



Simulation of hydrocarbon reflection from carbon and tungsten surfaces and its impact on codeposition patterns on plasma facing components

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ABSTRACT

In order to investigate the redeposition characteristics of hydrocarbons released by chemical sputtering, a Monte Carlo simulation of the transport in edge plasmas is performed, where the reflection and dissociation efficiencies at tungsten (W) and carbon (C) surfaces are calculated using molecular dynamics simulation. The redeposition probability for W and W–C mixed material is strongly suppressed due to strong break-up of hydrocarbons on the surface. Sticking coefficient for ion species increases with increasing plasma temperature, whereas for low plasma temperature (<3 eV) it approaches to the value for neutral species which is independent of the temperature. Our calculations reproduce the redeposition distribution and the difference between C and W roof-like limiters in ¹³CH₄ injection experiments at TEXTOR. The redeposition distribution is more localized for physical sputtering at a W–C mixed layer formed on the W limiter than for chemical sputtering of hydrogenated and amorphized carbon on the C limiter.

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1. Introduction

Computer modeling is widely used to study the performance of plasma facing components. A key issue with carbon based materials for plasma facing walls (PFW) is chemical sputtering. Transport and redeposition of hydrocarbons released by chemical sputtering is an important mechanism for the tritium inventory on the PFW. Simulation of the hydrocarbon redeposition requires (1) chemical sputtering yields of the carbon, (2) exact cross sections for complex reactions of the hydrocarbons in plasmas, and (3) reflection/sticking coefficients of the PFW for the break-up products that result from the plasma reactions. On the terms of (1) and (3), molecular dynamics (MD) of collisions between hydrogen/hydrocarbons and materials is a reliable method. Recently, some MD simulation codes were developed for chemical sputtering and reflection/sticking of hydrocarbons by several groups [1–6]. We have investigated hydrocarbon interactions with fusion-relevant C and W by using a MD simulation, where hydrogenated and amorphized C and W–C mixed surfaces are prepared as a starting surface. Moreover, a Monte Carlo simulation of transport and redeposition of CH₄ is performed in order to investigate the redeposition characteristics. The calculated redeposition patterns are compared with the patterns

observed between C and W limiters in ¹³CH₄ injection experiments in TEXTOR [7–9].

2. Calculation models

2.1. Molecular dynamics simulation of hydrocarbon reflection on different surface conditions

A classical MD simulation scheme is used for the dynamics of a many-particle system composed with H, C and W atoms. We used the interaction potential based on analytic bond-order scheme, which was developed for the ternary system W–C–H by Juslin et al. [10]. Atomistic trajectories in a temperature-controlled simulation cell are followed using a conventional technique [11]. When a W surface is bombarded by C ions with the energies of several tens of eV or more, the surface is eroded but some C ions are implanted in the surface layer of W. In order to prepare a W–C mixed layer, a W crystalline cell comprised 10 × 10 × 20 unit cell was bombarded by 100 eV C ions with the fluence of 5 × 10¹⁶ cm⁻² along [001]. Since the bombardment by low-energy (10 eV) C ions with the fluence of 5 × 10¹⁶ cm⁻² results in the formation of amorphized C layer on W, the hydrogen uptake in the amorphized carbon was followed by simultaneous bombardment with 0.025 eV C and 1 eV H with the total fluence of 2 × 10¹⁶ cm⁻². Fig. 1 shows hydrogen and C depth profiles of

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hydrogenated amorphous carbon and of the W–C mixed layer on W, respectively, which are used for simulation.

Since the impact position and molecule direction of an incident particle clearly influence whether it reflects from or sticks on the surface, 100 particles for each hydrocarbon, CH_x ($x = 0-4$), with random direction are landed at random position of the top surface for the calculation of the reflection coefficient. The incident angle is 45° against the surface normal.

2.2. Monte Carlo simulation of hydrocarbon transport in edge plasmas and its redeposition on surfaces

The rectangular volume above part of the surface with an area of $10 \times 10 \text{ cm}^2$ is the simulation volume, where the thickness of the plasma with constant temperature and density is 10 cm. The angle of magnetic field lines with the toroidal direction is 5° and the lines are inclined by 30° against the poloidal direction; the magnetic field strength is 5 T. 10^5 CH_4 molecules with a thermal velocity distribution are released from a position on the surface and their complex dissociation/ionization reactions are followed using atomic data package from Janev/Reiter [12]. When a particle produced by the reaction is charged, it gyrates in the magnetic field and experiences friction and thermal gradient forces parallel to the magnetic field lines, cross-field diffusion, sheath and presheath accelerations [13]. In our simulation volume, constant plasma temperature is assumed; however, the thermal gradient force is important in that it competes with the friction force. Thus, for simplicity, the temperature gradient per meter was assumed to be equal to the plasma temperature. The particles returning to the surface can either stick (redeposit) or move back (reflect) into the plasma as different types of hydrocarbons, according to the emission probability for each hydrocarbon calculated by using our MD code.

Erosion and redeposition at C and W test limiters with roof-like surfaces in $^{13}\text{CH}_4$ injection experiments [8] are modeled by exposure to the scrape-off layer plasma of TEXTOR. The redeposition rate and its distribution are sensitive to the plasma parameters which also influence the bombarding energy of ionized hydrocarbons on the surface. Therefore, two sets of background plasma parameters (constant density and temperature) in the same simulation volume as mentioned above are assumed to simulate erosion- and deposition-dominant conditions for both C and W: $5 \times 10^{12} \text{ cm}^{-3}$ and 40 eV, and $2 \times 10^{12} \text{ cm}^{-3}$ and 20 eV, respectively [9]. Furthermore, deposition of the background plasma impurities, such as ^{12}C , is not taken into account. The inclination angle of the limiter surface against the toroidal magnetic field lines is 20° and the field strength is 2.25 T.

3. Results and discussion

3.1. Reflection of methane and its break-up on a hydrogenated and amorphized graphite and a tungsten and carbon mixed material

Fig. 2 shows emission probabilities of CH_4 and the break-up products for the incident of CH_4 . With increasing impact energy, due to the break-up of incident molecules, the emission of CH_4 is suppressed due to strong dissociations on the surface. Carbon atoms emitted from a W surface are much larger than for a graphite surface and a small amount of hydrogen is retained in W [14]. Both amorphization of graphite and hydrogen uptake in amorphized graphite reduce the reflection coefficients (or increase sticking probability) and codeposition with hydrogen dominates the process. The mixing of W with C atoms also reduces the reflection coefficients but there emitted much more C atoms (and hydro-

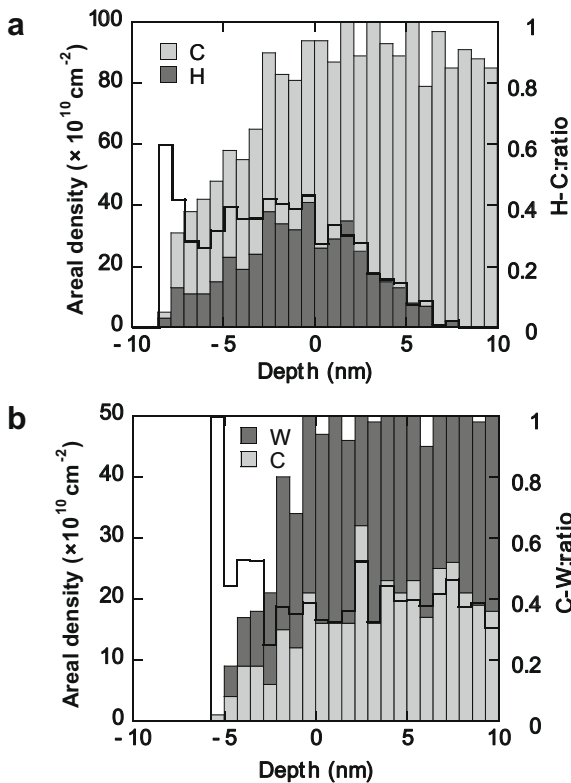


Fig. 1. Depth profiles of (a) hydrogen and (b) C in a hydrogenated/amorphized graphite and a W–C mixed layer on W, respectively, which are prepared as a starting surface for our simulation.

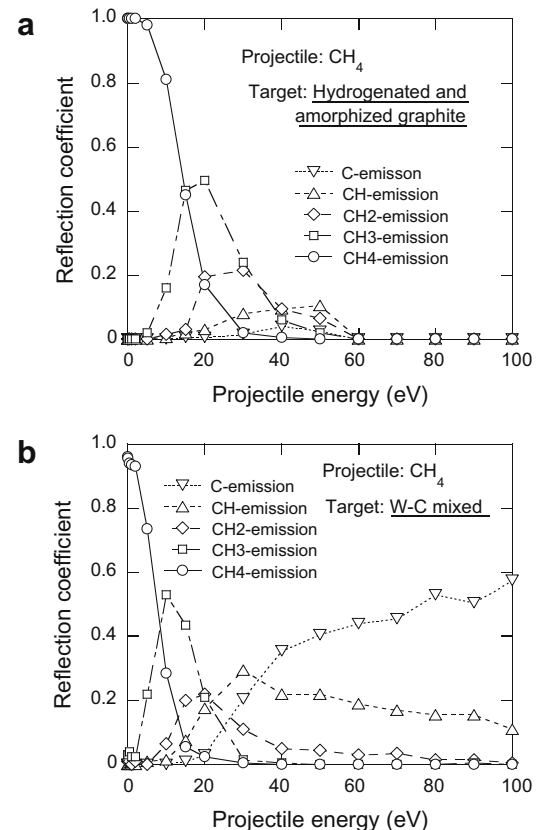


Fig. 2. Reflection probability as each break-up products of incident CH_4 at a hydrogenated/amorphized graphite surface and a W–C mixed surface.

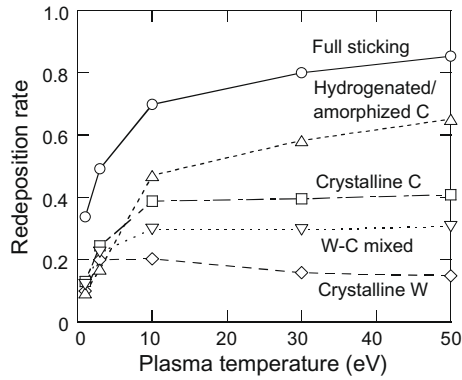


Fig. 3. Redeposition probability for CH_4 and the break-up products at different structures of C and W.

carbons with a few hydrogens, such as CH) than that for all structures of graphite calculated (Fig. 2).

3.2. Redeposition probability and species at different structures of carbon and tungsten surfaces in a constant plasma

After repetitive reflection/dissociation at the W and W–C mixed surface, the resultant small molecules and atoms are easily transported to outside of the simulation volume above the surface. Therefore, as shown in Fig. 3, the redeposition probability is much lower than for hydrogenated/amorphized graphite. At low plasma temperatures (<3 eV), it is dominated by neutral species of C atoms and hydrocarbons whose reflection coefficients are so high that the

redeposition probability is not largely influenced by the surface conditions. The redeposition characteristics for ionized species of C atoms and hydrocarbons are clearly different from those for neutral species. Fig. 4 shows the sticking coefficient of each constituent hydrocarbon and C atom, which is deduced from the present transport/redeposition simulation. According to each reflection probability, for hydrocarbons with less hydrogens (CH_2 and CH) and C atoms, both ion and neutral species are larger than for hydrocarbons with more hydrogens (CH_3 and CH_4). Due to repetitive impact and break-up at the surface, small molecular ions and atomic ions are more energetic than large molecular ions (not shown here). It should be noted that the sticking coefficient for the ion species strongly depends on the plasma temperature due to their sheath acceleration before the bombardment of the surface. Nevertheless, with increasing plasma temperature, the sticking coefficient for ion species on the W–C mixed surface is saturated or decreased due to an increase in multi-charged atomic components with small gyroradii, which are easily transported outside the simulation volume. On the other hand, the sticking probability of neutral species is independent of the plasma temperature.

3.3. Comparison with redeposition patterns on C and W roof-like limiters in $^{13}\text{CH}_4$ injection experiments at TEXTOR

Fig. 5 shows a simulation calculation of redeposition distribution on the roof-like limiters in $^{13}\text{CH}_4$ experiments at TEXTOR [8]. Most of hydrocarbons and the break-up products were redeposited in the vicinity of the position released from the limiter, which is placed in the injection hole with the diameter of 2 mm drilled into the limiter. Since our calculation assumes a zero-sized hole, the redeposition at the positions of -1 mm to $+1$ mm around the injec-

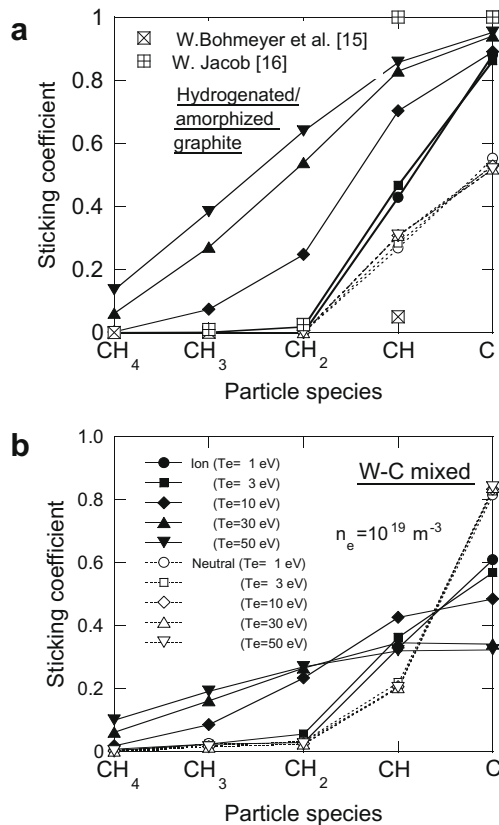


Fig. 4. Sticking probabilities of neutral and ionized methane families and C atoms on a hydrogenated/amorphized graphite surface and a W–C mixed surface. Symbols are deduced from Bohmeyer et al. [15] and Jacob [16].

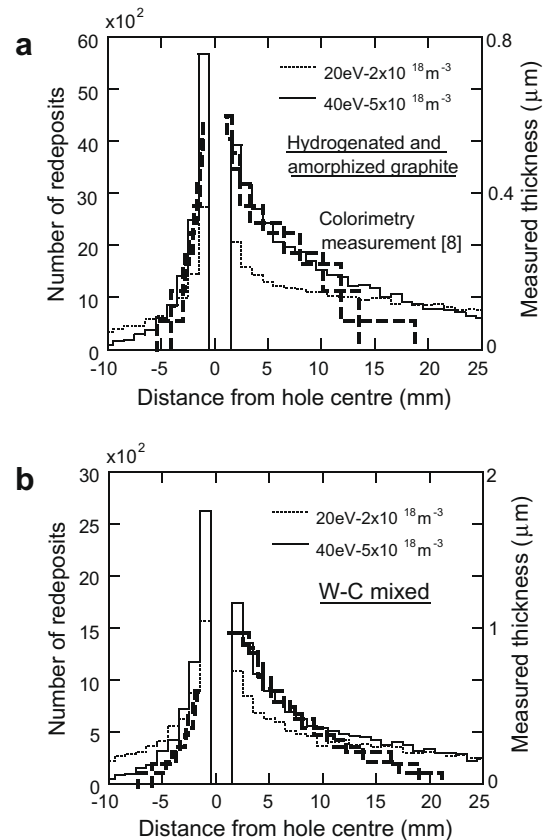


Fig. 5. Redeposition distributions along the C and W roof-like limiter surface in the toroidal direction. The distributions obtained by means of colorimetry measurement [8].

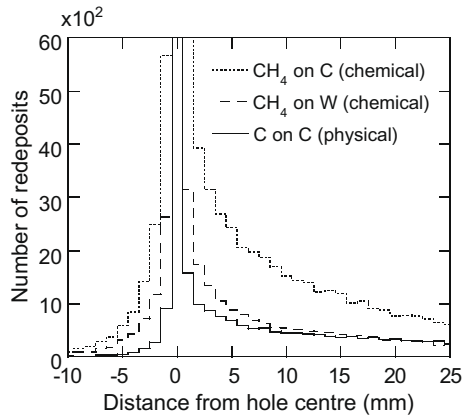


Fig. 6. Redeposition distributions of CH₄ (chemical sputtering) and C atoms (physical sputtering) on hydrogenated/amorphized graphite surface and a W-C mixed surface, respectively.

tion centre are omitted so that the redeposition probability on the limiter is decreased to be half value or less. The probabilities calculated to be 0.52–0.56 for the hydrogenated and amorphized graphite and 0.23–0.24 for the W–C mixed material. The redeposition probability is of two order magnitude higher than the ¹³C deposition efficiency estimated by the experiment; 0.17% and 0.11% on C and W, respectively. This large difference between the calculated and observed results indicates that most of redeposited hydrocarbons and C atoms are re-eroded by subsequent bombardment of plasma ions. Nevertheless, the probability on the hydrogenated and amorphized graphite is approximately twice higher than that on the W–C mixed material, which is similar to the observed difference. Furthermore, the calculated distribution is in fair agreement with the thickness distribution obtained by means of the colorimetry measurement, and it is broader for the case of low density and temperature (20 eV and $2 \times 10^{18} \text{ m}^{-3}$) than for high density and temperature (40 eV, $5 \times 10^{18} \text{ m}^{-3}$). However, for spherical limiters [7,9], there observed a large difference in the efficiency of 0.3% for W and 4% for graphite and a much broader distribution for graphite than for W. The large difference is not clear but one of the possible reasons is proposed to be the different redeposition characteristics between physically sputtered C atoms and chemically sputtered hydrocarbons, which dominates the C release from the W–C mixed layer on W and hydrogenated/amorphized graphite [17], respectively. Since hydrocarbons and the break-up products redeposited on the hydrogenated/amorphized graphite will be re-eroded by chemical sputtering, the redeposition pattern broadens discharge by discharge due to high reflection probability of low-energy hydrocarbons. On the other hand, Due to their small radii and sheath acceleration of ionized or multi-ionized C atoms, the redeposition of physically sputtered C atoms is more localized by prompt redeposition in comparison with hydrocarbons (Fig. 6).

Nevertheless, very recent experiments with polished and unpolished C limiters reveal the influence of surface roughness on the redeposition rate and the distribution [18]. Further simulation calculations modeled the roughness, such as dynamic simulation of surface topography changes [19], are necessary for the detailed discussion.

4. Conclusions

The redeposition probability for W and W–C mixed material is strongly suppressed due to dominant break-up events on the surface, which are easily transported inside the plasma. Sticking coefficients of the surfaces are estimated using the transport/redeposition simulation of injected CH₄ molecules. The sticking coefficient of ion species of hydrocarbons increases with increasing plasma temperature, whereas for low plasma temperature (<3 eV), it approaches to the value for neutral species which is independent of the temperature. Our calculations reproduce the redeposition distribution and the difference between C and W roof-like limiters in ¹³CH₄ injection experiments at TEXTOR. The redeposition distribution is more localized for physical sputtering at a W–C mixed layer formed on the W limiter than for chemical sputtering of hydrogenated amorphous carbon on the C limiter. Nevertheless, the calculated redeposition probability is much higher than the values observed by the experiments where the redeposited particles are repeatedly re-eroded by chemical and physical sputtering.

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