Journal of Nuclear Materials 447 (2014) 254–270

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

Reflection and implantation of low energy helium with tungsten surfaces

Valery Borovikov *, Arthur F. Voter, Xian-Zhu Tang

Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, USA

ARTICLE INFO

Article history:
Received 20 February 2013
Accepted 13 January 2014
Available online 24 January 2014

ABSTRACT

Reflection and implantation of low energy helium (He) ions by tungsten (W) substrate are studied using molecular dynamics (MD) simulations. Motivated by the ITER divertor design, our study considers a range of W substrate temperatures (300 K, 1000 K, 1500 K), a range of He atom incidence energies ($\leqslant$100 eV) and a range of angles of incidence (0–75°) with respect to substrate normal. The MD simulations quantify the reflection and implantation function, the integrated moments such as the particle/energy reflection coefficients and average implantation depths. Distributions of implantation depths, reflected energy, polar and azimuthal angles of reflection are obtained, as functions of simulation parameters, such as W substrate temperature, polar angle of incidence, the energy of incident He, and the type of W substrate surface. Comparison between the MD simulation results, the results obtained using SRIM simulation package, and the existing experimental and theoretical results is provided.

1. Introduction

Plasma surface interaction (PSI) at the first wall and divertor of a fusion reactor not only poses a materials challenge in terms of radiation damage due to the extreme plasma and neutron irradiation flux, but also introduces a controlling factor on the boundary plasma conditions through recycling and impurity production. The latter effect has a direct impact on fusion power output since edge plasma is known to affect the performance of fusion-producing core plasmas. Presently both solid wall and liquid wall designs are being actively studied. The design of ITER chooses a combination of beryllium (Be) first wall and tungsten (W) divertor. A number of current tokamak upgrades and proposed future machines have been exploring a configuration of all-tungsten first wall and divertors. The primary benefits are the high melting temperature, the low sputtering yield, and the excellent thermal conductivity of refractory metals in general and tungsten in particular [1].

The plasma ion irradiation flux to the tungsten surface in a fusion reactor is made of deuteron (D) and triton (T), which are unburned fusion fuel, and helium (He), which is the fusion product. Unlike D and T, helium is chemically inert, but can bring severe damage to the tungsten surface by clustering in the form of subsurface bubbles, which can burst and induce complicated surface morphology known as fuzz. Also unlike D and T, helium cannot aggregate on the tungsten surface as a deposited He layer. The incoming helium is either implanted below the W surface or reflected upon impact. The implanted He can migrate to the tungsten surface on a diffusive time scale. The desorption of He from a tungsten surface is energetically favorable so a mostly clean tungsten surface is maintained in a He plasma. In a working fusion reactor, the recycling of He will be complicated by the presence of triton and deuteron at the tungsten surface. Here we will focus on the pure He plasma situation. This simplification is helpful in establishing a better understanding of the fundamental process of He ion interaction with a tungsten surface. It is also practically important because, due to heating power constraint for accessing high (H) confinement mode, there is a proposed pure He plasma phase in the ITER program start-up.

Our emphasis here is on low energy helium ions, in the range of 1–100 electron volts (eV) at the time of impact with the tungsten surface. This is to be consistent with the design goal/choice that takes advantage of the negligibly small sputtering yield of light ions on tungsten surface at low energy. For an impacting He ion with energy E_i, incident polar angle θ_i and azimuthal angle φ_i, the probability of it being reflected by the tungsten surface with an outgoing energy E_r into a differential solid angle $d\Omega \equiv \sin\theta_r d\theta_r d\varphi_r$ about θ_r and φ_r, is $\mathcal{T}(E_r, \theta_r, \varphi_r | E_i, \theta_i, \varphi_i) d\Omega$. Evidently $\mathcal{T}(E_r, \theta_r, \varphi_r | E_i, \theta_i, \varphi_i; \Sigma, T)$ is also a function of the tungsten surface type Σ and its temperature T. The total probability of the He ion being reflected upon impact is

$$R(E_i, \theta_i, \varphi_i; \Sigma, T) = \int_0^\infty dE_r \int_0^{\pi/2} \sin\theta_r d\theta_r \int_0^{2\pi} d\varphi_r \mathcal{T}, \quad (1)$$

* Corresponding author. Present address: Division of Materials Sciences and Engineering, Ames Laboratory, Ames, IA 50011, USA. Tel.: +1 5134322070.

E-mail addresses: valery@lanl.gov (V. Borovikov), afv@lanl.gov (A.F. Voter), xtang@lanl.gov (X.-Z. Tang).

http://dx.doi.org/10.1016/j.jnucmat.2014.01.021
0022-3115/Published by Elsevier B.V.

and the average energy of the reflected He is given by

$$\langle E_r \rangle = \int_0^\infty dE_r \int_0^{\pi/2} \sin\theta_r d\theta_r \int_0^{2\pi} d\varphi_r E_r \mathcal{T}. \quad (2)$$

The so-called energy reflection coefficient for mono-energetic He ion striking the tungsten at a particular orientation is given by

$$R_E(E_i, \theta_i, \varphi_i; \Sigma, T) \equiv \frac{\langle E_r \rangle}{E_i}. \quad (3)$$

The reflection function $\mathcal{T}$ provides the energy and angular distribution of the reflected He atoms $F_r(E_r, \theta_r, \varphi_r)$ for any given impacting He ion distribution $F_i(E_i, \theta_i, \varphi_i)$,

$$F_r(E_r, \theta_r, \varphi_r) = \int_0^\infty dE_i \int_0^{\pi/2} \sin\theta_i d\theta_i \int_0^{2\pi} d\varphi_i \mathcal{T}(E_r, \theta_r, \varphi_r | E_i, \theta_i, \varphi_i; \Sigma, T) F_i(E_i, \theta_i, \varphi_i). \quad (4)$$

F_r provides the wall feedback flux to the boundary plasma, which is described by a set of combined plasma/neutral evolution equations. In other words, F_r sets the boundary condition for a boundary plasma model that can inform us on the energy and angular distribution of the impacting He ions. The importance of this recycling process is that it provides a crucial link in the feedback loop of PSI that governs the boundary plasma condition in a fusion reactor.

Particle conservation implies that $1 - R(E_i, \theta_i, \varphi_i; \Sigma, T)$ is the probability of the impacting ion being implanted into the tungsten. For the implanted He ions, the final resting position gives the so-called range distribution function $\mathcal{S}(l, \theta_s, \varphi_s | E_i, \theta_i, \varphi_i; \Sigma, T)$ with l the distance from the surface, θ_s the polar angle and φ_s the azimuthal angle, all relative to the point of initial impact at the tungsten surface. By definition,

$$\int_0^\infty l^2 dl \int_0^{\pi/2} \sin\theta_s d\theta_s \int_0^{2\pi} d\varphi_s \mathcal{S}(l, \theta_s, \varphi_s | E_i, \theta_i, \varphi_i; \Sigma, T) = 1 - R(E_i, \theta_i, \varphi_i; \Sigma, T). \quad (5)$$

The average projected range or implantation depth normal to the surface for an impacting He ion of $(E_i, \theta_i, \varphi_i)$ is

$$L(E_i, \theta_i, \varphi) = \int_0^\infty l^2 dl \int_0^{\pi/2} \sin\theta_s d\theta_s \int_0^{2\pi} d\varphi_s x \mathcal{S}, \quad (6)$$

where

$$x \equiv l \cos\theta_s, \quad (7)$$

the projected range. For an impacting He distribution of $F_i(E_i, \theta_i, \varphi_i)$, the total range distribution $S(l, \theta_s, \varphi_s)$ is

$$S(l, \theta_s, \varphi_s) = \int_0^\infty dE_i \int_0^{\pi/2} \sin\theta_i d\theta_i \int_0^{2\pi} d\varphi_i \mathcal{S}(l, \theta_s, \varphi_s | E_i, \theta_i, \varphi_i; \Sigma, T) F_i(E_i, \theta_i, \varphi_i). \quad (8)$$

The range distribution $S(l, \theta_s, \varphi_s)$, or equivalently, $S(x, \theta_s, \varphi_s)$, provides the source information of implanted He atoms for understanding their eventual effect on the bulk and surface properties of the tungsten divertor and first wall. This is the materials side of plasma-surface interaction, in contrast to $F_r(E_r, \theta_r, \varphi_r)$ which provides the influence of plasma-surface interaction on the plasmas. Specifically for tungsten, implantation of He can cause He-bubble formation, blistering and formation of W nanostructure ("fuzz") on the surface [2–4]. This can lead to rapid erosion and significant degradation of the mechanical properties and heat load resistance of the material. Interaction of He with W surfaces has been investigated experimentally and theoretically for the last four decades [5–10]. There were also a number of simulation studies. In particular, Henriksson et al. [11,12] studied He bubble formation and initial stages of blistering in He implanted Li et al. [13] studied temperature effects on low energy He bombardment of the W surface. However, only the W (100) surface was considered and only bombardment with incident direction normal to the surface was studied.

The primary objective of this paper is to quantify $\mathcal{T}$ and $\mathcal{S}$ for low energy He ion bombardment of W surfaces. This information is required for further studies of wall recycling on boundary plasmas ($\mathcal{T}$) and plasma irradiation on materials properties ($\mathcal{S}$). Molecular dynamics is arguably the method of choice to provide $\mathcal{T}$ via direct numerical simulations. This will become obvious as one encounters the detailed multiple multi-body collision processes as opposed to single binary collision in He reflection by W surfaces. For the low energy He ion considered here, MD is also an excellent tool for quantifying the range distribution for the He implantation since the contribution from electronic stopping is small. We have performed MD simulations of low energy He bombardment of three W surfaces, using three W substrate temperatures, a range of He incident energies and a range of angles of incidence with respect to substrate normal. We have also compared the results of MD simulations with the results obtained using the SRIM simulation package [14], as well as with the existing experimental and theoretical results. For the purpose of completeness in documenting simulation data of $\mathcal{T}$ and $\mathcal{S}$ as boundary and initial conditions for boundary plasma modeling and studies of He transport in tungsten, we provide a large number of tables and plots.

The rest of the paper is organized as follows. The set up and the procedures of our MD simulations are described in Section 2. The simulation results are given in Section 3. Specifically, a summary of the integrated quantities for reflection and implantation, namely the particle and energy reflection coefficients, and the average range of implantation, are shown in Section 3.1 as a function of substrate temperature, surface type, incidence energy and angle. The range distribution is taken up in Section 3.2. The energy and angular distributions of the reflected He are examined in Sections 3.3 and 3.4, respectively. For comparison, we also perform SRIM calculation in Section 3.5, and MD simulations, using a second EAM potential, in Section 3.6. Our results are contrasted with existing ones in Section 4, before concluding remarks in Section 5.

2. Molecular dynamics simulation procedure

Molecular dynamics is used in our atomistic studies of He reflection and implantation with a tungsten surface. To describe the interatomic interaction between W atoms we used the Ackland–Thetford embedded atom method (EAM) potential for W [15], modified by Juslin and Wirth [16]. To describe the interaction between He and W atoms we used the W–He pairwise potential recently developed by Juslin and Wirth [16]. We considered three bcc W surfaces ((100), (110), (310)), three simulation temperatures (300 K, 1000 K, 1500 K), a range of He deposition energies (0.5–100 eV), and a range of deposition angles with respect to substrate normal (0–75°). For better statistics, we simulated 1000 He impacts for each set of simulation parameters. In those cases where the initial deposition angle with respect to substrate normal was not 0°, the azimuthal angle for each deposition was drawn randomly (ranging from 0° to 360°). This corresponds to a distribution of impacting He ions f_i that is independent of φ_i, *i.e.*, $f_i = f_i(E_i, \theta_i)$.

In the case of a W (100) surface, the size of the simulation system varied from 6750 atoms (~47.5 Å × 47.5 Å × 47.5 Å) to 54,000 atoms (~95 Å × 95 Å × 95 Å), depending on the initial energy of the He ion. In cases where the channeling effect [17] was especially pronounced, we used a simulation system elongated in the z direction (up to ~220 Å). For (110) and (310) surfaces we used similar system sizes. Periodic boundary conditions were applied in the x and y directions. In the z direction there are free-standing top and bottom surfaces. With relatively large system sizes we did not need to use a thermostat for temperature control during the MD simulations of He impact with W surfaces, because