Final Progress Report

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"Plasma Surface Interactions: Bridging from the Surface to the Micron Frontier through Leadership Class Computing"

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I. Introduction

The choice of material for the plasma facing components (PFC), in particular, for divertor targets, is one of the main issues for future tokamak reactors. There are two major requirements for the PFC's material: acceptable level of tritium retention and durability in a harsh environment of fusion grade plasma. Based on these criteria, some years ago it was decided that tungsten is an acceptable material for divertor targets in ITER. However, further experimental studies reveal that the irradiation of tungsten even with low energetic (well below sputtering threshold!) He containing plasma causes significant modification of surface morphology, formation of the layer of He nano-bubbles (in the temperature range T<1000 K), "fuzz" (for 1000 K<T<2000 K), and pinholes (for T>2000 K) (e.g. see Fig. 1). Recall that He, being an ash of D-T fusion reactions, is an inherent impurity in fusion plasma.

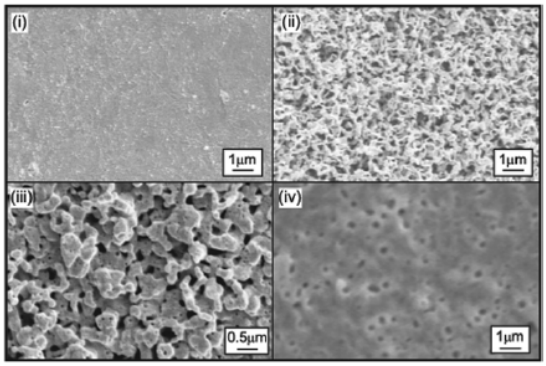

Fig. 1a. Pinholes and "Fuzz" on tungsten surface after irradiation of He plasma. (Kajita et al., NF, 2009)

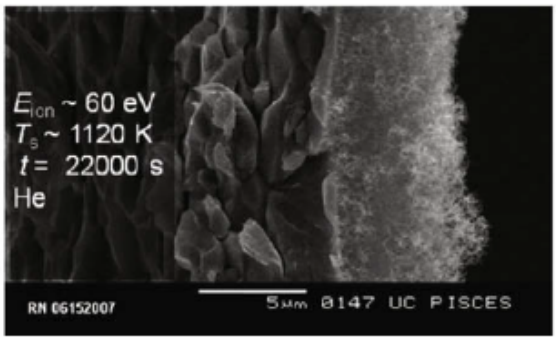

Fig. 1b. "Fuzz" on tungsten surface after irradiation of He plasma. (Baldwin et al., JNM, 2009)

The goals of the UCSD Applied Plasma Theory Group was: i) investigate the mechanisms of the formation of He nano-bubble layer and fuzz growth under He irradiation, as well as the physics of transport of hydrogen species in tungsten lattice, and ii) develop physics understanding of the models suitable for the incorporation into the Xolotl-PSI code based on the reaction-diffusion approach, which is the flagship of the whole SciDAC project [8], which can guide both numerical simulations and experimental studies. Here we just highlight our major accomplishments.

II. Hydrogen transport in tungsten

As we have mentioned above, hydrogen transport and retention in the PFC's material is one of the key issues for the choice of the PFC's material. The hydrogen retention is associated with the hydrogen trapping in the imperfections (traps) of material's lattice. One of the experimental tools allowing to determine the trapping (binding) energies of hydrogen is the Temperature Desorption Spectroscopy (TDS), which is based on the study of the rate of hydrogen desorption as a function of ramping up sample temperature. To deduce both trap densities and trapping energies from the TDS data, researches are usually use the reaction diffusion models and adjust both spectrum of trapping energies and trap density distribution to fit experimental data. However, this is an "ill posed" problem which include both hydrogen diffusion and re-trapping and it's solution does not give you 100% proved answer. To understand the limitations of the TDS-based approach we perform very thorough study of an impact of different processes (including diffusion and re-trapping) on the accuracy of the post-processing of the TDS data [7, 11]. As a result, we found some useful criteria for the validity of the parameters, which can be deduced from the TDS data.

However, experimental data from tokamaks suggest that the majority of hydrogen is trapped in a co-deposits, which may have very complex atomic structure and, as a result, a broad-band distribution of traps over trapping energies. For this case the conventional approach to the analysis of the TDS data, based on just few different traps, does not work. Therefore, to study the broad-band effects on the TDS we introduce the continuum approximation of the traps over the trapping energies. Our analytic studies confirmed by numerical simulations with our newly developed code FACE [3, 13] demonstrated that hydrogen dynamics in co-deposits for the case of a broad-band trapping energies is very different from a "standard" case of just few traps. In particular we have demonstrated that hydrogen dynamics for the case of a broad-band trapping can be described (depending on trap distribution) by sib- or super-diffusion processes. As a result, hydrogen long-time outgassing from co-deposits can follow $t^{-\alpha}$ where α can differ from 0.5, which follows from a standard diffusion law. This can explain experimentally observed in both JET and Tore-Supra tokamaks a long-time outgassing from co-deposits proportional to $t^{-0.7}$.

Finally, we have addressed an issue of hydrogen desorption from tungsten surface with the Molecular Dynamic (MD) simulations. We have shown that standard H-W Tersoff interaction potentials, widely used in different MD simulations describing the interactions of hydrogen with tungsten, cannot properly explain experimental data of predominantly molecular hydrogen thermal desorption [6]. It appears that the reason for such discrepancy is the

overestimation of the impact of tree-body interactions in a standard H-W Tersoff potential. By a proper change of this part of a standard H-W Tersoff potential we were able to fit available experimental data (see Fig. 2 taken from Ref. 6). Nonetheless, this fact is razing the question of the validity of available W-H potential at tungsten surface.

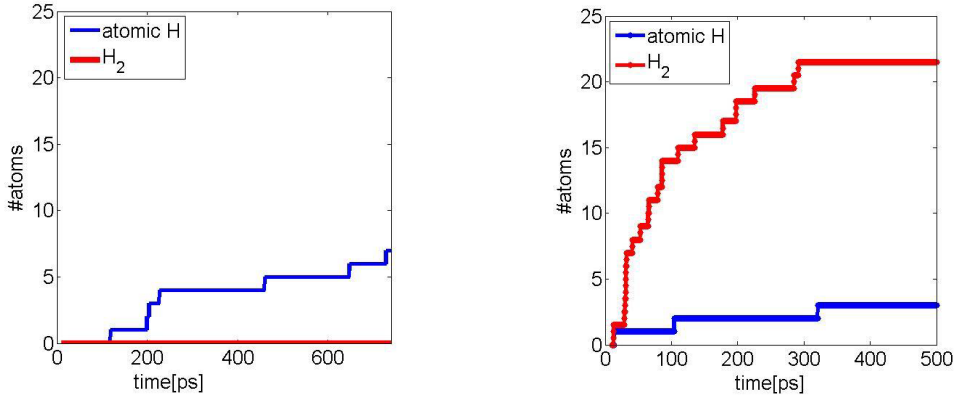

Fig. 2. The rates of molecular vs atomic hydrogen thermal desorption from tungsten surface for a standard (left) and modified (right) H-W Tersoff interaction potentials.

III. Helium transport in tungsten

One of our early model of the fuzz formation caused by He irradiation (Krasheninnikov, *Phys. Scripta*, 2011) used, in particular, *ad-hoc* postulated enhanced tungsten plasticity for the case of large amount of He atoms embedded into tungsten lattice. In order to verify this assumption we performed the MD simulations of tungsten yield stress as a function of He concentration. Our results confirm our assumptions and demonstrated a significant reduction of the yield, supporting so-called "visco-elastic" model of the fuzz growth [1].

In Refs. 2, 9 we analyze the formation of the layer of nano-bubbles, observed in experiments (e.g. see Fig. 3), based on He self-trapping and He trapping to available lattice defects.

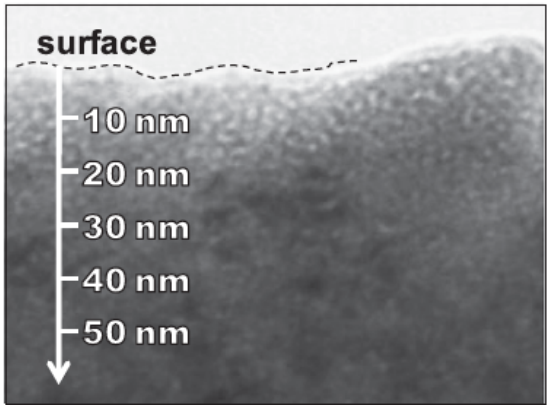

Fig. 3. Layer of experimentally observed nano-bubbles. Miyamoto, JNM, 2011

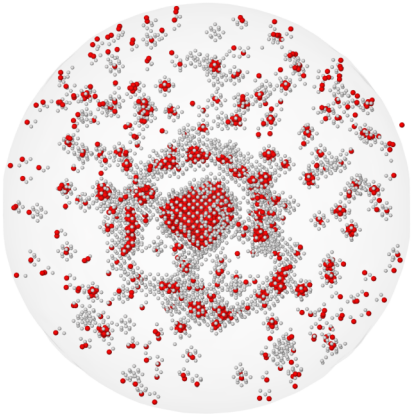

Fig. 4. He trapping in dislocation loops caused by the growth of nano-bubble [5].

Based on He cluster dynamics described by reaction-diffusion equations we found analytic and semi-analytic solutions [2] predicting that if the formation of He nano-bubbles is due to He self-trapping: i) it cannot explain the formation of the nano-bubbles in the tendrils of the fuzz seen in experiments, ii) the thickness of the layer of He nano-bubbles in thick tungsten sample should strongly increase with decreasing the flux of He impinging to the surface. In Ref. 9 these conclusions were confirmed by numerical solution of the system of equations describing He cluster dynamics. However, experimental data show that the thickness of the layer of He nano-bubbles in tungsten sample virtually does not depend on He flux.

The way out of this "inconsistency" was suggested by the results of our MD simulations of growth and coalescence of nano-bubbles [4]. It appears that both growth and coalescence of nano-bubbles are accompanied by the formation of the dislocation loops, which serve as He traps promoting the growth of other bubbles (see Fig. 4). The model for such avalanche-like processes developed and solved in Ref. 5, 12 gave very good agreement with all major experimental observations of the parameters of the layer of He nano-bubbles.

IV. Conclusions

Our UCSD Group was very productive in this SciDAC project, publishing 13 papers in refereed journals, developing understanding of the physics of helium/hydrogen interactions with tungsten, bringing up novel ideas, and guiding both comprehensive numerical simulations and experimental studies.

Publications in refereed journals

[1] R.D. Smirnov and S.I. Krasheninnikov "On the shear strength of tungsten nano-structures with embedded helium", *Nucl. Fusion* **53** (2013) 082002. (doi:10.1088/0029-5515/53/8/082002)

[2] S.I. Krasheninnikov, T. Faney, and B.D. Wirth "On helium cluster dynamics in tungsten plasma facing components of fusion devices", Nucl. Fusion **54** (2014) 073019. (DOI: 10.1088/0029-5515/54/7/073019)

[3] R.D. Smirnov, S.I. Krasheninnikov, J. Guterl, M.J. Baldwin, and R.P. Doerner "Modeling of hydrogen retention and outgassing from co-deposits with distributed energy states", *Contrib. Plasma Phys.* **54** (2014) 610-614. (DOI 10.1002/ctpp.201410033DOI 10.1002/ctpp.201410033)

[4] R.D. Smirnov, S.I. Krasheninnikov, and J. Guterl, "Atomistic modeling of growth and coalescence of helium nano-bubbles in tungsten", *J. Nucl. Materials* **463** (2015), 359–362. (doi:10.1016/j.jnucmat.2014.10.033)

[5] S.I. Krasheninnikov and R.D. Smirnov, "He cluster dynamics in fusion related plasma facing materials", *Nucl. Fusion* **55** (2015), 073005. (doi:10.1088/0029-5515/55/7/073005)

[6] J. Guterl, R.D. Smirnov, S.I. Krasheninnikov, B. Uberuaga, A.F. Voter, and D. Perez, "Modeling of hydrogen desorption from tungsten surface", *J. Nucl. Materials* **463** (2015), 263–267. (doi:10.1016/j.jnucmat.2014.12.086)

[7] J. Guterl, R.D. Smirnov, S.I. Krasheninnikov, M. Zibrov, and A.A. Pisarev, "Theoretical analysis of deuterium retention in tungsten plasma-facing components induced by various traps via thermal desorption spectroscopy", *Nucl. Fusion* **55** (2015), 093017. (doi:10.1088/0029-5515/55/9/093017)

[8] B.D. Wirth, K.D. Hammond, S.I. Krasheninnikov, and D. Maroudas, "Challenges and Opportunities of Modeling Plasma Surface Interactions in Tungsten Using High Performance Computing", *J. Nucl. Materials* **463** (2015), 30–38. (doi:10.1016/j.jnucmat.2014.11.072)

[9] T. Faney, S.I. Krasheninnikov, and B.D. Wirth "Spatially dependent cluster dynamics model of He plasma surface interaction in tungsten for fusion relevant conditions", Nucl. Fusion **55**, 013014 (2015). (DOI: 10.1088/0029-5515/55/1/013014)

[10] R.D. Smirnov, S.I. Krasheninnikov, and J. Guterl "Atomistic modeling of growth and coalescence of helium nano-bubbles in tungsten", *J. Nucl. Mater.* **463** (2015) 359-362. (http://dx.doi.org/10.1016/j.jnucmat.2014.10.033)

[11] J. Guterl, R.D. Smirnov, S.I. Krasheninnikov, "Revisited reaction-diffusion model of thermal desorption spectroscopy experiments on hydrogen retention in material", *J. Appl. Phys.* **118** (2015) 043302 (http://dx.doi.org/10.1063/1.4926546)

[12] S.I. Krasheninnikov and R.D. Smirnov, "He cluster dynamics in W in the presence of cluster induced formation of He traps", *Phys. Scripta* **T167** (2016), 014021. (doi:10.1088/0031-8949/T167/1/014021)

[13] R.D. Smirnov, J. Guterl, and S.I. Krasheninnikov, "Modeling of multi-species dynamics in fusion related materials with FACE code", *Fusion Sci. Technol.* **71** (2017) 75-83. (doi: 10.13182/FST16-125)