An EDDY-PIC Simulation of Co-deposition of Hydrogen Isotopes on a Castellated Structure of Plasma Facing Tiles

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To investigate the sputtering and the co-deposition processes on plasma-facing tiles with castellation geometry, a PIC (particle-in-cell) simulation of the sheath layer near the surface was incorporated into a dynamic plasma surface interaction code, EDDY. From the PIC simulation, the gyro-motion of the hydrogen isotope ions was found to be strongly affected the incident angle of their bombardment. The most probable angle in the angular distribution was found to be smaller than the angle of the magnetic field (measured from the surface normal) in fusion devices. Therefore, the sputtering yield, which calculated by using the angle of the magnetic field as an incident one, was overestimated. On the other hand, as the angle of the magnetic field increased, chemically eroded hydrocarbons were redeposited far from the released position after successive dissociation in the plasmas. Moreover, $E \times B$ drift became an important process for the redeposition distribution. The radial electric field E was caused by the gradient of the potential profile in the sheath layer. Realistic plasma profiles of the sheath layer are important for the precise estimation of the co-deposition rates of hydrogen isotopes.

Keywords: hydrocarbon, sputtering, redeposition, Monte Carlo simulation, particle-in-cell simulation

1. Introduction

Castellated armor tiles are anticipated to withstand intense heat fluxes on the first wall and divertor of ITER. However, the introduction of castellated structures presents serious concerns such as the accumulation of impurities and the fuel retention in the gaps between the cells [1]. In a previous paper [2], the castellated structure with the cells tilted against the toroidal direction was studied in order to minimize the redeposition in the gaps. On the tilted surface with the poloidal and the toroidal gaps, the plasma profiles in the vicinity of the surface, i.e. the sheath layer, are affected by the inclination angles of the magnetic field. Detailed discussions are required for understanding the effects of the angle of the magnetic field and the geometry of the tiles in order to control the accumulation of impurities and fuel retention.

In this study, we incorporated a PIC (particle-in-cell) simulation into a dynamic plasma surface interaction code, EDDY [3]. We focused our attention on the sputtering and the co-deposition process of hydrocarbons.

2. Simulation model

2.1 Particle-in-cell simulation code

The plasma in the scrape-off layer is divided into three regions; collisional presheath, magnetic presheath and Debye sheath. In order to simulate the magnetic presheath and Debye sheath regions, we have developed a one dimensional kinetic code with three dimensions in velocity space. Figure 1 shows the coordinate system used in this study. The x axis is taken to be normal to the wall surface and the system length (or the position of the wall) is denoted by L. The plasma profiles, such as density and potential, in the vicinity of the surface are assumed to vary only in the x direction. However, the magnetic field lines are inclined against the surface normal so that the gyro-motion of the ions must be taken into account. The case considered in this paper is the fully ionized magnetized plasma with one species of singly charged ions, which bombard on a perfectly absorbing and electrically floating wall. The electric field at the wall is determined by the charge density on the wall. The code is based on the analysis of the equations of motion and the integration of Poisson's equation to obtain the self-consistent electric field that accelerates the ions. We integrate the equations of motion for both electrons and ions with a leap-frog method. For the ions, we use a shifted Maxwellian with a velocity cut-off only in the direction of the magnetic field that satisfies the generalized Bohm criterion at the electrostatic sheath entrance. The injected electrons are assumed to be Maxwellian. In this study, we use $n_e = 10^{18}\mathrm{m}^{-3}$, $T_i = T_e$, B = 5 T. However, the effective temperature of the ion is varied with the cut-off velocity, $v_{ci} = 0.6 \times \sqrt{T_i / m_i}$, taken from [4].

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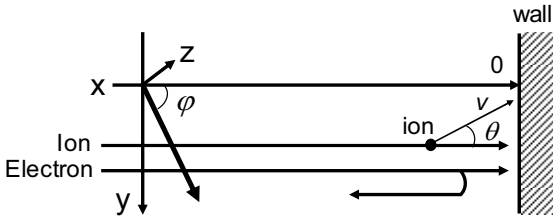

FIG.1 Coordinate system used in the PIC simulation.

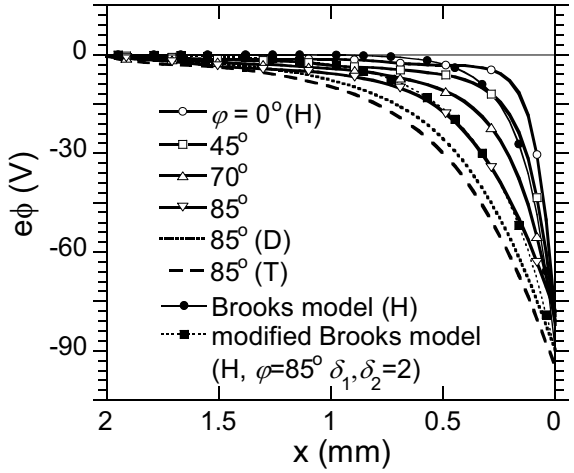

FIG. 2 Potential profile at a plasma temperature of 30 eV for the different angle, φ, of the magnetic field line with respect to the surface normal and for the different sources of plasma used, i.e. proton (H), deuterium (D) and tritium (T).

2.2 EDDY code

The EDDY code simulates the deceleration of the projectile ions in the material and the formation of recoil cascades leading to processes such as ion reflection and physical sputtering [3]. Moreover, EDDY simulates the transport process of chemically eroded hydrocarbons in the plasma [5]. The released hydrocarbon molecules experience complex collisional processes in the plasma. The rate coefficients for electron-impact ionization, dissociation, dissociative recombination, proton-impact ionization and charge exchange processes of CH_4 and the fragments were calculated using fitting formulae taken from Janev and Reiter [6]. If a particle produced by a collision was charged in the plasma, it gyrates and receives various forces, such as friction and thermal gradient forces, cross-field diffusion and sheath acceleration.

Reflection/sticking coefficients at the tile surface were considered by using a classical molecular dynamics (MD) simulation [7]. We used the interaction potential based on the analytic bond-order scheme, which was developed by Juslin et al. [8] for the ternary system W-C-H. In our MD simulation the hydrogenated and amorphized graphite was prepared as a starting surface by bombardment with C and H. Since the direct coupling of the transport/redeposition code with the MD is very time-consuming, a database based on the results of the MD simulation for incident

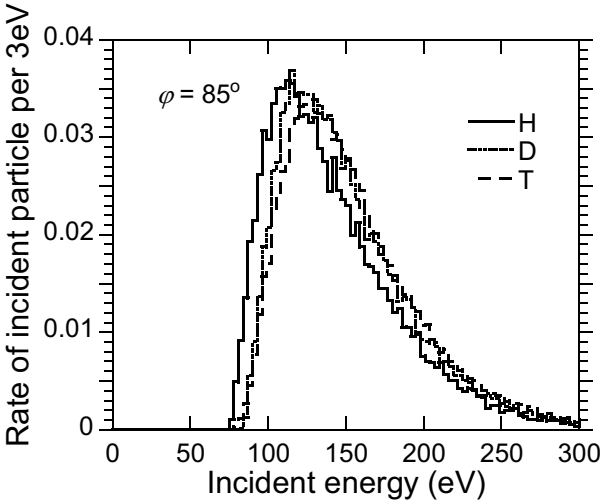

FIG. 3 The energy distributions at the wall for the hydrogen isotopes examined.

angle of 45° against the surface normal were employed in EDDY.

2. Results and Discussion

Figure 2 shows the potential profile in the vicinity of the wall surface at a plasma temperature of 30 eV for different angles, φ, of the magnetic field line with respect to the surface normal, and for the different sources of plasma used. These sources were proton (H), deuterium (D) and tritium (T). The thin solid line corresponds to the profile of the Brooks sheath model [9]. The potential profile of the Brooks model was similar to the present profile at 45°. The boundary between the magnetic presheath and the Debye sheath was not clear, and the width of the Debye sheath was almost independent of the magnetic field strength. The width of the magnetic presheath was roughly proportional to the Larmor radius of the thermal ion as found by Chodura in Ref. [10]. The width of the magnetic presheath increased when the magnetic field was almost parallel to the surface. Moreover, when the source plasma consisted of the heavier hydrogen isotopes, i.e., D and T, which have larger Larmor radii than H, the width of the magnetic sheath increased.

The energy distributions of the hydrogen isotopes bombarding the wall are shown in Fig. 3. Since the potential drop is the same, the energy distributions do not depend on the angle of the magnetic field. Moreover, plasma ions are accelerated by the wall potential, therefore, the minimum bombarding energy is given by the wall potential. The energy distribution was shifted slightly to a higher energy when the source plasma consisted of the heavier hydrogen isotopes (i.e. D and T). This is because the wall potential drops increased for the heavier ions. The angular distributions of the incident H ions on the wall are shown in Fig. 4 for the different angle, φ, of the magnetic field lines. The gyro-motion strongly affects the incident angle of the ions. The most probable angle of the angular

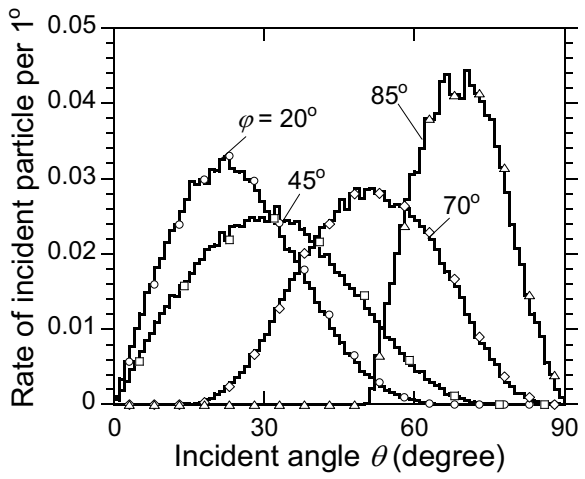

FIG. 4 The angular distributions of incident H ions at the wall for the different angle, φ, of the magnetic field line.

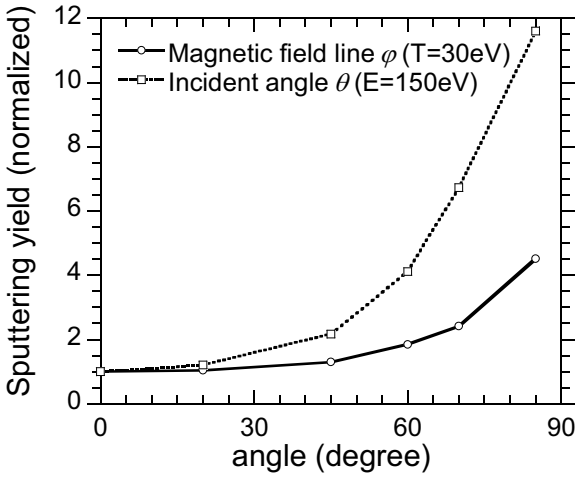

FIG. 5 The dependencies of the sputtering yield of C impacted by H ions on the angle of the magnetic field line and the constant incident angle using the average incident energy. The sputtering yield was normalized at the yield of the angle from the surface normal.

distribution was smaller than the angle of the magnetic field except for the case of the nearly normal magnetic field to the surface. This tendency is found in Ref. [11].

These energy and angular distributions affect the sputtering and the reflection processes from the wall material by the ion impacts. The dependencies of the sputtering yield of C impacted by H ions on the angle of the magnetic field are shown in Fig. 5. The sputtering yield for each energy and angle of the bombarding ions (Figs. 3 and 4) was calculated by the EDDY code. This result was compared with the sputtering yield using the average incident energy (~150 eV, dotted line). The calculated angular dependence (solid line) was substantially weaker than using the average incident energy (dotted line). Also the sputtering yield was less at the angle of more than 20° (data not shown). In addition, the same tendency was obtained for the reflection coefficient of H ions. This indicates that both the sputtering yield and the reflection coefficient in the fusion devices, where the strong magnetic field is applied, were overestimated in previous studies. On the other hand, at small angles of the magnetic field (< 20°), both the sputtering yield and the reflection coefficient were underestimated due to the distribution of the bombarding angle. In general, the sputtering yields of carbon bombarded by hydrogen isotopes have peaks around 70-80 degrees. In this calculation the peak angle of the sputtering yield is near 90 degree although it may be too high.

We performed a simulation of the transport of the chemically eroded hydrocarbons and the redeposition on the tile. In order to study the local redeposition characteristics of the hydrocarbon, the rectangular volume above part of the tile with a surface area of 10×10 cm^2 is simulated where the thickness of the plasma is 10 cm. A neutral methane (CH_4) molecule with a Maxwellian velocity distribution corresponding to a temperature of 0.1 eV was released at the center of the tile surface. For each angle of the magnetic field, 10^5 CH_4 molecules were launched from the tile, and each particle was traced until the particles redeposited on the surface or escaped from the simulation volume. In this simulation, we employed the PIC calculation or the Brooks sheath model. Additionally, in order to introduce the effect of the angle of the magnetic field, we propose the Brooks model with the following modification:

$$\phi(\vec{r}) = \phi_0 \exp[-l(\vec{r}) / \lambda] \qquad (1)$$
$$\lambda = \delta_1 \sin\varphi \lambda_{Li} + \delta_2 (1 - \sin\varphi) \lambda_{De}$$

where $\phi_0 \approx -3kT_e / e$, λ_{Li} is the gyro-radius of the plasma ion, λ_{De} is the Debye length, l is the distance from the surface and δ_1, δ_2 is an arbitrary constant. In Fig. 2, the thin dotted line corresponds to the profile of the modified Brooks sheath model. We obtained the fitting parameters, $\delta_1, \delta_2 = 2$. The potential profile of the modified Brooks model was similar to the profile calculated by the PIC simulation.

Figure 6 shows the spatial distributions of carbons and hydrocarbons redeposited in the (a) toroidal and (b) poloidal direction on the surface at a plasma temperature of 30 eV. The asymmetry between the positive and negative directions was shown in both directions when the magnetic field approached parallel to the surface. Furthermore, the redeposition near the released position decreased and the redeposition pattern broadened. This indicated that the hydrocarbons were transported far from the released position. This is because the ionized hydrocarbons and carbons move along the magnetic field lines, i.e., the toroidal direction. Furthermore, in the poloidal direction, the redeposition distribution of the ionized hydrocarbon in the vicinity of the surface has a peak (~5 mm), because the ionized hydrocarbons moved in the positive direction due to $E \times B$ drift, where the radial electric field E, was caused by the gradient of the potential profile in the sheath

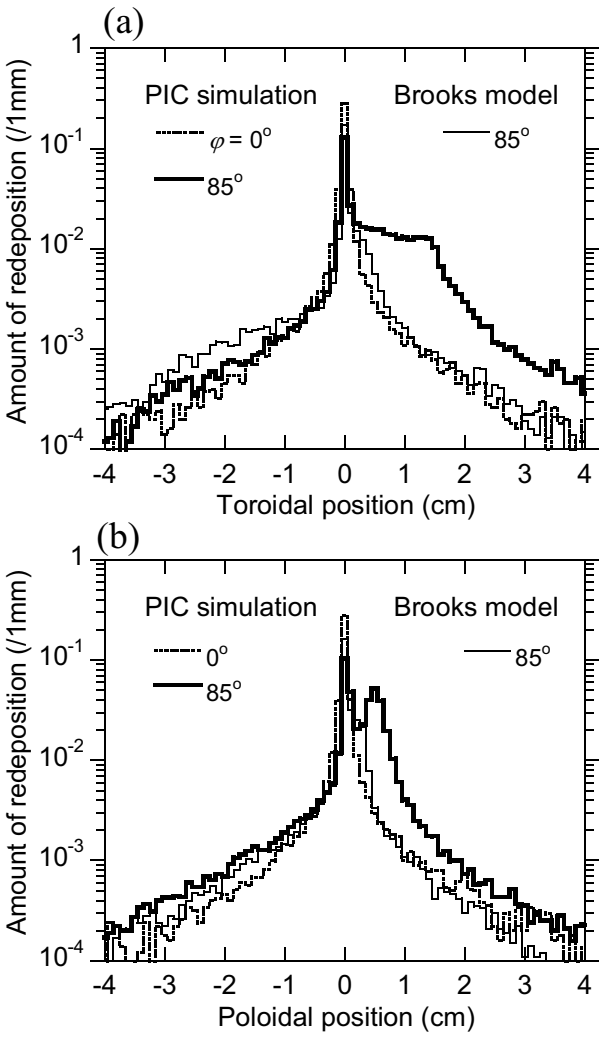

FIG. 6 The spatial distributions of carbons and hydrocarbons redeposited in the (a) toroidal and (b) poloidal direction on the surface at a plasma temperature of 30 eV using the original Brooks model and using the plasma profile calculated by PIC simulation.

layer. However, most of ions were redeposited promptly using original Brooks model since the sheath profile decayed steeply. Using the modified Brooks model, the redeposition profile was similar to the profile using the PIC simulation result (data not shown).

As shown in Fig. 7, the redeposition of the ion species was slightly affected by the magnetic angle, φ (T_e = 10 eV). Due to the lack of acceleration in the sheath, the neutral species are not shown here. As the angle of the magnetic field increased, the redeposition of the small particles such as carbon ions increased as a result of successive dissociations of hydrocarbons in the background plasma. This is because the flight path along the magnetic field line becomes longer for larger angles of the magnetic field. In general, at large magnetic field angles, the prompt redeposition became a dominant process. At high plasma temperatures (>10 eV), the redeposition of CH_4^+ dominates (data not shown). However, according to the MD

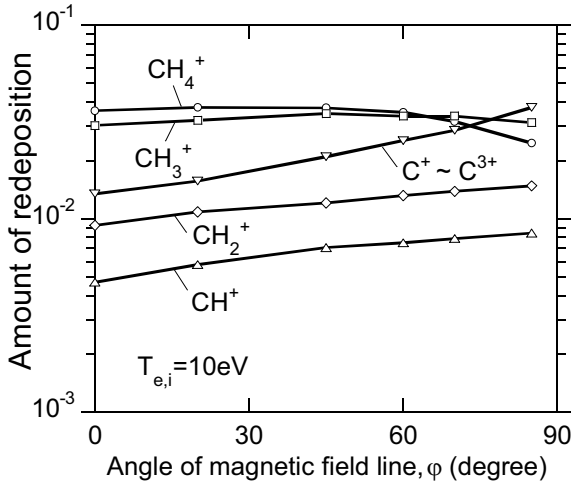

FIG.7 The redeposition amount for the different angle, φ, of the magnetic field line using the plasma profile calculated by PIC simulation.

simulation, the methane family with thermal energy has a rather higher chance of reflection from hydrogenated and amorphized graphite. Furthermore the rate coefficients for electron impact ionization decrease at temperatures of less than 10 eV [5]. Therefore, hydrocarbons were reflected at the surface and the redeposition species was complex and dependent on the bombarding energy.

The redeposition distribution of hydrocarbon is affected by the potential profile in the sheath layer. Realistic plasma profiles are important for precise estimation of co-deposition rates of hydrogen isotopes. Although the reemission from a material, such as the secondary electron, is not taken into account in present PIC simulation, it will be valuable to simulate more realistic conditions. This will be reported at a later date.

3. Conclusions

A PIC (particle-in-cell) simulation was incorporated into a dynamic plasma surface interaction code, EDDY, in order to investigate the sputtering and the co-deposition process. The gyro-motion strongly affects the incident angle of the hydrogen isotope ions bombarding the surface. The most probable angle of the angular distribution of the incident ions is usually lower than the angle of the magnetic field line (φ >20°). Therefore, the change of the sputtering yield due to inclination of the magnetic field was weakened in fusion devices. The usage of the angle of the magnetic field as an incident leads to the overestimation of the sputtering yield.

The hydrocarbons were redeposited far from the released position and dissociated successively when the angle of the magnetic field against the surface normal became large. Moreover, $E \times B$ drift became an important process. As a result, the determination of a

realistic plasma profile of the sheath layer is important for precise estimation of the co-deposition rate of hydrogen isotopes.

Acknowledgement

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References

[1] A. Litnovsky et al., J. Nucl. Mater., in press.
[2] K. Inai, K. Ohya, Y. Tomita, A. Kirschner, A. Litnovsky, T. Tanabe, J. Nucl. Mater., in press.
[3] Y. Hamada S. Ebisu and K. Ohya, Jpn. J. Appl. Phys. **43**, 6385-6391 (2007).
[4] G. Kawamura and A. Fukuyama, Phys. Plasmas **14**, 083502 (2007).
[5] K. Inai and K. Ohya, Jpn. J. Appl. Phys. **46**, 1149 (2007).
[6] R.K. Janev, D. Reiter, Rep. Forschungszentrum Jülich, Jül-3966 (2002).
[7] K. Inai, Y. Kikuhara, K. Ohya, Surf. Coat. Technol., **202** 5374-5378 (2008).
[8] N. Juslin et al., J. Appl. Phys. **98**, 123520 (2005).
[9] J.N. Brooks, Phys. Fluids B **2** 1858 (1990).
[10] R.Chodura, Phys. Fluids **25** 1628 (1982).
[11] G. Kawamura, A. Fukuyama and Y. Tomita, J. Nucl. Mater., in press.