] D. A. Terentyev, T. P. C. Klaver, P. Olsson, M.-C. Marinica, F. Willaime, C. Domain, and L. Malerba, «Self-Trapped Interstitial-Type Defects in Iron», *Phys. Rev. Lett.*, **100**, 145503, (2008).

[3] L. Malerba, M. C. Marinica, N. Anento, C. Björkas, H. Nguyen, C. Domain, F. Djurabekova, P. Olsson, K. Nordlund, A. Serra, D. Terentyev, F. Willaime, and C. S. Becquart, «Comparison of empirical interatomic potentials for iron applied to radiation damage studies», *Journal of Nuclear Materials*, **406**, 19, (2010).

[4] M.-C. Marinica, L. Ventelon, M. R. Gilbert, L. Proville, S. L. Dudarev, J. Marian, G. Bencteux, and F. Willaime, «Interatomic potentials for modelling radiation defects and dislocations in tungsten», *Journal of Physics: Condensed Matter*, **25**, 395502, (2013).

[5] M.-C. Marinica, F. Willaime, and J.-P. Crocombette, «Irradiation-Induced Formation of Nanocrystallites with C15 Laves Phase Structure in bcc Iron», *Phys. Rev. Lett.*, **108**, n025501, (2012).

Molecular Properties of Neutral and Charged CsH in the Context of the Heating and Current Drive Systems [1*]

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We present molecular data for neutral and charged CsH that can be formed in negative H/D ion source used in TOKAMAK plasma heating. Negative ion production is a crucial issue for the International Thermonuclear Experimental Reactor (ITER) [1]. It is important to know the chemistry and dynamics of Cs in this source because it can help to control the unwanted Cs transport to the reactor and minimize unfavourable compounds formation with impurities in the background plasma. Chemistry of Cs is rather complex and accurate molecular data on the structure and properties of Cs compounds are still lacking [2,3].

We report the results of quantum-chemical study the structure and molecular properties of CsH. Neutral, cationic and anionic species are studied using multi-reference Complete Active Space Perturbation Theory (CASPT2). In addition, we present also preliminary results for Cs_2. Common denominator of our approach is the application of high-level computational methods of quantum chemistry for the calculations of reliable data (spectroscopic properties, ionization potentials, electron affinities, spin-orbit corrections) within "chemical accuracy" [4]. It is expected that our results will form complementary set to existing experimental data and could help experimentalists in optimal design of the Cs oven that is an important part of the RF-driven negative ion source.

References

[1] E. Speth, H.D. Falter, P. Franzen, U. Fantz, M. Bandyopadhyay, S. Christ, A. Encheva, M. Froschle, D. Holtum, B. Heinemann, W. Kraus, A. Lorenz, C. Martens, P. McNeely, S. Obermayer, R. Riedl, R. Suss, A. Tanga, R. Wilhelm, D. Wunderlich: Overview of the RF source development programme at IPP Garching. Nucl. Fusion 46 (2006) S220.

[2] W. Kraus, U. Fantz, P. Franzen, M. Froschle, B. Heinemann, R. Riedl, D. Wunderlich: The development of the radio frequency driven negative ion source for neutral beam injectors (invited). Rev. Sci. Instr. 83 (2012) 02B104.

[3] U. Fantz, P. Franzen, D. Wünderlich: Development of negative hydrogen ion sources for fusion: Experiments and modelling. Chem. Phys. 398 (2012) 7.

[4] F. Aquilante, L. De Vico, H. Ferre, G. Ghigo, P.A. Malmqvist, P. Neogrady, T. Pedersen, M. Pitonak, M. Reiher, B. Roos, L. Serrano-Andrés, M. Urban, V. Veryazov, R. Lindh: MOLCAS 7: The next generation. J. Comput. Chem. 31 (2010) 224.

[*] This contribution is dedicated to Dr. Peter Franzen who was the initial *Spiritus movens* in our research.

Positron annihilation lifetime measurement and X-ray analysis on energetic heavy ion beam irradiated polycrystalline tungsten

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In future fusion reactors, a large number of high-energy neutrons will be generated by deuterium–tritium fusion reactions. These neutrons will irradiate the reactor wall and in turn the physical properties of reactor wall material will get modified [1]. Tungsten is considered as the most likely material to be used in divertor section of ITER like Tokamak, because of its attractive physical properties e.g. it can withstand high temperatures, low activation, does not transmute into long-lived radioactive isotopes and has a low erosion rate [2]. In fusion reactor, the flux of high-energy neutrons (14 MeV) will create a large number of displacement damages in tungsten and it will lead to change in physical properties of tungsten [3].Thus, it is imperative to understand the effect of radiation induced damage, on properties of tungsten, and its implications for use of tungsten in a reactor environment. Energetic heavy ion irradiation method is taken as a proxy for neutron irradiation to simulate radiation damages in tungsten.

In order to simulate radiation damages in tungsten, potential plasma facing materials in future fusion reactors, gold ion beam is employed to induce damages in tungsten. Tungsten specimens were irradiated with gold ions of energy 120MeV at different fluences. Positron annihilation lifetime measurements were carried out on pristine and annealed tungsten before and after energetic heavy ion beam irradiation. The variation in positron annihilation lifetime in ion beam irradiated tungsten specimens confirms evolution of vacancy clusters under heavy ion irradiation. The structural properties of pristine and annealed tungsten before and after energetic heavy ion beam irradiation have been investigated by employing X-ray diffraction method. Substantial modifications have been in observed in structural parameters. The induction of damages in metallic tungsten is mainly attributed to high electronic energy losses, which is 40keV/nm in present case as obtained from SRIM software. The detail results and their interpretation will be discussed during presentation.

1. M. R. Gilbert, S. L. Dudarev, S. Zheng, L. W. Packer, J. –Ch Sublet, Nucl. Fusion 52 (2012) 083019.

2. G. Pintsuk, I. Uytdenhouwen, Int. J. Refra. Metl. Hard Mater. 28 (2010) 661.

3. V. Barabash , G. Federici, M. Rodig, L. L. Snead, C. H. Wu, J. Nucl. Mater. 283-287 (2000) 138.

Modeling of hydrogen desorption from tungsten surface

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Hydrogen retention and recycling on metallic plasma-facing components are among the key-issues for future fusion devices due to both safety and operational reasons. Understanding of

these processes requires proper description of hydrogen desorption from metallic surface, which is usually modeled by the desorption flux $\Gamma_{out} = Kc_s^{\gamma}$. Here the desorption rate constant K is often approximated by $K = K_0 e^{-E/T}$. However, for tungsten, which has been chosen as divertor material in ITER, desorption parameters (E, K_0,γ), experimentally measured for fusion-related conditions, show a large discrepancy[1]. Indeed, various complex phenomena may affect recombination of surface hydrogen atoms into molecules (e.g atomic islands, roughness, surface reconstruction, impurities, etc) [2]. Understanding the processes governing hydrogen desorption from tungsten and their dependencies on material conditions is thus required to provide hydrogen desorption models reproducing experimental data.

In this work, we therefore investigate hydrogen recombination and desorption on tungsten surfaces using molecular dynamics simulations and accelerated molecular dynamics simulations to analyze adsorption states, diffusion, hydrogen recombination into molecules, and clustering of hydrogen on tungsten surfaces. The quality of tungsten hydrogen interatomic potential is discussed in the light of MD simulations results, showing that three body interactions in current interatomic potential do not allow to reproduce hydrogen molecular recombination and desorption. Effects of surface hydrogen clustering on hydrogen desorption are analyzed by introducing a kinetic model describing the competition between surface diffusion, clustering and recombination. Different desorption regimes are identified and reproduce some aspects of desorption regimes experimentally observed.

[1] R. Causey, Journal of Nuclear Materials 300 91–117 (2002)

[2] S. Markelj, et al., Applied Surface Science 282 478-486 (2013).

Macroscopic rate equations modelling of trapping/retrapping of hydrogen isotopes in W materials

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Macroscopic rate equations (MRE) are an efficient way to investigate migration and trapping of hydrogen isotopes (HIs) in metallic materials from nanometer to centimeter scales. In MRE, HIs are split into two populations: mobile and trapped. Mobile species are subject to diffusion in the metallic matrix and can be trapped in specific sites with various trapping energies. To get relevant forecasts for tritium inventory in ITER, MRE codes are often used and need critical inputs like diffusion coefficients, trapping energies, trap densities… These parameters can be derived from experimental data such as Thermal Desorption Spectrometry (TDS), Ion Beam Analysis (IBA) and tritium gas absorption/desorption.

Here, we present results of a MRE code called MHIMS (Migration of Hydrogen Isotope in MetalS) developed at IRFM in the case of HIs in tungsten. We use the code to model several existing experiments. To obtain relevant data, each experimental step has to be studied from the implantation to desorption phase including the resting phase corresponding to the duration during which the sample waits at room temperature between implantation and desorption. Indeed, experimental parameters (temperature, flux, pressure and time) are of first importance for predicting the behavior of HIs in materials.

First, we use TDS spectra and IBA depth profiles to constraint trapping parameters (energies and densities of traps). With a jump attempt frequency of 10^{13} s^{-1}, detrapping energies of 0.85 eV, 1.00 eV and 1.5 eV are inferred. The density of traps is ~5×10^{-4} trap/tungsten atom. During ion implantation, if the flux is > 10^{18} D/m²/s, a trap creation process is introduced leading to trap density greater than 5×10^{-4} in the ion stopping zone which is correlated with the IBA depth profiles [1,2]. With these trapping parameters, we investigate the effect of experimental condition (temperature, fluence) on HI inventory for ions implantation. First we modelled the evolution of retention with fluence for implantation at both 300 K and 500 K. The results obtained are then confronted to experimental results [3, 4]. It is observed that for implantation temperatures > 600 K, the hydrogen inventory decreases by several orders of magnitude which is also noted in experimental observation [5]. Finally, the effect of resting time between implantation and TDS is investigated. It is shown that, after implantation at 300 K, the overall inventory of HIs can significantly decreases due to outgassing from the 0.85 eV trap during resting time. The corresponding peak in TDS spectrum disappears and the HIs are much deeper implanted in the bulk.

[1] V. Kh. Alimov, J. Roth, M. Mayer, J. Nucl. Mater. 337-339 (2005) 619-623

[2] W. Wang, J. Roth et al, J. Nucl. Mater. 299 (2001)124-131

[3] O.V. Ogorodnikova et al., J. Nucl. Mater. 313-316 (2003) 469-477

[4] Z. Tian et al., J. Nucl. Mater. , 399 (2010) 101-107

[5] J.P. Roszell, J. W. Davis, J. Nucl. Mater. 429 (2012) 48-54

Impact of transient events on DEMO PFC

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Thermo-hydraulic analysis of design concept of mono-block type water cooled DEMO PFC module with Cu alloy/EUROFER tube have been performed for DEMO operations with the mitigated and unmitigated ELMs under different water cooling conditions . It is shown that for DEMO I operation with ELMs all material temperatures saturate. However, for unmitigated ELMs the W surface temperature exceeds the melting point at the ELM peaks positions and the tube material temperatures could remain within allowable range only for PWR-like cooling conditions. For mitigated ELMs all temperatures remain within allowable temperature range for PWR-like cooling. For DEMO II operation with unmitigated ELMs the maximum temperatures also saturate within the allowable range, except W, which melts at the ELM peaks positions. The saturation occurs due to W vapor shielding which results in reduction of heat flux to the water coolant under PWR-like cooling conditions. For DEMO II operation with mitigated ELMs the material temperatures increasing and exceeding allowable upper limits and the overheating occurs under PWR-like cooling conditions due to absence of vapour shielding effect. For modified PWR cooling condition with lower inlet water temperature material temperatures saturate and are within allowable limits, except EUROFER and W, which maximum temperature is still much higher than the upper limit, although stays below the melting point.

Multi-timescale modeling of helium-induced nano-fuzz structure formation on tungsten surfaces

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Although tungsten is a promising candidate for the surface material of divertors mounted in Tokamak type fusion reactors, fuzz-like structure growth is reported on the plasma facing tungsten surface at a high temperature under He ion irradiation. The detailed mechanism of this surface reaction is still not well understood at the atomistic level. Molecular dynamics (MD) simulations revealed several basic atomistic events, such as the migration of interstitial He and bubble formation, resulting in W interstitial creation. However, due to the restriction of the time scale, surface topography change simulated solely by MD is quantitatively far from the experimental observation. In order to take the effects from rare events into account we have developed a direct combination model of MD and lattice kinetic Monte Carlo simulations. He concentration, stress from He bubbles, and mobility of W surface adatoms are evaluated and the surface structure evolution is in excellent agreement with the experimentally observed evolution speed under the same conditions.

Ab initio modeling of the dislocation-carbon interaction in ferritic steels

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Under high energy neutron irradiation, the associated kinetics can be strongly modified and new solutes such as He solutes come into play. As a starting point for the treatment of plasticity and embrittlement, the present work focusses on impurity dislocation interactions at the atomic scale. These dislocation-impurity interactions are driving forces for solute strengthening/softening. While long-range dislocation interactions are well-described by elasticity theory, short-range interactions with crystal lattice and impurities depend on the local interatomic interaction, thus requiring an accurate description of atomic bonding, down to the electronic structure level. In this work, we investigate the effect of carbon interstitial solutes on screw dislocations in body-centered cubic (bcc) iron using Density Functional Theory (DFT) calculations.

In bcc metals, plasticity is governed by the motion of screw dislocations with ½<111> Burgers vector. These dislocations are subjected to a lattice resistance that can be described through the two-dimensional energy landscape of the dislocation in the {111} plane, the so-called 2D Peierls potential. Ab initio electronic structure calculations showed that iron has a specific and surprising behavior compared to the other bcc transition metals. In particular the hard core position is a monkey saddle between adjacent easy core energy minima, at variance with empirical potentials for iron that behave strikingly different with the hard core being the maximum of the Peierls potential [1, 2].This new picture of the Peierls potential in iron has major consequences on the dislocation-solute interaction in iron. The interaction between a screw dislocation and an interstitial carbon atom is investigated for various solute positions in the neighborhood of the dislocation core. It is found that this interaction is strong enough to locally induce an inversion of the stability of the hard versus easy core configurations. A low energy configuration is indeed found, where the solute atom is trapped at the center of the dislocation core in the hard core configuration, forming a carbon centered regular trigonal prism similar to the cementite building unit. None of the existing empirical potentials for FeC are able to reproduce this core reconstruction. These new findings have an important impact on the carbon enrichment on dislocations. Indeed we show that the strong attractive carbon-dislocation interaction energy involved in this unexpected configuration leads to the dislocation core saturation by carbon atoms at room temperature and below, even for very low bulk carbon concentrations.

[1] L. Ventelon, F. Willaime, E. Clouet and D. Rodney, "Ab initio investigation of the Peierls potential of screw dislocations in bcc Fe and W", Acta Mater. **61**, 3973-3985 (2013).

[2] L. Dézerald, L. Ventelon, E. Clouet, C. Denoual, D. Rodney and F. Willaime, "Ab initio modeling of the two-dimensional energy landscape of screw dislocations in bcc transition metals", Phys. Rev. B **89**, 024104-13 (2014).

Reaction-diffusion based modelling of deuterium retention in Be

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Beryllium and W-based material systems, as well as their interaction with hydrogen isotopes and impurities, both intrinsic and seeded, represent a particular interest for ITER and future reactor-scale devices Multi-scale approaches combining simulations, semi-analytical methods and data from dedicated laboratory experiments seem to be promising in describing the properties and evolution of such complex material systems.

As a starting point, a model based on coupled reaction-diffusion systems (the CRDS code [1]) is used in this work to interpret experimental results on hydrogen retention in Be. The model allows introducing multiple diffusing species including mobile traps and was successfully applied to explain temperature-programmed desorption (TPD) experiments with monocrystalline and polycrystalline Be irradiated to low D^+ fluences ($\sim 3\times10^{19}$ m^{-2}) in the Artoss facility [1]. The model uses results of DFT simulations [2] to address the diffusion and trapping properties of a D/Be system.

In this contribution, the CRDS code is modified by implementing multiple trapping in mono-vacancies with a consecutive reduction of the de-trapping energy. The code is applied to interpret the TPD spectra obtained after the implantation of D ions into Be. For fluences above 2×10^{23} D^+/m^2, additional low-temperature peaks were observed below 500 K, which are attributed to over-saturation of the surface layer with D, leading possibly to Be amorphization and hydride phase formation. The effect is observed both in monocrystalline and polycrystalline Be, with a higher peak intensity in the polycrystalline case. An overview of the CRDS code and a comparison of experimental and modelling results will be presented.

[1] R. Piechoczek et al., J. Nucl. Mater. 438 (2013) S1072

[2] A. Allouche, J. Phys. Chem. C 114 (2010) 3588

Software engineering strategies for fast development and growth of fusion modeling tools

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Controlled nuclear fusion is one of the most daunting technological challenges of our time; as such, a significant amount of effort has been aimed at the development of computational tools to study phenomena associated with the design and operation of fusion devices. However, this effort has not been fully articulated; the amount of legacy code, development duplicity and difficulty in interfacing codes are just some of the manifestations of this lack of coordination. To make better use of the human and hardware resources available for computational efforts in fusion, a universal platform for code development should be implemented. As physicists, engineers and computer scientists involved

in the field, an effort should be made to develop such platform, which would allow community-based development of useful codes, better interaction among different codes, faster evolution and enhancement of modeling capabilities. This could be implemented by borrowing concepts already well-established within the software development community and standardized coding practices, just as it was proposed by the EFDA Integrated Tokamak Modeling effort, and accomplished to a certain extent with the European Transport Solver code as an example. As a case study, the conceptual design of two tools, an edge plasma impurity MC transport code (think DEGAS, EIRENE) and a Monte Carlo particle transport in solids code (think TRIM , ERO and all its derivations) to study plasma-material coupling will be selected. The analysis of the two codes and their interaction from an UML point of view will be presented and discussed.

Development of interatomic potential for W-N-H system

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Tungsten monocarbide (WC) and mononitride (WN) are getting more attention from physicists and material scientists due to their unique physical and chemical properties such as extreme hardness and chemical inertness. These compounds belong to the most promising engineering materials with wide range of industrial applications.

N_2 or noble gases will most likely be used as seeding species to reduce the power loads on the tungsten divertor target of ITER in relevant heated scenarios. The seeding species will interact with the plasma-facing materials beryllium and tungsten, and, in the case of nitrogen, also form chemical bonds with the wall surfaces as well as with plasma hydrogen isotopes. This raises a special interest in for W-N and N-H interactions in the fusion community.

Since interatomic potentials for W-Be (Björkas et al. 2010) and W-C-H (Juslin et al. 2005) interactions have already been developed, the W-N-H potential is a new important piece of a potential puzzle, soon hopefully containing all possible interactions between the fusion reactor materials.

In this work the potential development process will be discussed and possibly some preliminary results will be shown.

Retention of deuterium and helium in monocrystal of tungsten

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Beginning with self-atoms damaged mono-crystal of W, we bombard the surface with D and He at the impact energy of 30 eV in order to predict the retention rate of the impinging atoms as well as their distribution inside the material. Our calculation is based on molecular dynamics simulation using high-performance computing. The goals was to distinguish between alternative outcomes: (1) the retention rate is proportional to the number of vacancies – consistent with recent experiments on the retention of D in damaged W, (2) vacancies will be filled by aggregates of D or He, leading to unstable surfaces, e.g., bubbling and blistering of the surface, and (3) some fraction of deuterium will fill the interatomic space in the W crystal lattice, creating a “protective layer” close to the surface, even in absence of significant tungsten lattice defects.

First-principles and Monte-Carlo modelling of phase stability and point defects in ternary Fe-Cr-Ni alloys

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Fe-Cr-Ni alloys and austenitic steels form an important class of high temperature structural materials developed for nuclear and related applications. Despite the fact that Fe-Cr-Ni alloys are one of the most extensively studied ternary alloy systems, the relation between their phase diagram, magnetic phase stability and defect structures formed under irradiation is not known.

We investigate structural and magnetic properties as well as the phase stability of ternary Fe-Cr-Ni alloys by using a combination of several simulation methods [1]. Density functional theory (DFT) and Cluster Expansion methods are combined in order to derive the cluster expansion parameters characterizing bcc and fcc crystal structures. DFT-based Monte Carlo (MC) simulations are then used for predicting the fcc-bcc phase stability and order-disorder transitions in Fe-Cr-Ni at elevated temperatures. Enthalpies of formation obtained from MC simulations at finite temperatures, as well as order-disorder temperatures and short-range order parameters predicted for a broad range of temperatures are compared with available experimental data. The DFT results for $Fe_{69}Cr_{19}Ni_{12}$ structure generated from MC simulation are compared with these obtained for the special quasi-random structure (SQS) and from Magnetic Cluster Expansion [1,2]. The point defect properties of Fe-Cr-Ni alloys are investigated for selected representative structures generated using MC simulations.

This work was supported by the Accelerated Metallurgy Project, which is co-funded by European Commision in the 7th Framework Programme (Contract NMP4-LA-2011-263206), by the European Space Agency and by the individual partner organisations. It has been carried out also within the framework of the EUROfusion Consortium and has received funding from the *Euratom research and training programme* 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

[1] J.S. Wróbel, D. Nguyen-Manh, M.Yu. Lavrentiev, S.L. Dudarev, http://arxiv.org/abs/1410.0548

[2] M.Yu. Lavrentiev, J.S. Wróbel, D. Nguyen-Manh, S.L. Dudarev, Phys. Chem. Chem. Phys. 16, 16049 (2014).

He embrittlement at grain boundary of bcc transition metals: Systematic study

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To investigate what atomic properties largely determine vulnerability to He embrittlement at grain boundaries (GB) of bcc metals, we introduced a computational model composed of first principles density functional theory and a He segregation rate theory model. Predictive calculations of He embrittlement at the first wall of the future DEMO fusion concept reactor indicated that variation in the He embrittlement originated not only from He production rate related to neutron irradiation, but also from the He segregation energy at the GB that has a systematic trend in the periodic table.

Molecular Dynamics Study of Interstitialcy diffusion in fcc and bcc metals

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Neutron irradiation of reactor materials creates energetic primary knock-on atoms (PKA) in the material, which cause collision cascades in the material resulting in Frenkel pairs. These Frenkel pairs can diffuse and recombine to neutralize each other and reduce damage, form vacancies and interstitial clusters, thereby changing the material properties. Simulations across various length and time-scales are necessary to model and predict the change in material properties [1]. An important parameter in such a multi-scale study is the surviving number of Frenkel pairs. The number of Frenkel pairs and their spatial distribution from the cascade simulations will be an input to lattice and/or object Kinetic Monte Carlo (KMC) simulations [2] of diffusive-recombination of the Frenkel pairs to form voids and interstitial clusters. We carry out MD simulations of a single interstitial in fcc Cu, bcc Fe and bcc W to demonstrate interstitialcy diffusion in time scales less than a nanosecond. A cube of 10×10×10 unit cells is used. A single atom is introduced close to the center of the crystal and an NPT ensemble is used to equilibrate the system at 0 bar pressure. Periodic boundary conditions are used in all three directions with a time step of 1 fs. After equilibration, an NVE simulation is carried out to study the interstitial transport. For Cu, Fe and W, MD simulations were carried out in the temperature range 300K – 1200K, 300K – 1800K and 300K – 3500K respectively.

Stoller et al report time-scales of a micro-second for interstitial diffusion in crystals [1]. Our simulations show that interstitialcy diffusion – wherein an interstitial displaces a lattice atom, thereby making the lattice atom an interstitial – has time-scales of a few tens of pico-seconds. We therefore propose that the "interstitialcy diffusion" mechanism can play a major part in the diffusive-recombinations of the Frenkel Pairs created during the cascade. Initial results of the interstitialcy diffusion are presented. The diffusion coefficients and migration energies from the study can be used in dynamic Monte Carlo simulations and macroscopic models of defect transport to scale up in (I) number of interstitials simulated, (II) size of crystal simulated and finally (III) time simulated.

1. R.E . Stoller and L.K. Mansur, ORNL report, ORNL/TM-2005/506 (2005).

2. C. Bjorkas, et al, Phys. Rev. B, 85 (2012) 024105.