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The role of the adatom diffusion in the tungsten fuzz growth

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Abstract

The model of the tungsten fuzz growth due to adatom diffusion is considered. Adatoms are created by helium ions bombarding the fuzz surface and diffuse along the fiber in both directions (towards the top and bottom). Only if there is an external force making movement towards the top preferential, the fiber can grow. We assume that this force is due to change of the surface binding energy of the adatom while it moves to a fiber top. The molecular dynamics (MD) simulations were performed to determine the surface binding energy dependence on the surface curvature. Adatom flow and a fiber length change were obtained by using this dependence. A square root time dependence of the fiber length was found. Numerical estimates are consistent with the experimental data.

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Keywords: plasma-exposed tungsten; diffusion; surface structure and morphology; molecular dynamics simulations; fuzz.

1. Introduction

Tungsten is considered as a primary candidate material for high heat load plasma-facing components in next generation magnetic fusion devices, in particular ITER. It was experimentally observed that filamentary nano-structures, called fuzz, can grow on tungsten surfaces irradiated with plasma containing helium. A morphologic

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modification of plasma-facing materials due to the fuzz growth can cause their increase in erosion. Therefore, an understanding of the fuzz growth process is of significant practical interest.

The formation of the fuzz was also observed on molybdenum [Kajita et al. (2011)], rhodium, nickel, iron ,and titanium. Thus, it seems that "fuzz" is a generic phenomenon of metal interactions with helium.

Necessary conditions for the formation of tungsten fuzz are the bombardment by He^+ ions with energies above 20–30 eV and the target surface temperature within 1000–2000 K. According to the experimental data of Baldwin and Doerner (2008), the dynamics of the "fuzz" growth is sensitive to the sample temperature, T, and also depends on the flux of helium ions, Γ_{He}. However, for helium flux exceeding ~10^{22} $m^{-2}s^{-1}$ the dependence on Γ_{He} vanishes and the thickness of the "fuzz", L_{fuzz}, scales with plasma irradiation time, t_{irrad}, as $L_{fuzz} \propto t_{irrad}^{1/2}$.

However, the physical mechanism of the "fuzz" growth is not clear. At this moment there are a few various opinions on this point.

A qualitative picture of the ''fuzz'' growth was suggested by Kajita et al. (2011). It is based on the formation of small bubbles the coalescence of which results in bursting blisters and further formation of the bubbles at the bottom of protrusions. However, this model has difficulties explaining how impinging helium can penetrate through thick "fuzzy" layer of tungsten all the way to the bottom of the protrusions. Another model [Krasheninnikov (2011)] is based on the assumption of enhanced plasticity of tungsten with large concentration of entrained helium atoms and clusters, which can play the similar role to that played by lattice defects resulting in the well known irradiation creep. This model explains the appearance of nanosized fibers by their growth due to a viscous flow of tungsten atoms caused by a stress gradient induced by the pressure of helium bubbles occurring inside the finger-like fibers. However, until recently there have not been results directly supporting the enhanced tungsten plasticity in the presence of large amount of helium atoms and clusters in the tungsten lattice. It should be noted that the structure of tungsten fuzz has much in common with the structures of films observed in tokamaks [Martynenko and Nagel' (2011)], which consist predominantly of carbon, sometimes with a significant amount of dissolved hydrogen. These films exhibit a large variety of structures depending on the conditions of formation, mostly on the deposition rate and substrate temperature, which have been explained [Martynenko and Nagel' (2009)] in terms of dendrite growth from individual adsorbed atoms (adatoms). It is believed that the fuzz structure on tungsten is also formed by growth from adatoms, but those appear on the substrate surface as a result of bombardment with He+ ions rather than due to deposition from the gas phase.

In the present work, we assume that the "fuzz" fingers grow due to tungsten adatoms flow. Adatoms are created by helium ions bombarding the fuzz surface and diffuse along the fiber in both directions (towards the top and bottom). Only if there is an external force making movement towards the top preferential, the fiber can grow. We assume that this force is due to change of the surface binding energy of the adatom while it moves to a fiber top. To verify this assumption, a Molecular Dynamics (MD) simulation was performed. The MD simulation results were used for determination of an adatom flow which leads to the fiber growth.

2. MD simulation on a surface binding energy of tungsten adatoms

To determine the surface binding energy of tungsten adatoms, we made use of the LAMMPS molecular dynamics (MD) code [Plimpton (1995)], which allows modeling a wide variety of atomic interactions and arrangements. In the simulations of tungsten atomic systems we used the multi-body Embedded Atom Model Finnis-Sinclair potential produced by Ackland and Mendelev [http://www.ctcms.nist.gov/potentials/W.html].

The tungsten structures simulated in this work were initially constructed as bcc monocrystals with the lattice constant a=0.31652 nm and then relaxed using the system energy and inter-atomic force minimization methods.

The tungsten structure (plane or cone) was first constructed and then an additional atom was added to the system. At the beginning, the distance between the additional atom and the surface is large and their interaction is negligible. The interaction of the additional atom and bulk atoms was determined by the same potential as for other atoms. But forces for the additional atom were switched off. Thus the system energy was monitored at a certain position of the additional atom.

When the atom approaches the surface, the energy of the system changes. Firstly, the energy decreases which means that the atom is in an attractive field. Then the atom achieves a stable position and the energy decrease stops.

Since the force for the additional atom is absent, its movement continues. After passing a stable position, the atom is in a repulsive field and the energy increases. An energy change ΔE at the stable position is of interest.

Simulations were performed for different trajectories of the additional atom. Trajectories of the atom were close to each other. A step of neighbouring trajectories is less than the period of the lattice.The energy change ΔE was obtained for each trajectory.

The energy change for the plane is shown in Fig. 1(a). The plot is periodic due to the lattice periodicity. Since atoms tend to occupy positions of minimal energy, only maximal values should be considered. The largest value obtained for the plane is ΔE=5.2 eV. The energy change for the cone is shown in Fig. 1(b). The highest value ΔE=8.6 eV is achieved at a fiber tip. A red line indicates the largest value for the plane. The energy change decreases to a value for the plane with distance from a cone top.

The change of surface binding energy was associated with a surface curvature ρ (E_0 – energy change for the plane, a and ρ_0 – constants):

$$\Delta E = E_0\left(1+\frac{a}{\rho+\rho_0}\right) \tag{1}$$

The resulting relation between the binding energy and the surface curvature was used to find the adatom flow toward the fiber top.

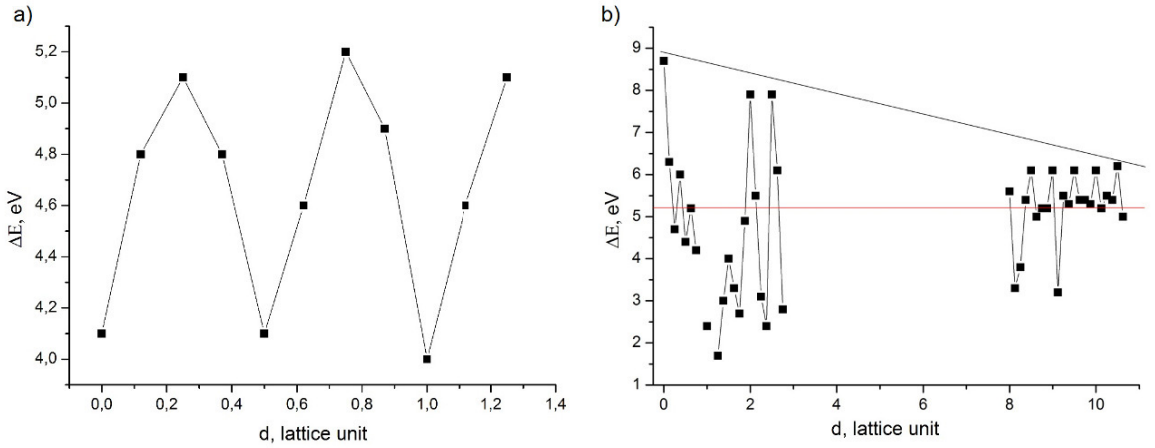

Fig. 1. The energy change for different trajectories of the additional atom (a) for a plane; (b) for a cone. The red line indicates the largest value for the plane.

3. The growth rate of the fiber due to the adatom flow

The gradient of the surface binding energy near the tip of fiber causes adatom flow. The flow can be expressed as:

$$j = -D\frac{\partial C}{\partial x} + C < \vartheta >_F, \tag{2}$$

where D is an adatom diffusion coefficient, C is a surface adatom concentration and $\langle \vartheta \rangle_F$ is average velocity due to an external force. If the concentration C of adatoms on the surface is determined by the rate of their recombination with vacancies, then it can be expressed as

$$C = \left(\frac{q}{D} \right)^{1/2}, \tag{3}$$

where q is the rate of adatom formation under ion bombardment. Assuming that the concentration is uniform we neglect the first term in (2). Average velocity can be expressed through the mobility and the external force. The mobility is given by

$$M = \frac{D}{T} \tag{4}$$

And the external force is

$$F = -\nabla E \tag{5}$$

Then the adatom flow is

$$j = \frac{(qD)^{1/2}}{T}(-\nabla E) \tag{6}$$

The rate of fiber growth due to the flux of adatoms to the fiber tip can be expressed as follows:

$$\frac{dl}{dt} = j \cdot \frac{2\pi R}{\pi R^2 n} \tag{7}$$

where l is the fiber length, R is the fiber radius, and n is the number of atoms per unit volume. Integration of (7) gives:

$$l = \left[\frac{1}{(R+\rho_0)^2} (qD)^{1/2} \frac{4E_0}{T} \frac{at}{n} \right]^{1/2} \tag{8}$$

It should be noted that a square root time dependence of the fiber length was obtained, which agrees with the experimental data. The increase of the fiber length can be expressed through an effective diffusion coefficient:

$$l = \sqrt{2D_{eff} t} \tag{9}$$

The estimates of the D_{eff} were made. They were compared with data of Baldwin and Doerner (2008) (Fig. 2). The fuzz formations were observed at 1120 and 1320 K. The kinetics of the layer growth is found to obey Fick's law characterized by an effective diffusive mechanism (9). Estimates of the D_{eff} are consistent with the experimental data.

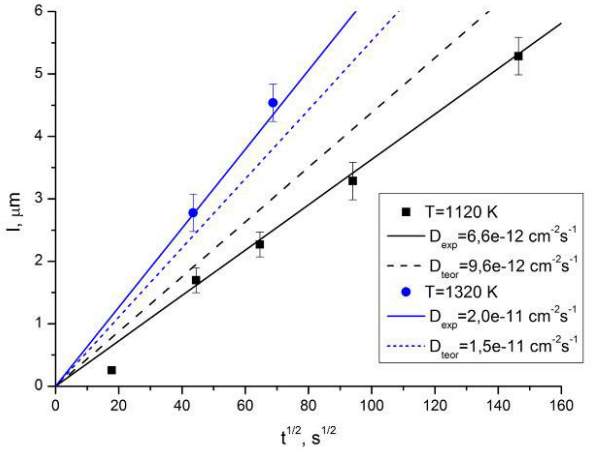

Fig. 2. The fiber length plotted against the square root of time. Data are shown for exposure temperature regimes of 1120 and 1320 K. The points and the straight lines correspond to the experimental data. The dashed lines correspond to theoretical estimates of the effective diffusion coefficient.

4. Conclusions

The model of tungsten fuzz growth due to tungsten adatoms is considered. Adatoms are created by helium ions bombarding the fuzz surface and diffuse along the fiber in both directions (towards the top and bottom). Only if there is an external force making movement towards the top preferential, the fiber can grow. We assume that this force is due to the change of the surface binding energy of the adatom while it moves to a fiber top.

To verify this assumption a Molecular Dynamics (MD) simulation was performed. Surface binding energies of adatoms at different positions were obtained. It was found that the surface binding energy increases towards the tip, which supports our assumption.

The change of surface binding energy was associated with the surface curvature. The resulting relation between the binding energy and the surface curvature was used to find the adatom flow toward the fiber top.

Proceeding from the adatom flow a square root time dependence of the fiber length was obtained. It was compared with experimental data. The estimates of the D_{eff} were made. Estimates are consistent with the experimental data.

Acknowledgements

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