Simulation of hydrogen bubble growth in tungsten by a hybrid model

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ABSTRACT

A two dimensional hybrid code (HIIPC-MC) joining rate-theory and Monte Carlo (MC) methods is developed in this work. We evaluate the cascade-coalescence mechanism contribution to the bubble growth by MC. First, effects of the starting radius and solute deuterium concentration on the bubble growth are studied; then the impacts of the wall temperature and implantation ion flux on the bubble growth are assessed. The simulation indicates that the migration-coalescence of the bubbles and the high pressure inside the bubbles are the main driving forces for the bubble growth, and that neglect of the migration and coalescence would lead to an underestimation of the bubble growth or blistering.

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1. Introduction

The hydrogen isotopes (HI) retention in tungsten (W) is a key issue for future fusion devices. Recent experiments observed the fuel inventory is increased remarkably due to the existence of bubbles and blistering, in which there is a substantial fraction of HI retained as molecules [1]. It is important to take the contribution of HI molecules in bubbles into account to understand the HI retention. However, the growth of bubbles is an important experimental complication that yet prevents a full understanding of HI retention processes.

In our previous work, a rate-theory model was developed to investigate bubble growth in plasma-irradiated W [2], in which the wall temperature, trap site concentration, and incident deuterium (D) flux and fluence dependencies of bubble growth were studied and well explained. However, the model was limited in that the migration and coalescence of the bubbles were not included, which may lead to an underestimation of the bubble growth. To overcome the shortcomings of the previous model, a two dimensional hybrid code (HIIPC-MC) based on rate-theory and Monte Carlo (MC) methods [3] is developed in this work. The cascade-coalescence mechanism contribution to the bubble

growth is evaluated by MC. The solute and trapped HI retention is simulated by the rate theory method using HIIPC2D [4], in which a source term is introduced to include the sink/source generated by HI molecules inside the bubbles. For each bubble, HI molecules are produced through recombination processes on the inner surface of the bubble where the solute HI reactants are supplied by HIIPC2D, and HI molecules can also dissociate themselves into solute atoms due to the very high pressure inside the bubble [5].

With this hybrid code, the HI bubble growth as well as blistering in W can be simulated. The simulation results indicate that the migration-coalescence of the bubbles and the high pressure within are the main mechanisms driving the bubble growth. The high pressure mechanism plays a dominant role when the wall temperature is low and the bubble radius is big; whereas the role of the migration-coalescence mechanism on the bubble growth increases with the wall temperature for very small bubbles. The molecules inventory is increased by the growing bubbles before they burst.

2. Simulation model

HIIPC2D [4] is applied to simulate the solute and trapped D retained in materials. The simulation domain is shown in Fig. 1: D^+ flux is implanted at the plasma-facing surface (PFS), and the material is W with an initial uniform density distribution of very small bubbles produced by vacancy clusters and voids at grain boundaries. After entering the material, D ions are first slowed down to thermalize and neutralize, then the D atoms may be trapped by trap sites, may diffuse back to the surface, or diffuse into bubbles, where they combine into molecules [2]. The following set of reaction–diffusion equations are used:

$$\frac{\partial C_s(x,y,t)}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial C_s(x,y,t)}{\partial x}\right) + \frac{\partial}{\partial y}\left(D\frac{\partial C_s(x,y,t)}{\partial y}\right) + S \qquad (1)$$

$$S = (1 - R_0)\Gamma_0\phi(x,y) - \frac{\partial C_t(x,y,t)}{\partial t} - \sum_i g_i(x,y) \qquad (2)$$

$$\frac{\partial C_t(x,y,t)}{\partial t} = \frac{2Da_0}{3}C_s\left(C_t^0 - C_t\right) - w_0 C_{t,i}\exp\left(-\frac{E_{HdTrap}}{k_b T}\right) \qquad (3)$$

where C_s and C_t are the solute and trapped D concentration, respectively; D is the diffusion coefficient, Γ_0 is the implantation D^+ flux, R_0 is the backscattering coefficient, ϕ is the implantation profile; $g_i(x, y)$ is the source/sink terms associated with molecular D in the ith bubble, a_0 is the lattice constant, C_t^0 is the intrinsic trap site density, w_0 is the bounce frequency of HI in traps [6], E_{HdTrap} is the binding energy of D within a trap and T is the material temperature. The PFS boundary condition assumes recombination of D atoms into D_2 molecules that desorb at the surface [4].

To take the cascade-coalescence process of the bubbles into consideration, a MC method based on Refs. [3,7] is improved upon and applied in this work. An initial population of 10,000 bubbles (changeable) is set up in the material with a uniform distribution as shown in Fig. 1. The bubbles are assumed to be ideally spherical. To add variation, the starting radii are treated to have a Gaussian distribution [3]. The averaged starting radius is set as r_{b0} = 1 nm unless otherwise stated, and the width of the distribution is $2r_{b0}$. The source/sink term $g_i(x, y)$ in Eq. (2) can be expressed as [2]

$$g_i(x,y) = \frac{\partial N_{b,i}}{\partial t} = 2\left(k_r C_s^2(x,y,t) - k_1 f\right)4\pi r_{b,i}^2 \qquad (4)$$

where C_s is obtained by HIIPC2D simulation, $r_{b,i}$ is the radius of the ith bubble, k_r is the recombination rate (unit, $m^4\,s^{-1}$), k_1 is the adsorption rate (unit, $m^{-2}\,s^{-1}\,Pa^{-1}$) and f is the fugacity of the D gas inside the bubble. The molecule content $N_{b,i}$ in the ith bubble can be calculated via Eq. (4). The pressure of a bubble is calculated from its molecule content, bubble radius, and the D_2 equation of state [2]. At very high pressures, fugacity is used instead of pressure, and it is expressed as [8]

$$\ln(f/p) = \int_0^p \left(v(p',T)/RT - 1/p'\right)dp' \qquad (5)$$

where p is the bubble pressure, $v(p, T)$ is the molar volume of the D_2 gas [9], and R = 8.31447 J mol^{-1} K^{-1} is the universal gas constant.

The pressure inside the bubble is assumed to satisfy the Greenwood mechanical equilibrium condition [10]

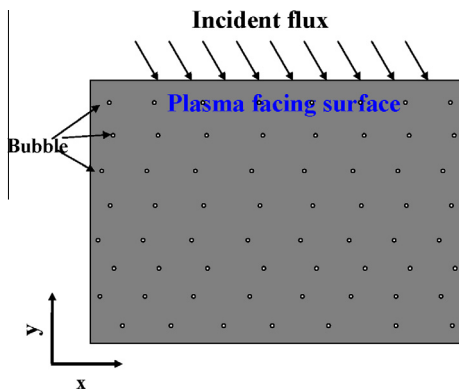$$P_{LP} = \frac{2\gamma}{r_b} + \frac{Gb}{r_b},\ G = G_0\left(1 - \alpha\frac{T}{T_m}\right) \qquad (6)$$

where $b \approx 3 \times 10^{-10}$ m is the dislocation loop Burgers vector, γ = 2.65 N/m is the surface tension of the bubble interface, while G is the shear modulus of W, where G_0 = 163.4 GPa is the shear modulus at zero temperature, T_m = 3700 K is the melting temperature of W, and α = 0.18 is a material constant [11]. When the bubble internal pressure exceeds P_{LP}, the bubble grows so that the Greenwood mechanical equilibrium condition is always satisfied during the growth process.

The random motion of the bubbles can be simulated according to surface diffusion kinetics, using the bubble diffusion relation [12]:

$$D_b = (3\Omega^{4/3})/(2\pi r_b^4)D_s = 0.301D_s\left(\frac{a_0}{r_b}\right)^4 \qquad (7)$$

where $D_s = D_{s0}\exp(-E_s/kT)$ is the surface diffusivity, and its value is taken as D_{s0} = 9.0 × 10^{-10} m^2 s^{-1} for a D bubble in W, E_s = 0.295 eV [13], and a_0 = 316 pm is the lattice constant of W. The bubble motions are then described by standard random-walk theory, in which the jump step for a bubble moving in a time interval Δt follows the Einstein relation [7]: $l = \sqrt{6D_b\Delta t} = \sqrt{1.806\Delta t D_s}a_0^2/r_b^2$. It is easy to obtain that for a bubble with radius r_b the jump step in a given time step (Δt) is proportional to $1/r_b^2$. For each time step, after all the bubbles are moved, then they are tested against their neighbours. When they touch each other, migration occurs, in which the two bubbles are assumed to coalesce instantaneously into a new spherical bubble with radius $r_b = (r_{b1}^3 + r_{b2}^3)^{1/3}$. If the bubbles move out of the material surface, the molecules within are lost and the bubbles are removed from the system. It is worth noting in the present work that the motion of bubbles has been neglected in the third dimension, which may make the description of the motion of the spherical bubble not as precisely as 3D modeling, such as the bubble radii and positions, especially at the beginning period. However, this approximation would not affect the drawn conclusions. During the growth of the bubbles, to make the simulation more realistic, their swelling effect on the surrounding W matrix is included by uniformly increasing the system size at regular intervals by an appropriate amount. At the same time all the bubble positions are changed by keeping their relative positions within the system constant [12]. In this work, the formation of extrinsic traps during swelling is neglected for simplification.

The flow chart of the present HIIPC-MC code is shown in Fig. 2. The MC code is applied to simulate the bubble growth, random-walk, cascade-coalescence and swelling of the system. The molecules inside the bubbles come directly from solute D, which is supplied by the rate-theory based on the HIIPC2D calculation. From this hybrid coupling, the bubble growth, including migration and coalescence, can be simulated during the D^+ flux irradiation.

3. Simulation results

In this work, the simulation domain is 10 μm × 10 μm, representing only the near PFS region.

3.1. Monte Carlo simulation

First, we use the MC module by itself to study the bubble growth to make it much easier to understand the essence of this process. Unless otherwise specified, the solute D concentration C_s is fixed to 10^{24} m^{-3}, wall temperature T = 500 K, starting radius r_{b0} = 1 nm. The bubble radius distribution, in its initial state and 20 s later, and the evolutions of the averaged bubble radius and the number of retained molecules are shown in Fig. 3. It can be seen that the most probable bubble radius grows from 1 nm to about 27.7 nm during this process. Initially, there is a fraction of bubbles with very small radius (<0.5 nm). According to Ref. [2],

Fig. 1. Schematic of the simulation domain: the ion flux is injected at the PFS of W wall, in which small bubbles are distributed uniformly at the beginning.