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Low energy and low fluence helium implantations in tungsten: Molecular dynamics simulations and experiments

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HIGHLIGHTS

- MD simulations give He retention rate decreasing with increasing incident He number.
- MD simulations reveal He saturation level in W close to experiments.
- MD simulations show W flaking due to He accumulation.
- MD simulations show stratification phenomena of the He depth distribution in W.

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ABSTRACT

300 eV Helium implantation process into tungsten at 300 K has been studied with molecular dynamic simulations (MD). Predicted retention doses were compared to that obtained from experiments performed in equivalent conditions. A saturation phenomenon of the helium retention was evidenced for a number of impinging He atoms and a retention dose similar in both, experiments and simulations. From MD simulations it is learnt that observed Helium diffusion, formation and coalescence of clusters are the phenomena leading to the flaking of the substrate. These processes could explain the saturation of the Helium retention observed experimentally at low energies.

1. Introduction

Due to its low sputtering yield and high melting point, tungsten is the material chosen to compose the first wall of the divertor of ITER fusion reactor. This part of the chamber will face the most severe conditions of the plasma, such as high fluxes of light particles with a wide range of energies and high heat loads [1–3]. Studies on plasma material interactions are currently carried out to anticipate the evolution of this metal while exposed to fusion plasma. Several reactors are developed to investigate the interactions of such fusion plasma on W such as Nagdis-I and II in Nagoya or Pisces in San Diego [4,5].

Gas implantation, diffusion and retention into metals are well-explored phenomena [6,7] Experimental studies have evidenced that He ion fluxes on W substrates lead to various surface morphology changes such as blistering, fuzz formation and even flaking [8–11]. Those features appearance is strongly dependent on the flux and incident energy of the ions; it also depends on the substrate temperature during the implantation process. At high energies, keV to MeV, mean penetration depths are high (100 nm to microns) and defects induced by elastic and inelastic collisions lead to the formation of damages in the substrates. However at low ion energies (below W displacement thresholds: 90 eV transferred from the impinging ion) the formation of the characteristic damage features is still under investigation.

Experiments performed in Nagdis-II by Nishijima et al. [8] showed damages as holes appeared for high fluxes (10^{19} cm^{-2} s^{-1}) and high doses or number of impinging atoms (10^{23} cm^{-2}) for energies ranging from 5 to 30 eV at high temperature (1300–2950 K). It was also reported by Lee et al. [12] that a

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limited number of He could remain in the material for energies below W displacement threshold for implantations performed with fluxes ranging from 10^{14} to 10^{15} cm^{-2} s^{-1} and doses from 10^{17} to 10^{19} cm^{-2}. Simulations using molecular dynamics were also performed to study the phenomena involved in the implantation process at low energies. Henriksson et al. studied the behaviour of helium with doses below 10^{14} cm^{-2} and with energies varying from 50 to 200 eV at 0 and 300 K [13]. Li et al. investigated implantations of 10^{15} cm^{-2} impinging helium ions on W at 200 eV at temperatures from 300 to 1500 K [14,15]. Both observed formation of growing and exploding clusters which liberate their He content to the surface. In the case of slightly higher energies (300 eV–1 keV), the mean penetration of the He is observed to be deeper and no "cluster rupture" was identified due to simulations stopped too early in the course of He interactions [15].

In the present article, the objective is to describe the phenomena observed during the simulation of implantation process carried out at doses ranging from 10^{14} to 10^{17} cm^{-2} and with a kinetic energy of 300 eV at a temperature of 300 K the simulations were performed by molecular dynamics and SRIM [16] calculations. MD simulations initial conditions are chosen to closely fit with experiments. The aim is to explain the saturation of the retained He atom number which does not occur because of the "cluster ruptures" but is however evidenced for implantation experiments performed at energies below W displacement threshold.

Then after a review of the details of the simulation and experimental methods, the MD simulation and experimental results are discussed and compared.

2. Model and experiments

2.1. Model, calculations: starting parameters and data treatment

To investigate the phenomena occurring during the implantation of Helium into the tungsten, molecular dynamic simulations are carried out on an Alineos quadriprocessor 8 cores high performance computer using LAMMPS [17]. Besides, the SRIM code, which is widely referred to in ion/material interaction studies, is used in addition to compare the statistics of the resulting implanted atom concentration and depth profiles.

A (100) body-centred cubic tungsten crystal box consisting of 17 × 17 × 204 unit cells is built, for which dimensions are then 53.8 × 53.8 × 645.7 Å. Periodic boundaries conditions are set in the *x* [100] and *y* [010] directions, and free motion is allowed along *z* [001]. The temperature of the substrate is set to 300 K, thus matching the room temperature experiments. The bottom of the box is composed of a fixed layer of 6 unit cells (20.5 Å) which mimics the unperturbed bulk. The rest of the W atoms are maintained at the temperature 300 K by the mean of a Berendsen thermostat [18]. The thermostat is used because the fluxes of impinging atoms used in MD simulations are unphysically high as compared to the experiments in order to reduce the large calculation times and properly accounting He interactions with W and already He present in W. Then over a set time, velocities of the W atoms are re-evaluated and brought back to values matching the initially set global temperature of the substrate. The substrate atom W current velocities are modified using the multiplicative coefficient χ:

$$\chi = \left(1 + \frac{dt}{\tau}\left(\frac{T_s}{T_k} - 1\right)\right)^{\frac{1}{2}}.$$

where dt is the integration timestep (here 0.1 fs), T_s is the targeted temperature, T_k is the current temperature and τ is the time needed for reaching the targeted temperature T_s.

This thermostat allows proper energy relaxation of the substrate for mimicking energy dissipation in the experiment on a reasonable time scale: it is set here to 1 ps, a value consistent with a model of electron-phonon coupling [19,20] that allows estimation of the relaxation time τ by the formula:

$$\tau = \frac{2m_e\kappa\varepsilon_F}{\Theta_D T_e L n e^2 k_B Z}$$

Θ_D is the surface Debye temperature, T_s the substrate temperature, L the Lorentz number, n the electron density, e the electron charge, k_B the Boltzmann constant, Z the valence, m_e the electron mass, κ the thermal conductivity, ε_F the Fermi energy and T_k is the kinetic temperature. For W, τ = 1 ps and is used as the relaxation time of the Berendsen thermostat.

Substrate thickness is chosen in order to limit to 0.5% the implanted He atoms crossing the substrate through the fixed W atoms layer. This allows observing all the implanted He atoms, their localization and surrounding, considering the channelled atoms as well. Also, the high number of thermostated W atoms combined with the energy dissipation handled by the thermostat helps keeping the desired temperature of the substrate at 300 K such as in the experiments. Moreover the thickness is chosen in order to keep unperturbed thermostated layers at the substrate bottom and so observe a smooth transition toward the fixed bottom layers. Thus none of the perturbations of the W lattice are missing.

Helium ions are treated as atoms, as they are neutralized at the W surface, so classical MD simulations are then applicable. He atoms are injected one by one and in a direction normal to the surface from a randomly chosen position above the box. This allows avoiding any interaction before reaching the substrate's surface. The frequency of the helium atom injection is set between 2.5 and 5 $at.ps^{-1}$. Such impingement frequency allows no lateral interaction between induced perturbations in the W crystal during the dissipation time, due to the large enough substrate width. The kinetic energy of the impinging He is set to be 300 eV. The lattice displacement threshold for a W atom is of 90 eV, and the maximum energy transferred from a He atom to a W atom is 25 eV when the He collides with an energy of 300 eV. This value is obtained from the elastic collision energy transfer formula: $E_{tr} = E_i{}^*4m_1m_2/(m_1+m_2)^2$ [2]. The number of helium atoms impinging the W surface ranges from 2000 to 10000 for a surface of 53.8 × 53.8 $Å^2$. It corresponds to the experiment doses ranging from 10^{14} to 10^{17} cm^{-2}.

Handling molecular dynamics only requires the knowledge of inter-atomic potentials and a set of initial conditions. We use the Juslin and Wirth potentials [21]: W–W interactions are described by a modified Ackland-Therford potential and W–He interactions are modelled from DFT study. Finally, He–He interactions in the substrate are described by Beck's potential [22], which would allow He cluster growth.

Analysis of He retention rate, of snapshots during implantation simulations and of implanted He atom depth profiles will give insights into the interaction dynamics of the He with W. SRIM calculations are also carried out for determining retention rates and depth profiles using SRIM 2013 with 2008 stopping power parameters [16,23]. SRIM software uses Binary Collision Approximation and is commonly used in simulating implantation processes. It considers an amorphous substrate with a density matching the W structure (19.3 $g\ cm^{-3}$) and ignores either the interaction between He atoms or effect of the accumulation in the substrate. Moreover SRIM calculations do not account for recombination of interstitials with the vacancies, nor for defect clustering and irradiation-induced amorphization. Thus comparison with MD simulations,