Book of Abstracts

4th International Workshop on Models and Data for Plasma-Material Interaction in Fusion Devices (MoD-PMI 2019)

18 – 20 June 2019, National Institute for Fusion Science, Toki, Japan

This workshop is organized in cooperation with the International Atomic Energy Agency (IAEA).

MoD-PMI 2019

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MoD-PMI 2019 program

2019/6/18 (Tue)			
8:40	registration		
9:30	opening		
9:35	Takeo Muroga (Deupty Director General of NIFS)		Welcome address and introduction of NIFS
session 1 (Chair: Yves Ferro)			
9:50	I-1	Sergei Dudarev	What Drives the Evolution of Microstructure of Plasma Facing Materials: Energies of Defects or Elastic Stresses and Strains?
10:20	I-2	Tomoaki Suzudo	First Principles Modeling on Radiation Defects in W and W-based Alloys
10:50	break		
11:00	I-3	Tsuyoshi Miyazaki	Linear-scaling First-principles Molecular Dynamics Simulations of Complex Nano-structured Materials with the CONQUEST Code
11:30	I-4	Johann Bouchet	Vibrational properties of the actinides
12:00	lunch		
session 2 (Chair: Hong-Bo Zhou)			
13:00	I-5	Chris Van de Walle	First-principles modelling of defects and hydrogen in oxides
13:30	I-6	Christoph Freysoldt	Modelling of charged point defects with density-functional theory
14:00	break		
14:10	I-7	Byeongchan Lee	Atomistic calculations on random nature of irradiated damage in single crystalline tungsten
14:40	O-1	Duc Nguyen-Manh	Origin of outstanding radiation resistance in W-based high-entropy alloys
15:00	group photo		
session 3 (Chair: Duc Nguyen-Manh)			
15:30	I-8	Ryo Kobayashi	Construction of efficient machine-learning potential for W-H system
16:00	I-9	Tommy Ahlgren	Corrections to sink strengths used in rate equation simulations of defects in solids
16:30	O-2	Hong-Bo Zhou	Towards understanding the influence of Re on H dissolution and retention in W by investigating the interaction between dispersed/aggregated-Re and H
16:50	break		
17:00	O-3	Shin Kajita	Deposition effects on He induced fiberform nanostructure growth
17:20	O-4	Atsushi M. Ito	Sputtering and Re-deposition Effects during Fuzz Growth Process Simulated by BCA-MD-KMC Multi-hybrid Simulation
17:40	O-5	Zhangcan Yang	Helium Bubble Growth In Tungsten Nano-Tendrils
19:00 - 21:00	Workshop dinner at Yamagami Onsen (hotspring house) *Bus for Yamagami Onsen will depart at 18:30 from NIFS		

2019/6/19 (Wed)			
session 4 (Chair: Bastiaan J. Braams)			
8:40	I-10	Predrag Krstic	Quantum-Classical Molecular Dynamics Simulation of Synthesis of Boron-Nitride Nano-Structures at High-Temperature, High-Pressure Plasmas
9:10	I-11	Paul Erhart	Tools for the construction of atomic scale models for materials
9:40	break		
9:50	I-12	Thomas Morgan	Liquid metal vapour shielding in linear plasma devices
10:20	I-13	Kenzo Ibano	Weighted PIC simulation for vapor shielding at wall under transient heat loads
10:50	I-14	Jianmin Yuan	Modifications to the Photonic and Electronic Impact Ionization Cross Sections of Ions in Dense plasmas due to the Transient Localization of Continuum Electron Wavefunctions
11:20	break		
session 5 (Chair: Hiroaki Nakamura)			
11:30	I-15	Yonggang Li	Effects of Microstructures on Surface Damage and H/He Retention in W: A multi-scale Modelling
12:00	O-6	Yves Ferro	Surface coverage dependence of the diffusion/desorption mechanisms of hydrogen from the W(110) and W(100) surfaces: a model based on DFT and thermodynamics
12:20	lunch		
session 6 (Chair: Katsuyoshi Tsumori)			
13:20	I-16	Seiki Saito	Molecular Dynamics Simulation for Hydrogen Recycling on Carbon Divertor
13:50	O-7	Mizuki Sakamoto	Impact of a high temperature target on hydrogen recycling
14:10	O-8	Takato Hirayama	Potential Sputtering from Rare Gas Solid Surface by Multiply-Charged Ion impact
14:30	O-9	Miroslaw Zlobinski	D retention in bulk Be and D co-deposited in Be layers studied by 3 different thermal desorption techniques and their modelling by CRDS
14:50	break		
session 7 (Chair: Takuji Oda)			
15:00	I-17	Bastiaan J. Braams	Recent approaches to machine learning of interatomic potentials seen from a perspective of plasma material interaction and primary radiation damage
15:30	I-18	Linfeng Zhang	Deep Learning for Multi-Scale Molecular Modeling
16:00	I-19	Utkarsh Bhardwaj	Classification of Clusters in MD Simulations of Collision Cascades
16:30	break		
session 8 (Chair: Izumi Murakami)			
16:40	O-10	Noboru Yoshikawa	Microstructural Change of Au Thin Films by Microwave Irradiation
17:00	O-11	Yugo Nagata	A monoenergetic energy-tunable positronium beam and its applications
17:20	break		
poster session			
	P-1	Daiji Kato	Vacancy clustering and stabilization in tungsten by hydrogen trapping
	P-2	Hyung-Gyu Lee	The defect formation mechanisms and change of the mechanical properties under the irradiation in pure W and W-Re alloy: Molecular dynamics study
	P-3	Jie Nan	Molecular dynamics study of materials properties of pure W and W-10Re alloy before and after irradiation
	P-4	Harsh Hemani	Inclusion of Electronic Stopping and Validation in the Open Source Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)

17:30 - 18:20	P-5	Quan Shi	Investigation of temperature and ion energy threshold for tungsten fuzz growth by Monte Carlo Simulation
	P-6	SangHyuk Yoo	Study of proton irradiation in wurtzite GaN with a-type prism-edge dislocation using molecular dynamics simulations
	P-7	Woonghee Cho	Development of Potential Model with Three-body Interaction for Tungsten
	P-8	Lukas Pichl	Recent Machine Learning Algorithms for Classification of Time Series: Recurrent Deep Learning Networks with Potential for Plasma Applications
	P-9	Izumi Murakami	NIFS Atomic and Molecular Numerical Database for Collision Processes in Plasmas
	P-10	Naoko Ashikawa	Observation of trapped hydrogen in coated tungsten on titanium specimen

2019/6/20 (Thu)			
session 9 (Chair: Daiji Kato)			
8:40	I-20	Sabina Markelj	Displacement damage stabilization by hydrogen presence under simultaneous W ion damaging and D ion exposure
9:10	I-21	Thomas Schwarz-Selinger	Influence of the presence of deuterium on displacement damage in tungsten
9:40	O-12	Kazuhito Ohsawa	Anomalous Properties of Vacancy in Tungsten and Interaction with Hydrogen
10:00	O-13	Takuji Oda	Molecular Dynamics Simulation on Interactions between Hydrogen and Vacancy Clusters in Tungsten
10:20	break		
session 10 (Chair: Suguru Masuzaki)			
10:30	I-22	Takeshi Toyama	Deuterium trapping at irradiation-induced defects in tungsten studied by positron annihilation spectroscopy
11:00	O-14	Yuji Hatano	Deuterium retention in W and binary W alloys irradiated with high energy Fe ions
11:20	O-15	Yoshio Ueda	Hydrogen isotope exchange between H and D in damaged tungsten
11:40	O-16	Toshikio Takimoto	Development of functional material for deuterium permeation observation under divertor plasma exposures
12:00	closing		

What Drives the Evolution of Microstructure of Plasma Facing Materials: Energies of Defects or Elastic Stresses and Strains?

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Density functional theory (DFT) calculations have now provided extensive information about the stable structures of elementary defects formed in pure metals and alloys under irradiation. For many types of defects, DFT simulations have also identified defect migration pathways, achieving strikingly good agreement with experimental observations and resolving fundamental questions that, in the absence of DFT models, remained outstanding for decades.

Recently, DFT simulations, combined with atomistic simulations, have also been able to offer insight into phenomena traditionally thought not to be accessible to *ab initio* methods. The notions of dipole tensor and relaxation volume tensor of defects [1], directly computable from DFT [2], enable relating the data on the structure of defects derived from DFT simulations to strains and stresses that they produce in materials. Also, through the dipole tensor formalism, it is now possible to compute energies and forces acting between defects, and between defects and dislocations. Furthermore, using relaxation volume tensors of defects derived from DFT simulations, it is possible to predict, at a fairly high level of accuracy, the volumetric swelling of materials resulting from the accumulation of radiation defects. Taking advantage of the scaling properties of elasticity equations, we can also interpolate DFT results to larger defect structures, for example vacancy clusters, cavities, or mesoscopic dislocation loops [3], and even extend the treatment to complex entangled dislocation configurations, offering a way of “mechanistically” linking the information about the defect structures observed in a material using an electron microscope, with the deformations and stresses that such defect structures produce on the macroscale.

Recent applications of the method include the interpretation of data on strains and stresses produced by the accumulation of helium in ion-implanted tungsten [4], the formation of vacancy-dominated microstructures in materials exposed to self-ion irradiation, and the use of first principles approaches to the derivation of models for finite element simulations of macroscopic reactor components.

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[2] P.-W. Ma and S.L. Dudarev, *Universality of point defect structure in body-centered cubic metals*, Phys. Rev. Mater. **3** (2019) 013605
[3] D.R. Mason *et al*., *Relaxation volumes of microscopic and mesoscopic irradiation-induced defects in tungsten*, https://arxiv.org/abs/1812.06874
[4] F. Hofmann *et al*., *Lattice swelling and modulus change in a helium-implanted tungsten alloy*, Acta Materialia **89** (2015) 352

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I-2

First Principles Modeling on Radiation Defects in W and W-based Alloys

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Tungsten (W) metals and alloys are considered as a promising candidate for plasma-facing materials for future nuclear fusion devices because of its high melting temperature, high resistance to sputtering, and high thermal conductivity. However, radiation-induced effects, such as swelling and increase in tritium retention seem to threaten its actual applicability. Thus, understanding the radiation-induced defects are critical to the application of these materials.

Rhenium (Re) and Osmium (Os) are produced from W through nuclear transmutation, and they would naturally be solute elements of W crystals under neutron irradiation. In such alloys, stable solvent-solute mixed dumbbells appear because the SIA and Re and Os substitutional atoms are attractive. We analyzed the atomistic migration patterns of these two transmuted elements and indicated that the mixed dumbbells composed of Re (or Os) and W atoms occasionaly become separated, and the Re (or Os) atom jumps to the 1NN site forming another mixed dumbbell. Because the rotation of these mixed dumbbells is easy, these solute elements can be carried for long distance by iteration of jumping and rotation events, letting them be capable of fast three-dimensional (3D) migration [1,2,3].

We also examined stability and mobility of various solute interstitials in W crystals. Through the examination, Ti, V, Cr and Mo interstitials were found to form mixed-dumbbells in addition to Re and Os. Further detailed first-principles study suggested that Ti, V, and Cr are also capable of fast 3D migration [4].

It is commonly recongnized that the most enegetically-favored SIA configuration in W would be <111> dumbbells and <111> crowdions in W. However, some DFT results show that they are not necessariliy the most favored. We revisited stability and mobility of SIAs based on accurate DFT calculations.

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Linear-scaling First-principles Molecular Dynamics Simulations of Complex Nano-structured Materials with the CONQUEST Code.

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First-principles simulations based on the density functional theory (DFT) are powerful tools to clarify the structural and physical properties of various materials at atomic scale. However, usual DFT methods cannot treat large systems containing many thousands of atoms, since the calculation cost increases very rapidly, proportional to the cube of the number of atoms *N* in the system. To overcome this size limitation, we have developed a linear-scaling[1] or O(*N*) DFT code CONQUEST. Using a recently-developed approach (multi-site support functions or MSSF[2]), the code is capable of performing high accuracy calculations on up to 10,000 atoms, while with a linear scaling approach we can treat million-atom systems[3].

In this talk, I will give an overview of the methods used in the code and present our recent applications of nano-scale materials[4,5]. I will also demonstrate that the code can perform robust linear-scaling first-principles molecular dynamics simulations of large complex systems[6,7]. The combination of using machine-learning forces[8,9] with the code will be also discussed.

This work is done in collaboration with Prof. D. R. Bowler (UCL), Dr. J. Lin, Dr. A. Nakata and Dr. R. Tamura (NIMS). The CONQUEST code[10] is developed jointly by the groups of University College London (Prof. D. R. Bowler), National Institute for Materials Science (First-principles simulation group), and the University of Bordeaux (Dr. L. Truflandier). The code will be open to public soon with the MIT license.

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[4] A. Nakata, Y. Futamura, T. Sakurai, D. R. Bowler, and T. Miyazaki, J. Chem. Theor. Comput., 13 (2017) 4146.

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[9] R. Tamura, J. Lin and T. Miyazaki, J. Phys. Soc. Jpn. 88 (2019) 044601.

[10] http://www.linear-scaling.org

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Vibrational properties of the actinides

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Density functional theory (DFT) has been an extraordinary successful tool to understand the ground state properties of the actinides and to show the fundamental role played by the 5f electrons. The inclusion of temperature effects in the calculations is even more challenging but crucial for studying the rich phase diagram exhibited by these elements.

Usually, thermal vibrations of atoms can be taken into account via the so-called quasiharmonic approximation (QHA). In this framework, the phonon dispersion relations are calculated at 0 K using density functional perturbation theory (DFPT) and the temperature is included only via the thermal dilatation, i.e., by computing the phonon spectrum at different volumes. This method has been applied with success to Th. However with only one f electron and a fcc structure, Th does not show all the complexity found in the heavier actinides. In particular, this method cannot be used on structures stabilized at high temperature by anharmonic effects and therefore dynamically unstable at 0 K such as the bcc structure adopted by the whole actinide series before the melting point.

Here we show the results of a new method based on ab-initio molecular dynamics simulations to obtain the phonon spectrum of a material at high temperature and capture the anharmonic effects [1]. Whereas all previous attempts based on the QHA failed to reproduce the behavior of the phonon modes of uranium as a function of temperature, this method can capture the effects responsible for the CDW phase transition in α-U [2]. We also show the phonon spectrum of the γ bcc structure at high temperature. Using the phonon density of states we calculate the free energies of the α and the γ structure to obtain the transition line in pressure and temperature [3].

We also present new results for the phonon spectra of the α, δ and ε phases of plutonium and we discuss the different mechanisms governing the stability and the phase transitions of these structures [4]. We will also show recent results obtained on the U-Mo system.

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First-principles modelling of defects and hydrogen in oxides

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First-principles calculations based on density functional theory can provide accurate results for the formation and migration of point defects and impurities. I will first discuss the underlying methodology and computational advances [1]. Then I will illustrate the type of results that can be obtained with the example of Al_2O_3, for which we have calculated point defects [2,3] and impurities such as nitrogen and carbon (4].

I will devote particular attention to the behavior of hydrogen in oxides. I will describe some general principles [5], and again illustrate the results with the example of Al_2O_3 [6].

Finally, I will comment on how these calculations can be used to assess radiation hardness, and determine which point defects are most likely to result from irradiation.

Work performed in collaboration with M. Choi, C. Freysoldt, A. Janotti, J. Lyons, H. Peelaers, J. Varley, and J. Weber.

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Modelling of charged point defects with density-functional theory

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Point defects such as vacancies, interstitials, or impurities play an important role in diffusion-driven transformations and ageing. In insulating or semiconducting materials, defects may carry a charge and therefore are crucial for the electrical behaviour of such materials, even if their concentrations are low. Density-functional theory calculations have proven invaluable for assigning experimental signatures to specific defect types, and for further characterizing properties that are often challenging to obtain from experiment.

Yet, the simulation of charged defects is a challenge in its own, because typical simulation setups such as the supercell approach (in which the defect is modelled in a periodic structure) are biased by artificial defect-defect interactions that are absent if the defect occurs at low concentrations. We have shown how Coulomb interactions can be addressed systematically to extrapolate to the isolated-defect limit [1]. The case of Coulomb interactions (related to charge) can be contrasted to the elastic interactions (related to the elastic dipole tensor), which are relevant also for the interplay with extended defects. Last, I will then discuss the relevance of defect-defect interactions at finite concentrations.

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Atomistic calculations on random nature of irradiated damage in single crystalline tungsten

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Tungsten is one of the high-temperature materials, and in particular, a candidate material for divertors in fusion reactors, which experience high-energy neutron irradiation. The microstructural evolution during irradiation damage is often understood with atomistic calculations, in which a few approximations as well as numerical techniques are used. Here we try to visit some of these approximations and techniques to find rooms for improvement.

The first phase of the improvement involves rethinking of the system size, ensemble, and boundary conditions, and the results can be compared with microstructures in the tungsten sample prepared with the state-of-the-art processes, which contains micro-meter-size grains. Nevertheless, a complex interplay between various factors such as temperature and grain orientation is yet to be understood in detail from a further study.

From a micro-meter-scale single crystalline tungsten, the grain orientation dominates the irradiation damage, but because of that and because of many potential pathways with equal probability, the overall damage profile appears random. Last, we briefly discuss the way experiments and calculations are compared, and talk about ways to improve the fidelity of atomistic calculations.

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Construction of efficient machine-learning potential for W-H system

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Tungsten (W) is a promising candidate as a plasma facing material (PFM) in next generation fusion reactors. Thus a lot of experimental and computational researches have been done to understand the response of W to harsh environment such as high energy neutron and/or helium irradiation and hydrogen isotope contamination. Among some study approaches, molecular dynamics (MD) is a powerful simulation tool since it can provide information and insights that cannot be obtained by the other research approaches. The reliability of the MD simulation results depend strongly on interatomic potentials used. Recently a lot of machine learning (ML)-type interatomic potentials have been developed such as neural-network (NN)[1], linear-regression with LASSO[2], gaussian approximation potential (GAP)[3] and so on, that can achieve quantum-mechanical (QM) level accuracy by learning from big data of QM calculation. Since ML potentials usually requires high dimension descriptor to precisely differentiate atomic environment, the cost of ML potentials are much higher than those of classical interatomic potentials, which is limiting the application of ML potential to very large-scale and/or long-time simulations that are required to study defect evolution under harsh environment in PFM.
We here focus on the construction of efficient NN potential for W-H system. A small number of descriptors relevant to the system are selected from a lot of candidates without loosing the accuracy using a greedy algorithm. This approach is compared with some previous methods that are aimed to reduce dimensionality of descriptors such as LASSO and orthogonal series [4], and it is shown that this approach outperforms the other methods in terms of cost performance.

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Corrections to sink strengths used in rate equation simulations of defects in solids

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Mean-field rate equations have proven to be a versatile method to simulate defect dynamics and temporal changes in the micro-structure of materials. However, the reliability and usefulness of the method depends critically on the defect interaction parameters used.

We will show that the sink strength depends also on the detrapping or dissociation process. The sink strength is much larger, than is usually used, for defects that are detrapped. Theory how to determine the appropriate sink strength is presented.

Test simulations with kinetic Monte Carlo method is used to check the new theory. Results show that the rate equation method, in some cases, gives wrong results if the detrapping dependence on the sink strength parameter is neglected.

Quantum-Classical Molecular Dynamics Simulation of Synthesis of Boron-Nitride Nano-Structures at High-Temperature, High-Pressure Plasmas

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Boron-Nitride (BN) Nanostructures can be synthetized in various forms like fullerenes (hBN), nanocages, nanococoons, nanoflakes and nanotubes, similarly to the carbon nanostructures. The diamond-like forms (cBN) are also seen. The BN nanomaterial has exceptional features and its synthesis is carried out experimentally by a number of methods, with ultimate goals to reach high-rate production of impurity and defect free nanostructures. However, complete understanding of the BN nanosynthesis process at the atomic level has been missing so far.

With use of the DFTB {1, 2] and DC-DFTB-K [3] based BO Quantum-Classical Molecular Dynamics (QCMD) we were able to synthesize various BN nanomaterials by self-organization of atoms at high temperatures and pressures, mimicking partially the experiments on the BNNT nanosynthesis in the plasma environment. Interestingly, we could not obtain these structures by classical molecular dynamics simulations. We observed that hydrogen may have a profound effect in the BN nanosythesis process, altering the nanosynthesis outcomes that could lead to creation of an ultra-hard cubic BN material [2]. Based on the results of these simulations we are able to recommend the optimal precursors, temperatures and pressures for synthesis various BN material in plasma [3].

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Tools for the construction of atomic scale models for materials

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Modeling the thermodynamic and kinetic properties of materials commonly requires taking into account both vibrational and compositional degrees of freedom. While electronic structure calculations strictly speaking can provide the necessary information, they are computationally too demanding for any practical purposes. One therefore requires models that can reproduce the relevant parts of the potential energy landscape at a much smaller computational cost. Here, I will present a set of software packages that we developed over the course of the last years that allow one to rapidly construct and sample models that map vibrational and/or compositional degrees of freedom. These tools can be integrated in a homogeneous Python based workflow, which combines structure generation, electronic structure calculations, model construction, thermodynamic sampling, and subsequent analysis. I will mostly discuss the hiphive and icet packages, which respectively have been developed to obtain anharmonic force constant potentials and alloy cluster expansions. Example applications include the prediction of alloy phase diagrams, temperature driven phase transitions, thermal conductivities, and ordering phenomena.

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Liquid metal vapour shielding in linear plasma devices

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Liquid metals used in plasma facing components are attractive for DEMO due to the liquid's ability to self-heal against erosion, immunity to most of the negative impact of neutrons and ability to go beyond conduction-only based cooling. One extension of this cooling is vapour shielding, occuring under high heat loading of the liquid-metal surface by the plasma leading to strong evaporation. In such a situation the interaction between the vapour and the plasma leads to additional energy and momentum loss which reduce the power to the surface from the plasma by these additional volumetric processes. A series of experiments carried out in DIFFER's linear devices Magnum-PSI and Pilot-PSI have explored this phenomenon in detail for the first time. These machines are able to recreate the high density ($>10^{20}$ m^{-3}) low temperature (<5 eV) conditions expected close to the partially detached strikepoints of ITER or DEMO. It was found that the surface temperature of Sn based substrates becomes locked when the plasma pressure and vapour pressure become similar, and that this temperature locking persists over a power input range of 1-20 MW m^{-2}. Due to ion-neutral friction and electron ion collisions the plasma is strongly cooled from 2-3 eV to <0.5 eV driving strong recombination. The plasma cooling and radiation leads to an overall reduction of ~one third in the conducted power. Additionally the process appears oscillatory in nature due to the mutual interaction of the thermal cooling (slow) with the plasma processes (fast). For Li similar behaviour is also observed and appears a general phenomenon which would be expected to be present in tokamaks. The talk will discuss vapour shielding for liquid metals and the needs for atomic data to give a deeper physical understanding and predictive capabilities for these processes.

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Weighted PIC simulation for vapor shielding at wall under transient heat loads

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Erosion caused by transient heat loads is a serious concern for plasma facing components (PFCs) of the future fusion reactor. An inherent mitigation of the erosion, vapor shielding, is expected during the high heat loads. Melting and evaporation occurs on the PFC surface under the heat loads, and emitted vapor from the surface interacts with incoming plasma. Atomic-molecular reactions, i.e., elastic collision, ionisation/recombination, and radiation, cause a dissipation of incoming plasma energy. As a result, total absorbed heat flux at the wall can be reduced, and consequently the erosion is mitigated.

Question is how much mitigation can be expected from the vapor shielding. It is very difficult to experimentally study a transient heat loads equivalent to those for reactor condition. Thus, we have been developing a numerical simulation code, PIXY [1,2]. A particle-in-cell (PIC) model is applied for the plasma simulation because the plasma considered in the vapor shielding is not likely in Maxwellian. One issue of the PIC simulation is its expensive calculation cost due to huge numbers of super-particles. If a constant weight (number of real-particles in a super-particle) is used for all particles, the number of super-particles representing vapor particles increases linearly in accordance with the vapor emission rate, which is dependent strongly on the surface temperature. To solve this issue, a weighted particle model is applied for the PIXY code. Using different weight for each super-particle, the number of super-particles can be much reduced, and then the calculation cost becomes realistic. In the wall side, a 1-d heat transfer calculation is taken to determine the vapor emission rate as a function of the surface temperature. Combining plasma and wall models, the PIXY code simulates the plasma-wall interaction at the transient loads.

The PIXY code successfully reproduced experimental results of a plasma gun [1]. Then, the code was applied to simulations of the mitigated erosions of Be and W walls for reactor condition, where a rectangular ELM pulse was injected by assuming a fixed pulse width (0.2 ms) and a fixed plasma energy (2keV) [2]. In this study, we examine the sensitivity to the pulse width and the plasma energy. We also study the effect of pulse shape, such as a triangle pulse closer to the realistic transient loads in a reactor. These results can be applicable to estimate the erosion by ELM and disruption in ITER. In addition, the estimated erosion rates are beneficial information for the future DEMO reactor designs.

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Modifications to the Photonic and Electronic Impact Ionization Cross Sections of Ions in Dense plasmas due to the Transient Localization of Continuum Electron Wavefunctions

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Photonic and electronic impact ionization processes of ions in warm/hot dense plasmas play a key role in the determination of ionization balance, equation of state, and opacity. Here we propose the notion of a transient space localization of electrons produced during the ionization of atoms immersed in a hot dense plasma, which can significantly modify the fundamental properties of ionization processes. A theoretical formalism is developed to study the wavefunctions of the continuum electrons that takes into consideration the quantum de-coherence caused by coupling with the plasma environment. The method is applied to the photoionization of Fe16+ embedded in hot dense plasmas. We find that the cross section is considerably enhanced compared with the predictions of the existing free-atom model, and thereby partly explains the big difference between the measured opacity of Fe plasma [1] and the existing standard models for short wavelengths.

We also proposed that the transient space localization of the one electron states involved in the collision processes significantly modifies the wavefunctions of the scattering and ionized electrons resulting in big enhancements of these parameters. The theoretical formalism is applied to study the electron-ion collision processes in a solid-density magnesium plasma. The results show that not only the collision dynamics and the energy correlation of the two continuum electrons are greatly modified, but also the integrated cross sections and transition rates are dramatically increased in hot dense plasmas. Compared with the isolated ion model, the integrated cross section can be increased by one order of magnitude and the transition rate by two orders of magnitude, which supports the recent experimental evidences that the electronic impact ionization cross sections and collision rates in the solid-density Al [2] plasmas produced using X-ray free electron lasers (FEL) were underestimated by more than one order of magnitude.

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Effects of Microstructures on Surface Damage and H/He Retention in W: A multi-scale Modelling

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Microstructures greatly affect the behaviours of surface damage and H/He retention in plasma-facing materials (PFMs) during plasma-material interaction (PMI) in fusion devices [1]. Two new models are thus developed to investigate the key issues in complex materials under ion/neutron irradiation, i.e., a universal, computationally efficient and massively parallel 3D Monte Carlo code, IM3D [2,3], based on the binary-collision approximation for estimating ion implantation, sputtering and primary damage, as well as a spatially resolved cluster dynamics (CD) model, IRadMat [4,5], based on the rate theory for describing defect generation, diffusion, reaction and accumulation. A sequential multi-scale modelling framework is then constructed by coupling these two new models with atomistic approaches [5]. The effects of surface roughness and grain sizes on surface damage and H/He retention in PFMs like W are systematically investigated and quantitatively compared with experiments.

1) Influence of surface roughness on H/He implantation and sputtering [3]: Using the IM3D code and a random rough surface model, ion implantation and sputtering of W with a surface roughness varying between 0-2 μm have been studied for irradiation by 0.1-1 keV D^+, He^+ and Ar^+ ions. It is found that both ion backscattering and sputtering yields decrease with increasing roughness, due to the direct, line-of-sight deposition of a fraction of emitted atoms onto neighbouring asperities.

2) Effect of grain size on H/He retention and neutron irradiation damage [5,6]: By introducing the cellular sink strength of grain boundaries (GBs) into the CD model, defect accumulation and H/He retention in W with different grain sizes are studied under various ion/neutron irradiation conditions. It indicated that both the low vacancy diffusivity and high diffusion bias suppress the radiation tolerance of nanocrystalline W. H/He retention increases dramatically with grain size decreasing due to the enhancement of H/He capture ratio by GBs. Thus, we suggested that coarse-grained crystals should be selected for W-based PFMs in practice.

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Molecular Dynamics Simulation for Hydrogen Recycling on Carbon Divertor

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Plasma facing materials are bombarded by hydrogen plasma in magnetic confinement plasma devices such as Large Helical Device (LHD) in National Institute for Fusion Science, Japan. In the case of LHD, the divertor which directly contacts to plasma is made of carbon materials. When the divertor plates are irradiated by hydrogen ions, some hydrogen atoms reflect and back to the plasma while the other hydrogen atoms retain in the divertor.

Because plasma particles are neutralized by the recycling process on the divertor, many neutral particles of fuel exist in the edge plasma. These neutral particles affect the plasma parameters such as the electron and ion temperature and the plasma density by the interaction with plasma such as ionization, charge-exchange, and recombination processes. Moreover, the temperature of the neutral particles affects the electron temperature of detached plasma near the divertor. Therefore, the understanding of the transport of the neutral particles in the plasma is one of the critical issues for the achievement of effective fusion devices.

The transport of the neutral particles can be numerically simulated by neutral-transport code. However, when neutral-transport code is performed, the parameters of emitted neutral particles such as the energy distribution and the form (atom or molecule) of emitted neutral particles are usually decided artificially without logical reason because these parameters are not clearly obtained from experimental results. The effects of neutral particles on plasma parameter may depend on the parameters emitted neutral particles from the plasma facing material.

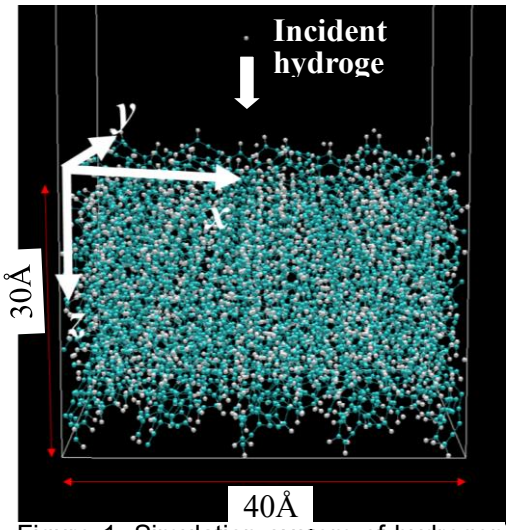

Figure 1. Simulation system of hydrogen injection ito amorphous carbon material. White and green ball denotes hydrogen and carbon atoms, respectively.

In this paper, therefore, as shown in Fig. 1, we develop an MD simulation model [1, 2] of hydrogen injection into an amophous carbon material to investigate the distribution of translational, vibration, and rotation energy of emitted hydrogen atoms and molecules.

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Recent approaches to machine learning of interatomic potentials seen from a perspective of plasma material interaction and primary radiation damage

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The starting point for my presentation is that for the study of material microstructure (as it is affected by radiation and as it affects hydrogen retention and transport) the fitted interatomic potential or force field is everything. Work in a recent International Atomic Energy Agency (IAEA) Coordinated Research Project on Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices [1] (as one of many applications for fusion materials) provides motivation to develop better interatomic force fields. One may think of systems such as W-H-He immediately after a primary knock-on atom (PKA) event; there is a local melt region and simulations (using molecular dynamics on a fitted force field) must provide accurate statistics for the microstructure after resolidification. The simulations are essential in connection with experiments that rely on surrogate (charged particle) irradiation or on irradiation by neutrons from fission, spallation or a stripping reaction and they are also essential to interpret the rather indirect measurements of microstructure.
Recent big data (machine learning) approaches to the development of atomistic force fields include use of Gaussian process approximation (kernel ridge regression) [2], spherical wavelet expansions [3] and deep neural networks (e.g. [4], [5]). At the same time, work done for the application domain of interatomic force fields is influencing research in computer science environments through the concept of deep neural networks that are invariant or covariant (equivariant) with respect to groups of discrete or continuous transformations: the point group of translations, rotations and reflections and the permutational symmetry group associated with the labeling of chemically identical atoms. Key words in the machine learning community include Point Cloud Convolutional Networks, Deep Sets, Spherical CNNs, Tensor Field Networks and Gauge Equivariant Neural Networks [6]. I will survey some of these developments in interatomic force fields and related machine learning research.

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Deep Learning for Multi-Scale Molecular Modeling

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Deep learning has emerged as a promising tool for a variety of applications in scientific modeling. However, while deep learning is a powerful tool for fitting data, constructing reliable and practical deep learning-based physical models is still a very non-trivial task. In this talk, we discuss the important issues and illustrate the relevant ideas in the context of constructing potential energy and free energy surfaces for molecular modeling. In particular, we will discuss the Deep Potential [1-3] and Deep Potential Generator scheme [4] for boosting ab-initio molecular dynamics and the Reinforced Dynamics [5] for enhanced sampling and free energy calculation. Important applications to various materials science problems will be introduced and used to illustrate these methods.

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Classification of Clusters in MD Simulations of Collision Cascades

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The structure of defect clusters formed in a displacement cascade plays a significant role in the micro-structural evolution during irradiation [1]. We present a novel method based on machine learning for pattern matching and classification of defect clusters from Molecular Dynamics simulations of collision cascades. The methods are applied on a database of collision cascades in Fe and W at energies ranging from 10 keV to 200 keV. The results show twenty six classes of cluster shapes providing new insights and parameters that can be used in simulations at higher scales. We discuss each step, starting from efficient identification of defects from simulation output to reduction of physics problems to machine learning stages viz. feature engineering, dimensionality reduction and unsupervised classification.

We characterised a cluster by the geometrical histograms of angles and distances between neighbouring defects in the cluster. We show the use of these histograms as similarity metric to search for similar cluster shapes. The dimensionality reduction helps in plotting each cluster as a point in a two or three dimensional space. The algorithm when used on the designed features (histograms) places similar clusters together. We show that clusters that are placed together also have similar types (interstitial / vacancy), sizes and dimensionality. The unsupervised classification separates out many already known categories of clusters such as crowdions, planar crowdion pairs, rings, etc. The distribution of different classes of shapes among cascades of different elements and energies shows the exclusivity of shapes to elements and energies. The cluster shape preferences for Fe and W agree with prior studies [2, 3]. The results also show new cluster shape classes and quantitative study of the sizes, dimensionality and preferences to elements and energies for each class. We discuss the key points and computational efficiency of the algorithms along with the various prominent results of their application.

We present an open-source software [4] implementing the methods and providing additional tools for analysis and interactive visualisations. The distribution of cluster shapes and structures along with the shape properties like diffusivity, stability, etc. can be used as input to higher scale models in a multi-scale radiation damage study. The machine learning methods can also be further extended to study shapes of subcascades and collision cascades.

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Displacement damage stabilization by hydrogen presence under simultaneous W ion damaging and D ion exposure

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In a future thermonuclear device such as DEMO the wall material will be irradiated by 14 MeV neutrons produced in the D-T nuclear reaction and at the same time exposed to a high flux of ions and neutrals of hydrogen isotopes (HIs) as well as helium. In most experiments where fuel retention in displacement-damaged tungsten (W) was studied by ion or plasma loading, the high energy ion damaging was performed as a surrogate for neutron irradiation and sequentially exposure to deuterium was done to determine the retention and properties of HI trapping. However, in real fusion devices creation of displacement damage and HI irradiation will take place simultaneously. This difference in the conditions at which damage is created, meaning with or without the presence of HIs, could be important when studying fuel retention. It was shown by positron annihilation spectroscopy that vacancy-hydrogen complexes have a higher barrier associated with their migration in metals like tantalum and niobium [1] compared to hydrogen free vacancies.

Here we will present experimental results of simultaneous exposures where polycrystalline W samples were irradiated by 10.8 MeV W ions and exposed to 300 eV deuterium (D) ions at different temperatures ranging from 450 K to 1000 K. After the simultaneous W/D exposure the samples were additionally exposed to low energy D ions at 450 K in order to populate all the defects created beforehand. The amount of damage created was evaluated by measuring D depth profiles and D thermal desorption spectra. Results are compared with data obtained in a sequential experiment where samples were first irradiated by 10.8 MeV W ions and only afterwards exposed to 300 eV D ions at 450 K to populate the created defects. At 450 K we observe a two times higher maximum D concentration for the simultaneous case as compared with the sequential case. At 600 K and 800 K the ratio between simultaneous and sequential decreases to about 1.6 and 1.2, respectively, and increases again to a factor of two at 1000 K. We attribute this temperature dependence to the change in the concentration of mobile and trapped D during the simultaneous exposures, which is in line with theoretical calculations predicting that trapped D in a vacancy prevents vacancy annihilation with self-interstitials [2]. From the comparison with the previous experimental series with D atoms [3] conclusions about the influence of retained D on damage stabilization will be drawn.

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Influence of the presence of deuterium on displacement damage in tungsten

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Among many other favourable properties intrinsically low fuel retention makes tungsten one material of choice as plasma-facing material. However, during operation of a fusion device defects in the tungsten lattice will evolve that will trap hydrogen isotopes. Experiments with neutron-irradiated samples as well as MeV-energy ion-irradiated samples showed that hydrogen isotope retention can reach values of the order of 1 at.% due to the displacement damage [1]. However, all these experiments were done sequentially: First damage was produced and only then transport and deuterium retention in this material was studied. First beam experiments where displacement damage was created with MeV tungsten ions while simultaneously dosing the samples with either atomic deuterium [2] or low energy deuterium ions [3] revealed increased retention by up to a factor of two compared to the sequential exposures.

Here a different experimental approach will be presented that allows studying the influence of hydrogen isotopes on damage creation. In this approach first 20 MeV tungsten is implanted into recrystallized tungsten to a level where damage cascades overlap and defect density saturates within the 2 µm deep implantation zone. Second, the created defects are decorated with deuterium with a low temperature plasma achieving a homogenous deuterium concentration of 1.8 at.%. In a third stage, these samples are again irradiated with 20 MeV tungsten. In this step not only tungsten atoms are displaced and defects are generated but also the retained deuterium atoms are de-trapped and hence mobilized. SDTrimSP calculations reveal that for the implantation parameters used, on average each D atom is recoiled at least once. Nuclear reaction analysis shows that during this second implantation no deuterium is lost from the sample, but it is only de-trapped and is effectively re-trapped again. When samples are again decorated with deuterium after the second self-damaging step, NRA and TDS reveals that deuterium retention exceeds the initial saturation value by nearly a factor of two [4]. These experiments clearly support the calculations by Kato et al. [5] and Middleburgh et al. [6] which predicted that hydrogen isotopes either stabilize vacancies or lower the vacancy formation energy which both leads to an increase in trap density.

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Deuterium trapping at irradiation-induced defects in tungsten studied by positron annihilation spectroscopy

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The development of fusion reactors like ITER has been improving. In plasma-facing components, energetic hydrogen is induced together with radiation damage due to exposure to fusion plasma. Since tritium is an essential fusion reaction source, it is necessary to constrain its retention in the plasma-facing components. Such constraints are also of great importance from a safety perspective. Tungsten is a primary candidate material for the plasma-facing components due to its high melting point and high sputtering resistance to energetic particles. The solubility of tritium in tungsten is very low (the lowest among metals), which is an advantage in reducing tritium retention during the operation of fusion reactors. However, recent studies have reported that irradiation cause significant enhancement of hydrogen retention in tungsten. This is ascribed to hydrogen trapping at irradiation-induced defects such as vacancies and vacancy clusters, however, it has not yet been clarified. We here employed positron annihilation spectroscopy (PAS) to reveal both irradiation-induced defects and hydrogen in neutron-irradiated tungsten [1].

Pure tungsten (4N) was neutron-irradiated at about 573 K for about 40 days to the dose of about 0.3 dpa, followed by post-irradiation annealing (PIA) at 573 K for 100 hours. The PIA was performed in a vacuum or in deuterium gas at about 0.1 MPa. In the as-irradiated state, the formation of vacancy clusters with the size of about V_{40} was revealed by positron lifetime measurement. After the PIA in vacuum, positron lifetime was almost the same as that in the as-irradiated state, indicating no change in the vacancy clusters. On the other hand, after the PIA in deuterium gas, positron lifetime was significantly shorter than that in the as-irradiated state, strongly suggesting positron annihilation with deuterium electrons at the vacancy clusters. To analyze chemical environment at the positron trapping sites, coincidence Doppler broadening (CDB) measurements were performed. CDB measurements clearly indicated positron annihilation with deuterium electrons, thus deuterium trapping at irradiation-induced vacancy clusters was revealed. This gives the direct observation of deuterium trapping at irradiation-induced defects, which is suggested to be the main origin of significant increase in hydrogen isotope retention in irradiated-tungsten.

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O-1

Origin of outstanding radiation resistance in W-based high-entropy alloys

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Understanding the phase stability under irradiation of alloys with multiple principal elements is one of the great chanllenges in developing materials engineering components such as the divertor or plasma-facing materials for fusion devices. Recently, a body-centered cubic tungsten-based refractory high-entropy alloy (HEA) with outstanding radiation resistance has been developed [1]. It was found that no sign of irradiation-created dislocation loops, even after 8 dpa, was observed. Furthermore, nanomechanical testing shows a large hardness of 14 GPa in the as-deposited samples, with near negligible irradiation harderning.

In this work, an ab-initio based constrained thermodynamic formalism for driven alloys, initially proposed by G. Martin, has been developed to model multi-component alloy system under irradiation for wich point defects are being considered as the additional elements in the system. It is found that the formalism can be mathematically respresented within matrix formulation for the K-component alloys via many-body cluster correlation functions which in turn can be computed efficiently from Monte-Carlo simulations in a combination with first-principles cluster-expansion Hamiltonian [2]. Applying the theory for bcc W-Ta-Cr-V based HEAs, it is predicted that there is a strong phase decomposition between W, Ta and Cr, V as a function of composition and temperature. The formation of Cr and V rich phase found from the MC simulations is in an excellent agreement with the precipitates oberserved with Atom Probe Tomography analysis for $W_{38}Ta_{36}Cr_{15}V_{11}$ alloy irradiated at T=1050K. The comptetion between phase segretation and radiation effects is discussed. The absence of irradiated damage in material ties the outstanding radiation resistance to maximum recombination probabilities between vacancy and interstitial defects in the investigated HEAs.

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O-2

Towards understanding the influence of Re on H dissolution and retention in W by investigating the interaction between dispersed/aggregated-Re and H

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Tungsten (W) and W alloys are considered as the most promising candidates for plasma facing materials (PFMs) in future fusion reactors. Rhenium (Re) is not only the typical alloying element but also the main production of transmutation in W-PFMs. The microstructure and mechanical properties of W as well as the behaviors of impurities in W will be influenced by the presence of Re. The deuterium retention in damaged W-3%Re at 750 K is two of magnitude lower than that in damaged Re-free W. Therefore, one can expect that Re should have significant effect on the behavior of H isotopes in W. However, little work has focused on this aspect so far.

Here, we have systematically investigated the effects of dispersed/aggregated Re on the behaviors of H in W as well as their interaction with point defects using a first-principles method in combination with thermodynamic models. It has been demonstrated that the influence of Re on H is strongly related to the distribution of Re in W. Re will aggregate and form clusters/ Re-rich precipitation phases under high energy ions/neutrons irradiation in W. The influence of Re clusters on H is extraordinary stronger than that of a single Re. The retention of H in W can be significantly suppressed by Re clusters, and their influences will be enhanced with the increasing of the number of Re atoms. On the contrary, it is found that the solution energy of H at most interstitial sites (> 80%) in W-Re sigma phase is much lower than that in pure W. Specifically, the H solution energy at most stable interstitial site in W-Re σ phase is only 0.47 eV, ~ 54% lower than that in pure W. This can be attributed to that W-Re sigma phase provides the larger available volume for interstitial H than the pure W, weakening the W-H repulsive interaction. Consequently, our calculations reveal that the Re-rich precipitation can serve as the strong trapping centers for H in W, while dispersed-Re/small Re clusters can be used to suppress H retention. These results provide an important reference to evaluate the influence of Re and other alloying elements on the behaviors of H isotopes in W-PFMs under future fusion conditions.

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O-3

Deposition effects on He induced fiberform nanostructure growth

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Helium (He) plasma irradiation to metals leads to various morphology changes accompanied by He bubble formations. In particular, fiberform nanostructures called 'fuzz' can be grown when the incident ion energy and the surface temperature satisfy a certain condition [1]. To understand the mechanisms for the He induced morphology changes, several models have been proposed and various simulations have been conducted. However, the growth process has yet to be fully understood. In particular, the growth process of a recently found enhanced growth process to large scale structures such as nanotendril bundles (NTBs) and mm-thick large-scale fiberform nanostructures (LFNs) [2,3] is a mystery. In this study we show LFN growth on several metals (W, Mo and Re) while metal particles (ions and neutrals) are precipitated on the samples which is exposed to He plasmas. When metal particles are precipitated on the surface, the growth process is not limited by some diffusion process. The height of nanostructure building block increased exponentially with irradiation time. Based on detailed transmission electron microscope (TEM) observations, the crystal orientation of the growth direction of linearly grown fiberform nanostructures identified on some HCP metals were identified. It is shown that HCP metals have a preferential growth orientation in *c*-axis direction. The results suggested that adatoms formed by He ion irradiation or metal ion precipitations diffuse on nanofibers and contribute to the growth at the tip of nanofibers in epitaxial crystal growth process.

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O-4

Sputtering and Re-deposition Effects during Fuzz Growth Process Simulated by BCA-MD-KMC Multi-hybrid Simulation

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Helium plasma irradiation induces the fuzzy nanostructure, ‘‘fuzz‘‘, on a tungsten surface[1,2]. The helium plasma is the ash of fusion reaction and the tungsten is used for the divertor plate in magnetic confinement fusion reactors. The heat lead of the divertor is regarded as a critical problem in the fusion reactor. Because the thermal conductivity of the tungsten material with fuzz is smaller than that of bulk[3], the generation of the fuzzy nanostructure on the divertor plate is a key issue of the research in plasma-wall interaction.

The growth mechanism of the fuzzy nanostructure has not been clarified, and the relation with the helium bubble, which is generated in the case that the fluence of helium ion is lower than the fluence to generate the fuzzy nanostructure, has been considered. Although, the formation mechanism of the helium bubble was well explained by using density functional theory(DFT)[4] and the molecular dynamics (MD)[5,6]. However, those simulations could not reproduce the generation of the fuzzy nanostructure because they cannot achieve the fluence necessary for fuzzy nanostructure formation, 10^{24} m^{-2}. We developed the BCA-MD-KMC triple hybrid simulation[7]. The hybrid simulation achieved the fluence of 10^{24} m^{-2} while the incident flux is kept low at 10^{22} $m^{-2}s^{-1}$, which is comparable with an experimental condition. As a result, the fuzzy nanostructure growth was reproduced. From this simulation, we clarified the transport of tungsten atoms for the growth of the fuzzy nanostructure is caused by the knocking out by the incident helium ion and the re-deposition of the tungsten atom knocked out.

We focused that the experiment requires that an incident energy of 6 eV or more is necessary for helium bubble growth[8] and an incident energy of 30 eV or more is necessary for fuzz growth[9]. From the DFT calculation[4], it is clarified that the incident energy required for helium atom to penetrate into tungsten is 6 eV. In the present work, we investigate incident energy dependence of the growth of the fuzzy nanostructure by using the BCA-MD-KMC multi-hybrid simulation. We consider that the incident energy threshold of 30 eV for fuzz growth is caused by the recoil (knocking out) threshold energy of tungsten on rough surfaces.

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O-5

Helium Bubble Growth In Tungsten Nano-Tendrils

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It is known that fuzz nanostructures will form when tungsten surfaces are exposed to low-energy helium plasma. These nanostructures appear as a tangled mass of disordered nano-tendrils with up to micrometer in length and several tens of nanometer in diameter. It is still unclear what continues to drive the formation of tungsten fuzz up to several micrometers in thickness. Recently, several studies have revealed that both helium bubbles and intratendril grain boundaries (GB) are present in the nano-tendrils. It may provide some insight to understand the mechanism of fuzz growth by investigating the growth of helium bubbles in the vicinity of GBs in nano-tendrils.

In this study, molecular dynamics (MD) simulations have been performed to systematically study the growth and bursting of helium bubbles near different GBs in nano-tendrils. The results show that the growth behavior of helium bubbles is very different from the cases in the bulk or near surfaces. Prismatic dislocation loops are rarely formed in the nano-tendrils. The results have also indicated that the resulting surface morphology depends on GB structures (see Figure 1). The movement of dislocations punched out by helium bubbles is also studied in details by analyzing the shear stress-field nephogram around the helium bubbles.

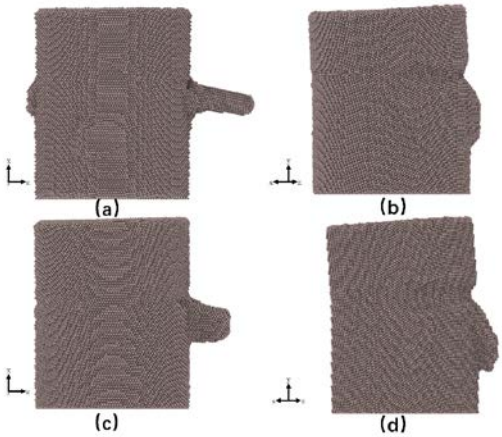

Figure 1. The evolution of surface morphology for 4 different GBs structure after He bubble bursts. (a) Σ3<111>{112} GB structure, (b) Σ5<100>{310} GB structure, (c) Σ7<111>{123} GB structure, (d) Σ17<100>{410} GB structure.

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O-6

Surface coverage dependence of the diffusion/desorption mechanisms of hydrogen from the W(110) and W(100) surfaces: a model based on DFT and thermodynamics

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The purpose of the present work is to establish the mechanisms for the diffusion of hydrogen in the sub-surface of tungsten and the mechanism for the recombination of molecular hydrogen on top of the W(100) and W(110) surfaces depending on the surface coverage in hydrogen.

Indeed, the interaction of tungsten with hydrogen is the aim of many theoretical and experimental modellings. In Laboratories, Temperature Program Desorption (TPD) is widely used to determine the behavior of hydrogen in tungsten depending on the temperature. These experiments are assisted by numerical simulation to understand the trapping mechanisms and to determine the type of defects with which hydrogen interacts. Nevertheless, the surface effects are currently not well understood and their dependence with the state of the surface in terms of hydrogen coverage remains unclear.

In this work, we first computed by DFT the energies of the most stable configurations of hydrogen adsorbed on the W(110) and W(100) surfaces from low coverages up to saturation. Based on these energies and on the vibrational properties of the system, we built a thermodynamic model that provides the hydrogen coverage of the W(110) and W(100) surfaces depending on the experimental conditions, which are the pressure and the temperature. These results are compared with experimental results from Low Energy Ion Scattering and Direct Recoil Spectroscopy.

The diffusion of hydrogen in the sub-surface and the recombination of H_2 on the W(110) and W(100) surfaces was then investigated. The related activation barriers were determined depending on the hydrogen coverage of the surface. We were finally able to determine the range of temperature and pressure in which the recombination mechanism becomes the rate limiting step during TPD experiments. This corresponds to temperature above 450K to 500K and pressure around 10^{-8} Pa, which falls in the conditions where the main of desorption peak is observed during TPD of hydrogen from tungsten.

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O-7

Impact of a high temperature target on hydrogen recycling

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Hydrogen recycling is one of the most important issues for stable steady state operation. Wall temperature plays a critical role on the hydrogen recycling [1]. In the tandem mirror GAMMA 10/PDX, the hydrogen recycling study has been carried out by using a temperature-controlled tungsten target which is exposed to the end loss plasma [2-3]. One of the features of GAMMA 10/PDX experiments is enough low neutral pressure during the plasma exposure to measure emissions of the recycling particles.

A device which is utilized in this study is installed in the west end region of GAMMA 10/PDX. It is named D-module and consists of a rectangular box (0.5 m square and 0.7 m in length) with an inlet aperture at the front panel and a V-shaped tungsten target (0.3 m in width and 0.35 m in length) inside the box. The end loss plasma flows through the inlet, and the target is exposed to the plasma. The target can be heated up to 573 K by sheath electric heaters. The open-angle of the V-shaped target was 45 degrees. Langmuir probes are installed on the upper target plate. The Balmer line and Fulcher-α band emissions of the plasma in front of the V-shaped target are measured by spectroscopies. Two dimensional image of the H_α line intensity is also measured by a fast camera with an interference filter (656 nm ± 10 nm).

When the target temperature (T_{target}) increased from room temperature to 573 K, the H_α and H_β intensities increased by a factor of two although the electron density increased by ~13 % (from ~2.3×10^{16} m^{-3} to ~2.6×10^{16} m^{-3}), indicating enhanced hydrogen recycling due to increasing the target temperature. The electron temperature was almost constant (~30 eV). The significant increase in the Balmer intensities are not caused by electron impact excitation, since the mean free path of excitation from n=1 to n=3 is ~100 m, which is much longer than the plasma size. A possible candidate of the mechanism of the increase in the Balmer intensities is production of excited hydrogen atoms by dissociation of vibrationally excited hydrogen molecules. The vibrational temperature which was evaluated with a Fulcher-α band spectrum was ~3400 K and constant relative to the target temperature, indicating the hydrogen molecules were vibrationally excited. The vibrationally excited molecules are considered to be produced by hot atom recombination on the tungsten target [4].

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Potential Sputtering from Rare Gas Solid Surface by Multiply-Charged Ion impact

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The potential sputtering phenomenon, widely observed on the surfaces of insulators, such as alkali-halides and oxides, is a desorption mechanism induced by the transfer of potential (internal) energy from incident multiply-charged ions (MCIs) to the solid surface [1].

Dynamic processes of sputtering can ideally be studied using rare gas solid (RGS), as it has the simple electronic structure similar to isolated atoms, along with very unique characteristics, such as very small cohesive energy (e.g., 0.02 eV/atom for Ne), large band gap energy (e.g., 21.6 eV for Ne), and long diffusion length of excitons (e.g., ~ 200 nm for Ne), which set it apart from the other materials.

We reported the relative ion yields of potential sputtering from solid Ne by Ar^{q+} (q = 1 − 7) impact and demonstrated the proportionality of the sputtering ion yields to the potential energy of the incident MCI [2]. Our absolute measurements of the ion sputtering yields revealed that the yields depend not only on the potential energy but also on the kinetic energy of the incident MCIs. In order to explain our results, we have proposed a new desorption mechanism, where ions are created in the solid by the charge transfer with the incident MCIs, and part of them desorb with surrounding neutral atoms [3].

To acquire more detailed and quantitative information on ion desorption process, we have developed a system for coincidence measurements of the ions desorbed and projectiles scattered from the surface of RGSs by MCI impact [4]. Recent progress including some preliminary results obtained by the new system will be presented at the workshop.

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O-9

D retention in bulk Be and D co-deposited in Be layers studied by 3 different thermal desorption techniques and their modelling by CRDS

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Hydrogen isotope retention in beryllium is an important issue for ITER especially concerning tritium due to the licence-limited inventory. Moreover, hydrogen retention has effects on the wall and the global fuel cycle. Therefore, understanding of the retention and release mechanisms for hydrogen implantation and co-deposition in Be layers is crucial. We present recent deuterium retention studies in Be/D co-deposits on W, D implanted in single and poly-crystalline Be and Be/W mixed materials ($Be_{12}W$). Modelling was performed by a Coupled Reaction Diffusion System (CRDS) [1], while the experiments were performed in two devices at FZJ that can handle Be:

The ARTOSS device combines many techniques of surface science in one UHV device: D implantation (1-2 keV/D) by a mass and energy separated ion source, Thermal Desorption Spectrometry (TDS) providing insight into the D binding states, Nuclear Reaction Analysis (NRA) for D inventory and X-ray Photoelectron Spectroscopy (XPS) to study chemical surface states.

The new FREDIS device [2] contains a TDS system for even larger samples and a Laser-Induced Desorption (LID) system that can scan full JET tiles with rapid sample heating by laser pulses. Both parts share the same Quadrupole Mass Spectrometer (QMS) system for quantification of the released gases.

ARTOSS recently revealed low energy binding states in Be for higher D implantation fluences (~ $10^{22}/m^2$). Very slow heating ramps of 0.01 K/s allowed to resolve three low energy binding states of D in Be for the first time. Secondary Electron Microscopy (SEM) imaging of the Be surface after D implantation showed fluence dependent blistering that might be correlated to these states.[3]

FREDIS showed similarly sharp low-temperature and broad high-temperature desorption peaks for co-deposited D in Be layers of 1, 10 and 20 µm thickness produced by High Power Impulse Magnetron Sputtering (HiPIMS) on ITER grade W and even sharper, instantaneous release in some cases. Additionally, it could be demonstrated that LID can desorb the D inventory completely under certain circumstances, opening a possibility for in situ desorption in the fusion device.[4]

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O-10

Microstructural Change of Au Thin Films by Microwave Irradiation

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For the purpose of fabricating interconnects in integrated electronic circuits, metal thin films are vapor-deposited and play their roles. In order to avoid thermal damages to the substrates, low temperature deposition is favored in the film fabrication (metallization) process. As a result, these films consist of small (nano) crystal grains, therefore, the films do not possess sufficient electric conductivity. Post annealing is conducted in order to improve their conductivity, which is again required to be minimized the thermal damage. Lamp heating is one of the currently-conducted processes in the electronic industry.

In our research group, microwave post annealing is investigated [1,2] because of its chracteristics of rapid and selective heating. In this paper, it is intended to present some results on the microstructural variations caused by microwave irradiation in comparison with the conventional (furnace) annealing.

Au films were sputter-deposited on SiO_2 substrates. Microwave at 5.8GHz was utilized for heating in a sigle mode microwave cavity at maxmum power 100W. The specimens were placed at the magnetic field maximum position in the cavity.

The films are also heated in an electric furnace for comparison. Temperature measurement was performed using the same optical method for the both heating methods. The post annealed specimens were evaluated their microstructures by means of AFM, SEM/EBSP, TEM and XRD.

Differences were demonstrated in microstructural evolution process of Au thin film by two anneling methods. It was observed that fine roughness of the film surface was reduced more by microwave than by furnace under conditions of low temperature annealings. However, by the higher temperature annealing, similar microstructures were obtained in both methods, eventually.

Considering various factors having possible influences on the film roughness variations, alteration of surface energy and/or surface diffusivity of atoms is one of the major effects for evolution of the film microstructures and the morphologies. Micro-plasma generated on the film surface is inferred to be related with alteration of the surface states.

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O-11

A monoenergetic energy-tunable positronium beam and its applications

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The positronium (Ps) atom is a hydrogen-like neutral system composed of an electron and a positron. The ground state splits into singlet (para-Ps) and triplet (ortho-Ps) spin states. They decay into gamma rays due to pair annihilation with very short lifetimes of 125 ps and 142 ns in a field free region, respectively [1]. Ps atoms are usually produced in materials such as gases, polymers, and liquids when positrons are injected into them. When metal surfaces are bombarded with positrons, they penetrate into the bulk, lose their energy and diffuse back to the surface. Some of the positrons are then converted to Ps atoms at the surface by capture of electrons and emitted.

For the detailed study of interactions between Ps atoms and materials, monoenergetic and energy-tunable Ps beams are needed. However, Ps atoms cannot be accelerated because they are electrically neutral. So far monoenergetic Ps beams have been produced in the energy range of 7 - 400 eV by using a charge-exchange reaction of energetic positron beams with gaseous atoms or molecules [2]. Unfortunately, extension to higher energy range has been limited because of decrease of the charge-exchange cross section.

Recently a high quality energetic Ps beam in the energy range of a few keV has been available by using photo-detachment of positronium negative ion (Ps^-) [3,4]. Ps^- is a three-body system composed of two electrons and a positron and can be accelerated using an electric field easily. This achievement was made possible by dramatic improvement of the efficiency for Ps^- production [5]. When positrons are injected into a tungsten surface coated with alkali-metal, the production efficiency of Ps^- increases to around 200 times larger than that obtained for uncoated surface. This method was applied for the first observation of the shape resonance of Ps^- [6]. In our present system, positrons from a ^{22}Na source are moderated and trapped by a buffer-gas trap [7]. The positrons are extracted from the trap as pulsed slow positrons synchronized with the laser for the photo-detachment [4].

In this talk, the details of our Ps beam system and its possible applications will be presented.

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O-12

Anomalous Properties of Vacancy in Tungsten and Interaction with Hydrogen

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Tungsten (W) is a plausible candidate as the divertor materials of the ITER and MEDO reactors which would be exposed to high-flux plasma particle and neutron irradiation. W is considered to be a promising plasma facing materials (PFMs) because of the high melting point, high thermal conductivity, and low hydrogen (H) solubility etc. H or H isotopes used in the fusion reactors as fuels usually do not accumulate in W specimens due to the low H solubility. However, a large amount of deuterium (D) retention were observed in the damaged zones of irradiated W materials. Tritium (T) retention in the PFMs will be a serious problem for the future fusion reactors. One of the candidates of traps for the H isotopes is vacancy-type lattice defects nucleated under the irradiation circumstance. So, we investigated the interaction of monovacancy with H atoms in terms of first-principle calculations based on density functional theory. Then, we found and examined two anomalous properties associated with a monovacancy in a bulk W.

H atoms can be accommodated in the vacancy-type lattice defects in bcc transition metals. Firstly, we investigated abnormal stable configurations of H atoms trapped in a W monovacancy [1, 2]. An interstitial H is located at a tetrahedral interstitial site (T-site). On the other hand, H atoms trapped in a monovacancy in bcc metals are located close to the octahedral interstitial sites (O-site) next to the monovacancy. Therefore, a maximum of 6 H atoms can be accommodated in the monovacancy in bcc lattice because 6 O-sites exist next to the monovacancy. However, stable configurations of H atoms trapped in a W monovacancy are remarkably reorganized as the number of H atoms increases. H atoms are largely shifted from the O-sites and they are finally located in the vicinity of T-sites. As a result, a maximum of 12 H atoms can be accommodated in the W monovacancy. This abnormal stable configurations of H atoms greatly affects the binding energy of H atoms to the monovacancy and zero-point energy of H isotope.

Secondly, we examined the stability of a divacancy in a bulk W [3]. Usually, a divacancy is supposed to be energetically stable than two separated monovacancies in metals. However, a repulsive or only slightly attractive interactions between two monovacancies is predicted in W by first-principle calculations. We confirmed the repulsive interaction by the calculations performed in a large supercell. On the other hand, the divacancy is considerably stabilized by H atom trapping.

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O-13

Molecular Dynamics Simulation on Interactions between Hydrogen and Vacancy Clusters in Tungsten

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Tritium retention and leakage behaviors in fusion reactor materials such as tungsten and steels are relevant with the safety and sustainability of fusion reactors. In order to accurately predict the tritium behaviors during reactor operation, understanding of interactions between hydrogen isotopes and irradiation defects is needed. Since vacancies basically act as strong traps of hydrogen in metals, many computational studies have been devoted to quantify the trap effects of vacancies, especially of mono-vacancies [1]. However, the knowledge on vacancy clusters is still limited, probably due to the fact that the first-principles calculation cannot easily deal with a large vacancy cluster and the accuracy of available potential models for H-V interaction is limited in molecular dynamics (MD) calculation.

In the present study, to investigate interactions between hydrogen and vacancy clusters in tungsten, we first developed a potential model with putting a high priority on reasonable description of H-V interaction energies. The potential model was fitted to energies, forces and stresses calculated by first-principles calculation using VASP code. Subsequently, with a developed potential model, MD calculations were performed using LAMMPS code. Systems of various hydrogen and vacancy concentrations were simulated. Two sorts of initial vacancy configurations were prepared: (1) vacancies are agglomerated as a single cluster and (2) vacancies are isolated as multiple mono-vacancies. The effective diffusivities of hydrogen, which is a good index to quality the strength of H-V interaction [2], and the H/V ratios in H-V complexes were evaluated,

The MD simulations showed that the hydrogen trapping energy in a H-V complex decreases as the number of trapped H atoms increases and increases as the number of involved vacancies increases. The trapping energy increases up to around the hydrogen trapping energy on a surface. The effective diffusivity of hydrogen is significantly reduced by vacancies. The reduction is often more significant when vacancies are isolated, not clustered. The trapping energy is reasonably correlated with the ratio of the number of trapped H atoms to the number of effective trapping sites in a vacancy cluster, which is calculated from the surface area of the vacancy cluster, rather than the number of vacancies involved in the vacancy cluster.

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O-14

Deuterium Retention in W and Binary W Alloys Irradiated with High Energy Fe Ions

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Trapping of hydrogen isotopes at radiation-induced defects in W is an important problem in evaluating tritium inventory in a vacuum chamber of future fusion reactor. In our previous study, deuterium (D) retention in W-5Re alloy after irradiation with Fe ions to 0.5 dpa was compared with that in pure W [1]. The addition of Re to W strongly reduced the concentration of vacancy-type defects and consequently D retention at irradiation temperatures ≥ 773 K [1]. According to DFT calculations by Suzudo et al. [2] a Re atom can form a dumbbell cluster with a W self-interstitial atom (SIA) to reduce the SIA's effective mobility and enhance recombination with a vacancy. However, the dependence of D retention on Re concentration and damage level has not been understood. The effects of other elements have not been examined. In this study, D retention in W-xM alloys (M = Cr, Ta, Mo and Re, and x is the concentration in at.%) after Fe ion irradiation to 0.5–2.5 dpa was examined systematically. These alloying elements were selected according to the DFT calculation of Suzudo et al. [2]. According to their predictions, the interaction of a W SIA with an atom of Mo and Ta is far weaker than that of Re, while a Cr atom forms a dumbbell cluster with a SIA as a Re atom.

Plates of W-(0.1-5)Re, W-(0.5-2.5)Mo, W-(1-5)Ta and W-3Cr alloys were irradiated at 1073 K with 6.4 MeV Fe ions to 0.5-2.5 dpa at the damage peak. The irradiated samples were exposed to D_2 gas at 0.1 MPa and 673 K, and the retention of D was measured by thermal desorption spectrometry (TDS).

No clear reduction in D retention was observed by Re addition at/below 1 at.%, while strong enhancement of vacancy annihilation was observed at 5 at.% up to 2.5 dpa. The addition of Mo and Ta resulted in no significant influence in D retention even at the highest concentrations examined, as expected from the above-mentioned results of DFT calculations by Suzudo et al. [2]. The experiments for W-Cr alloy are in progress and the results will be reported in the presentation.

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O-15

Hydrogen isotope exchange between H and D in damaged tungsten

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In ITER, full tungsten divertor will be used due to its low tritium inventory as well as low sputtering yield compared with carbon based materials. However, tritium retention during a DT phase could be significantly increased because neutron irradiation will make strong trap sites uniformly distributed in the bulk of W [1]. One of possible methods to remove the retained tritium would be hydrogen isotope exchange during plasma operation with deuterium [2]. In order to correctly evaluate a tritium removal rate by isotope exchange with deuterium, understanding of the mechanism and appropriate modeling are necessary. But few studies have been performed about isotope exchange at various tritium trapping sites. In this study, by using high energy Fe ion damage as a proxy of neutron damage, isotope exchange between deuterium and hydrogen was investigated.

Recrystallized tungsten specimens annealed at 2073 K for an hour with very low intrinsic trapping sites (concentration of less than 10^{-4}) were used. Ion damage was made at 473 K by 6.4 MeV Fe ion irradiation to about 0.2 dpa (average value within an ion range), corresponding to trap site concentration of about 10^{-2}. Implantation of 1 keV D ions or H ions at 473 K was performed by an ion irradiation device, HiFIT. Ion flux and fluence were 1.3 x 10^{20} $m^{-2}s^{-1}$ and 1.5 x 10^{24} m^{-2}, respectively. Under the temperature (473 K) and the fluence conditions, implanted D or H can fill all the ion damaged traps. In addition, new traps with their implantation were created. After D (H) implantation, H (D) ions were successively implanted also at 473 K with the fluences up to 1.5 x 10^{24} m^{-2} (the same fluence as the first implanted ions). Retention of D and H was measured by thermal desorption spectroscopy (TDS).

TDS spectra have a broad peak from 473 K (irradiation temperature) to about 950 K. In these spectra, two recognizable peaks were observed at around 550 K and 750 K, probably corresponding to vacancies (activation energy of~1.4 eV) and voids (activation energy of~1.8 eV), respectively. It is noted that even at irradiation temperature of 473 K isotope exchange took place in the whole TDS spectra (up to 950 K). In more detail, as the second ion fluence increased isotope exchange was firstly observed at low temperatures (weak trap sites), then it extended to high temperatures (strong trap sites). At the second ion fluence of 1.5 x 10^{24} m^{-2} (the same fluence as first ions), about 75% of first implanted species were removed. No clear isotope effects were observed, namely D to H exchange and H to D exchange behaved similarly. Considering difference in vibrational energies between hydrogen isotopes in lattices sites and defects sites, lighter ions may have higher trapping energies at defects, which may predict that isotope exchange from lighter ions to heavier ions (H to D) is slower than that from D to H. But our results did not show such tendency.

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O-16

Development of functional material for deuterium permeation observation under divertor plasma exposures

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It is known that plasma-induced permeation of hydrogen occurs at the plasma-facing wall in fusion devices. Accordingly, a quantitative evaluation on a hydrogen transfer to primary cooling system is necessary for the design of the DEMO. However, there is no precedent on a direct evaluation of hydrogen permeation in metallic walls under high heat flux plasma exposure in fusion devices. Therefore, in order to quantitatively evaluate the amount of hydrogen permeation in metallic walls during plasma exposure, the sample was newly developed that combines tungsten (W) and titanium (Ti).

We have produced the sample which is an integrated structure in which W is coated on palladium (Pd) coated side on Ti bulk considering the experimental environment in fusion devices. W is a prime candidate for divertor plates and plays a role as a plasma-facing material also in this sample. The reason for selecting the coated W is to facilitate the permeation of deuterium due to its thinness (~0.1 mm). The hydrogen permeated through W is collected by Ti that is a hydrogen storage material. This is the mechanism as a key of this new sample to measure the hydrogen permeation. Pd is a catalyst to facilitate a hydrogen transfer from W to Ti. The main role is to reduce the dissociative energy required in the process of hydrogen becoming an atom from a molecule at the interface of Ti.

In the initial samples, blisters on the surface and pores between Pd layer and Ti bulk by the cross-sectional images were observed. In order for Pd to perform its own role, it is necessary to strengthen the contact between Pd and Ti. Accordingly, for the purpose to improve the coating characteristics of Pd, heat treatment was applied to the sample after Pd coating. However, an issue was arisen that the Pd layer becomes unclear after heat treatments of 650 ℃. Therefore, we are promoting the improvement by temperature adjustment. We plan deuterium plasma exposures to the improved samples in the linear plasma device TPD-Sheet IV [1]. Retained deuterium permeated through coated W to Ti is evaluated by Glow discharge optical emission spectrometry (GD-OES).

In this presentation, we report that the improvement of Pd layer by heat treatments and retained deuterium after plasma exposure to the improved samples.

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Vacancy clustering and stabilization in tungsten by hydrogen trapping

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Tritium retention in tungsten is a key issue to qualify the full-tungsten option for DEMO reactors. Tungsten is known as a highly non-occluder metal to hydrogen, which is one of advantages for divertor materials. However, tritium will be trapped by vacancies created by plasma irradiations and fusion neutrons resulting in an increase of tritium retention. Nano-blistering of tungsten surfaces exposed to high-flux deuterium plasmas and enhanced deuterium retention at elevated temperatures are observed [1, 2]. Recently, deuterium retention in tungsten is investigated by self-ion damage experiments with co-injection of deuterium atoms [3]. Influence of hydrogen on vacancies and on its evolution in tungsten is a key issue to predict the tritium retention of DEMO reactors.

In this study, hydrogen (H) mediated vacancy (V) clustering and stabilization in tungsten (W) is investigated based on first-principle calculations of mutual interactions of W-H-V ternary system. The calculations based on density functional theory using VASP code [4,5] are corrected by adding surface exchange-correlation energy correction. The first-principle calculations predict that the di-vacancy formation in tungsten is energetically unfavourable. However, the di-vacancy formation is facilitated remarkably by trapping hydrogen atoms [6]. The formation energies for the di-vacancies trapping single hydrogen atom coincide with an experimental value for the di-vacancy in the first-nearest-neighbour configuration [7]. Similar calculations are conducted for Tri-vacancies [8]. Our calculations predict also that hydrogen clusters stacking with a mono-vacancy suppresses annihilation of the vacancy-SIA (111-crowdion) pair in tungsten [9].

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P-2

The defect formation mechanisms and change of the mechanical properties under the irradiation in pure W and W-Re alloy: Molecular dynamics study

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Tungsten is used plasma-facing material, because of good material properties for withstanding extreme operating condition. Under the irradiation condition, defects nucleation and transmutation into Re or Os occur, which causes the material properties changes. So, it is need to understand the material properties change and defect formation mechanisms of W and W-Re alloys under the irradiation. In this study, we performed molecular dynamics simulations to investigate the defect formation mechanisms and changes of the mechanical properties in bulk W and W-Re alloys. Three different temperatures (400, 700, 1000 K) are chosen to analyse the temperature effect on the displacement cascades. In all trials, irradiation dose reaches up to about 0.1 dpa with a PKA energy of 2 keV. As increasing the irradiation dose, Young's modulus and bulk modulus decreases. Also, formation mechanisms of 1/2 <111> or <100> dislocation loop are observed under the cascade overlapping simulation.

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P-3

Molecular dynamics study of materials properties of pure W and W-10Re alloy before and after irradiation

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Tungsten is expected to be used as plasma facing material (PFM) of fusion reactors, because W(tungsten) has high melting point, thermal conductivity and sputtering resistance. But some tungsten atoms transmute into the Re atoms and form some defects after the neutron irradiation. These lead to changes in material properties. Therefore it is necessary to understand the changes of material properties with temperature and irradiation. In this study, we calculate mechanical properties (Young's modulus and bulk modulus), thermal properties (thermal expansion coefficient, melting temperature) using molecular dynamics simulations of pure W and W-10Re alloy from 0K to 3000K. Before irradiation, pure W has larger Young's modulus and higher melting point than W-10Re alloy. After irradiation, pure W has lower melting point and smaller Young's modulus.

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P-4

Inclusion of Electronic Stopping and Validation in the Open Source Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)

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Electronic stopping (ES) of energetic atoms is not taken care of by the interatomic potentials used in molecular dynamics (MD) simulations. Several methods for inclusion of ES in MD simulations have been developed [1,2,3,4,5]. We use the Lindhard-Scharf (LS) formula [6] for electronic stopping and include it as a drag term for energetic atoms in the open source code LAMMPS. In order to validate the modified code, the total loss due to electronic stopping during the MD simulations is compared with the electronic stopping losses predicted by the NRT model [7] which also uses the LS formula. MD simulations of collision cascades at primary knock-on atom (PKA) energies of 5, 10 and 20 keV are carried out in W and Fe in 100 random directions. It is seen that the total ES losses from the MD simulations averaged over the 100 directions matches the loss predicted by the NRT model very well. The root mean square error from the MD implementation is around 10 % for both W and Fe in the PKA energy range explored.

An important parameter in the MD implementation is the cut-off energy (E_{CutES}) below which there is no electronic stopping. We expect this to be of the order of displacement energy (E_D) of the material, since ES occurs only if there is a physical displacement of atom from its lattice site to another location straddling a neighbouring atom/atoms. We have earlier obtained direction averaged displacement probability ($P(E_D)$) for atoms in W [8] and Fe by carrying out MD simulations in 1000 random directions in the PKA energy range 30-500 eV. It is seen that there exists a minimum energy, $E_{dmin,}$ below which the probability of displacement is 0 and a maximum energy, $E_{dmax,}$ above which the probability of displacement is 1. We show that the ES losses from MD matches the ES losses from the NRT model when E_{cutES} equals the average value of E_{DMin} and E_{dmax}, for both W and Fe.

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P-5

Investigation of temperature and ion energy threshold for tungsten fuzz growth by Monte Carlo Simulation

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Tungsten has been considered as the primary candidate for the wall material of the next generation fusion devices. The advantages of low sputtering yield, high melting point and excellent thermal conductivity are crucial factors for fusion operation environment. However, in recent decades, nanostructures on tungsten surface called ‘fuzz’, which is known to degrade the good properties of tungsten, have been discovered under helium plasma irradiation in many experiments [1,2]. Numbers of studies has been done to investigate the mechanism of fuzz growth in both experiment and simulation method. Ion inducement and migration is wide believed as the main reason of fuzzy structure generation [3]. A window of temperature and incident ion energy for tungsten fuzz growth has been rivaled [4]. The mechanism of fuzz growth can partly explain this parameter window, but the comprehension of these thresholds which fuzz can grow is still deficient.

We investigate this issue by using the three dimensional Monte Carlo code named SURO-FUZZ, which has simulated the early stage of tungsten fuzz growth in 1073K [5]. In this study, surface morphology is presented at different surface temperature and incident ion energy compared with experimental observations. The results indicate that diffusitive of helium particles and the capacity of tungsten for holding the bubble presure play important roles in the various behaviour of sungsten surface (nanobubbles, fuzz, large voids).

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P-6

Study of proton irradiation in wurtzite GaN with a-type prism-edge dislocation using molecular dynamics simulations

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LED and HEMT (High Electron Mobility Transistor) based on gallium nitride (GaN) was introduced in the aerospace industry decades ago because of outstanding features including large bandgap and high electron mobility. GaN also shows high radiation hardness, which is a major property considered in aerospace applications. In order to investigate radiation damage on GaN during operating in the space, researchers conducted experiments [1, 2]. From these studies, the relation between the degradations of properties in applications and non-ionizing energy (NIEL) were proved. Simulations were also carried out to improve the comprehension of the mechanism of radiation damages [3, 4]. However, dislocations in the GaN, which occurred necessarily due to the lattice mismatch in the experiments, were not considered in the simulation.

In this study, Primary Knock-on Atom (PKA) simulations with and without *a*-type prism-edge dislocations are conducted in order to predict displacement damage on bulk wurtzite GaN at 300K. The PKA energies coming from protons are selected based on the results of GEANT4 simulation. PKAs are chosen near the dislocations under 10 Å and its velocity is applied in the directions of the dislocation core. The defects statistics, recovery rate and changes of dislocation will be compared and discussed.

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P-7

Development of Potential Model with Three-body Interaction for Tungsten

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Tungsten (W) is considered as one of the candidate materials for plasma facing components in fusion reactors. Molecular dynamics (MD) simulation can be used in understanding the behavior of tungsten during the reactor operation. MD simulations are categorized into two types, classical MD (CMD) and first-principles MD (FPMD), which are different in the way they calculate the potential energy and atomic forces needed to simulate time evolution of a system. In the present study, we propose a method to systematically construct an accurate potential model for CMD simulation by using calculation results of FPMD, and construct a potential model for tungsten.

In the proposed potential model, we explicitly treat up to three body interaction and treat many body interactions above four body with an embedded-atom method (EAM) potential [1]. The coefficients of each term are optimized by minimizing the least square error from a set of energy, force and stress data calculated by FPMD. The VASP code is used for FPMD based on the density functional theory (DFT). The Perdew-Burke-Emzerhof (PBE) exchange correlation functional is utilized.

After construction of the potential model, physical quantities are calculated by CMD using the LAMMPS code. Subsequently, the quality of the potential model is evaluated by comparing the calculation results with experimental data and first principles calculation results. To be specific, equilibrium lattice constant, cohesive energy, surface energies, bulk modulus, vacancy formation energy, and the melting point are examined. The comparison shows reasonable correspondence for all properties tested. The constructed potential model can reproduce (100) surface reconstruction [2].

Finally, the calculation cost of the developed potential model is compared with the costs of other existing potential models for tungsten. The developed potential model has one-fourth speed of a bond-order potential [3], which also uses many body and angular interaction. This comes from the interpolation scheme that is used for three body terms in the present potential model, which we plan to improve in a future work.

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Recent Machine Learning Algorithms for Classification of Time Series: Recurrent Deep Learning Networks with Potential for Plasma Applications

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Applications of deep learning have recently become common and achieved substantial interest in various fields of science, such as plasma disruption modelling [1] and solar flares prediction [2].

In the proposed poster we review the recent recurrent neural network architectures from deep learning, such as the LSTM and GRU models [3] and focus on the regression and classification performance of related machine learning architectures for the case of time series. In particular, we illustrate the performance of our recent method [4] for autoregressive processes using the example of non-stationary cryptocurrency time series data. Preliminary results may also be shown for simple time series related to plasma applications.

We hope to establish possible collaboration in using the recurrent deep learning neural network techniques for plasma modelling applications.

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NIFS Atomic and Molecular Numerical Database for Collision Processes in Plasmas

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We have constructed and opened NIFS Atomic and Molecular Numerical Database for collision processes for public at http://dbshino.nifs.ac.jp/. Atomic and molecular (AM) data compilation started in 1970s [1] and the AM database system was first built in computer in 1980s [2]. Web accessible system with oracle relational database managing system was started in 1997 [3]. The database system was rebuilt with PostgreSQL and Ruby on Rails with JavaScript in 2017. We improved user interfaces introducing simple table skipping complex query form. This allows to find available data easily especially for molecular data. Numerical data can be seen in browser and graphical output is also available.

The database consists of 9 sub-databases, i.e. AMDIS ION (electron-impact ionization cross sections/rate coefficients, 2,943 records stored), AMDIS EXC (electron-impact excitation cross sections/rate coefficients, 725,718 records), AMDIS REC (recombination rate coefficients, 27,534 records), AMDIS DIO (dissociation cross sections, 202 records), CHART (ion-atom collision cross sections, 7,618 records), AMDIS MOL (electron – molecule collision cross sections/rate coefficients, 3,187 records), CHART MOL (atom – molecule collision cross sections, 2,139 records), SPUTY (sputtering yields, 2,349 records), and BACKS (back scattering coefficients, 485 records). Almost all data are compiled from publications, and information on papers are attached to the data records. Such publications with AM data are searched by human and extracting data to make data files are also done by human. Thus man-power is needed for data update. We tried to use data mining concept to search such publications many years ago, but there were many problems. We need such tool with a new technic to find publications to extract valid AM data.

Recently we have started to implement our database to Virtual Atomic and Molecular Data Centre (VAMDC) [4]. At the moment AMDIS ION is linked to VAMDC portal. Other sub-databases will be linked in future. This new activity will help users who need AM data for their researches.

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P-10

Observation of trapped hydrogen in coated tungsten on titanium specimen

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Estimations of leakage tritium amounts from plasma facing side to the coolant is important issue in DEMO [1]. In general, hydrogen isotope permeation is measured by a quadrupole mass spectrometry (QMS), which can detect widely integrated at regions around target areas [2]. Permeation measurements are not sufficient data evaluated directly the hydrogen permeation amount in metallic walls under high heat load plasma irradiation in magnetic confinement fusion devices.

Therefore, in order to quantitatively evaluate the amount of hydrogen permeation in the metallic wall during high heat load plasma irradiation, it is designed that a specimen, which was combined titanium (Ti) as a hydrogen trapping material, and tungsten (W) as one of candidate materials for plasma facing walls in DEMO. For high efficiency of hydrogen permeation from the W to Ti, palladium (Pd) is used as a hydrogen permeation catalyst between Ti and W.

Hydrogen isotope observations are planned from a plasma facing side and a backside of the specimen, which is Ti plate without connected to Pd layer, using sputtered analytical method such as glow discharge optical emission spectroscopy (GD-OES). It is required that optimizations of thickness of W, Pd layers, and Ti for sufficient intensities of deuterium.

In the case of thin Ti plate about 0.1 mm, a surface of the specimens show distortion for subsequent Pd and W coatings. Hence, the current design uses Ti plate of 0.5 mm. After deuterium plasma exposure in a linear plasma facility, TPD-Sheet IV, in Tokai University [3], deuterium at Pd side on Ti was detected. In this presentation, observations of deuterium at the backside of the specimen are shown, and characterizations of the specimen are discussed.

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