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Molecular dynamics and dynamic Monte Carlo studies of mixed materials and their impact on plasma wall interactions

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ABSTRACT

A molecular dynamics technique was used to study the sputtering characteristics of co-deposited carbon (C) and to investigate subsequent effects of introducing beryllium (Be) impurities. Amorphous C layers containing hydrogen (H) with atomic ratios of H/(C + H) < 0.3 together with a small amount of Be with ratios of Be/(C + H + Be) < 0.06 are produced on top of a tungsten (W). Noncumulative bombardment of the amorphous C layer without H (*i.e.*, H/(C + H) = 0) by H atoms, produces no atomic C sputtering at energies less than the threshold energy for physical sputtering, as calculated by a dynamic Monte Carlo code, EDDY. By examining the H uptake in the layer, it was observed that hydrocarbon sputtering occurs when the dominant emitted species are small radicals *e.g.* CH and at low H/(C + H) ratios (<0.1). When the ratio was increased, larger radicals (CH_2 and CH_3) were emitted. In the eV energy range, the larger molecules were the dominant emitted species, whilst C atoms were emitted even at very low energies. A small percentage of Be was implanted in the C layer, and was found to reduce sputtering of the large molecules, whereas the emission of the small molecules and the C atoms was slightly reduced or remained unchanged.

1. Introduction

Material mixing has attracted great interest since the International Thermonuclear Experimental Reactor (ITER) uses beryllium (Be), carbon (C) and tungsten (W) as its plasma facing components. It drastically changes the plasma surface interactions of the underlying substrate material. In previous work, we have extensively studied W–C mixed layers formed on a W/C twin test limiter which was exposed to TEXTOR edge plasmas. This used a dynamic Monte Carlo code, EDDY, based on a binary collision approximation (BCA) [1]. It was observed that the W–C mixed layers, on W, suppressed physical sputtering of the W, whereas the same layers placed on C strongly suppressed the chemical sputtering of C. However, the BCA breaks down in the low-energy regime (tens of eV or less) of bombarding particles, when many-body effects become important. This indicates that the BCA codes may not be applicable to low plasma temperatures (below about 10 eV) which is an important range in the detached plasma conditions in the ITER divertor. Furthermore, characterization of the erosion and deposition of the mixed layers requires more dedicated studies based on physical and chemical properties of the materials. Therefore, we have recently developed a molecular dynamics (MD) code for the collisions of hydrogen isotopes and eroded impurities with fusion related materials including hydrogenated amorphous C and W–C mixed layers [2].

Beryllium is used for most of the sections of the first wall of the reactor and is subjected to strong physical sputtering due to its low surface binding energy (3.32 eV) when compared with C (7.37 eV) and W (8.90 eV). This results in threshold energies of 15.4 eV (Be), 38.5 eV (C) and 416 eV (W) due to the impact of hydrogen (H) [3]. Since some of the eroded Be atoms migrate towards the divertor region, a more pronounced Be deposition and in addition the formation of Be–C and Be–W mixed layers will appear on the C and W divertor components, respectively. A critical issue with C divertor targets is the chemical sputtering due to the bombardment with high-flux hydrogen isotopes. The Be coverage effect of the plasma impurities on the C has recently been demonstrated in experiments at the plasma divertor simulator PISCES-B [4,5]. The method of seeding Be onto a plasma, in contact with a C target, was shown to decrease the chemical sputtering yield of carbon to negligible levels, even at Be concentrations ≈0.1% in the plasma. Dedicated studies are continuing to understand the interplay between erosion, deposition and material mixing and this includes an analysis of the transport of the eroded impurities in the plasma [6]. The present work has primarily focused on the Be–C mixed materials, although relevant work using hydrogenated amorphous C (a-C:H) layers has also been performed. This paper is devoted to studying the mixing effect of hydrocarbons and carbon sputtering, in the energy range ≤tens of eV (which approximates the threshold energy of physical

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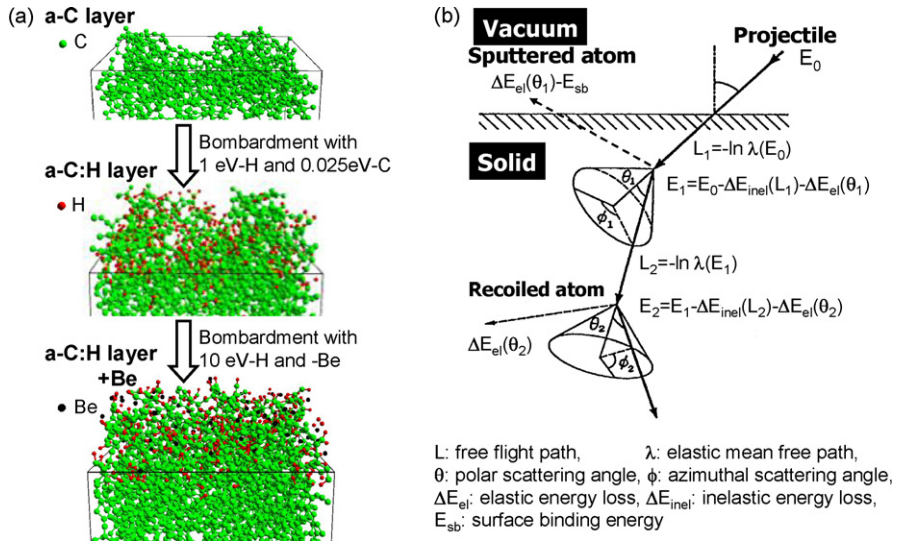

Fig. 1. (a) Mixed materials prepared by means of MD technique: amorphous carbon (a-C) layer, hydrogenated amorphous carbon (a-C:H) layer with the H atomic ratio, H/(C + H)~0.3, and beryllium-implanted a-C:H layer with the Be atomic ratio, Be/(C + H + Be)~0.06. (b) Schematic drawing for simulation models of EDDY for physical sputtering based on the binary collision approximation.

sputtering of C) together with a comparison between the MD and EDDY calculations.

2. Simulation method

2.1. Preparation of a-C:H and Be–C mixed materials

In a classical MD scheme, atoms in a system are traced by Newtonian mechanics where the force on each atom is calculated from the analytical derivative of the interaction potential. The atomic trajectories in a temperature-controlled simulation cell are followed using a variable-time-step Verlet algorithm. The temperature control of the cell uses a Langevin thermostat with a time constant of 0.1 ps at a temperature of 300 K, dissipating the excess heat between impacts. The atoms at the bottom surface of a computational cell are held fixed, which prevents the entire cell from moving downward when bombarded by energetic atoms. The top surface is free, and the sides of the cell have periodic boundary conditions.

At first, an a-C:H material, which represents a C deposition layer formed on the plasma facing walls, is prepared using the following technique. A crystal W (0 1 1) cell with dimensions of 3.17 nm × 3.17 nm × 6.33 nm, consisting of 4000 atoms in 10 × 10 × 20 conventional bcc unit cells is used as the initial computational cell. We use the interaction potential based on the analytic bond-order scheme, which was developed by Juslin et al. [7] for the ternary system W–C–H. The potential combines Brenner's hydrocarbon potential (C–C, C–H and H–H) [8] with the parameter sets of W–W, W–C and W–H interactions. The bombardment by low-energy (10 eV) C atoms with fluence of 5×10^{16} cm^{-2} results in the formation of an amorphized C layer with a thickness of more than 2 nm on the W, as shown in Fig. 1(a). The hydrogen uptake in the amorphous C layer was followed by simultaneous bombardment with 0.025 eV C and 1–30 eV H with a total fluence of 2×10^{16} cm^{-2}. Fig. 2(a) shows the H depth profile of the a-C:H layer with a thickness of ≈1 nm. The atomic ratio of H to (C + H) is approximately 0.30 on average over a −0.43 to 0.14 nm depth for the bombardment of 1 eV H. Here, the negative (positive) depth corresponds to the net deposition (erosion). The H depth profile can be controlled by changing the H impact energy, so that the H/(C + H) ratio is varied from 0.30 to 0.06 at impact energies from 1 to 30 eV.

As shown in Fig. 1(a), small amounts of Be atoms were implanted into the a-C:H layer by simultaneous bombardment with 1 eV H and

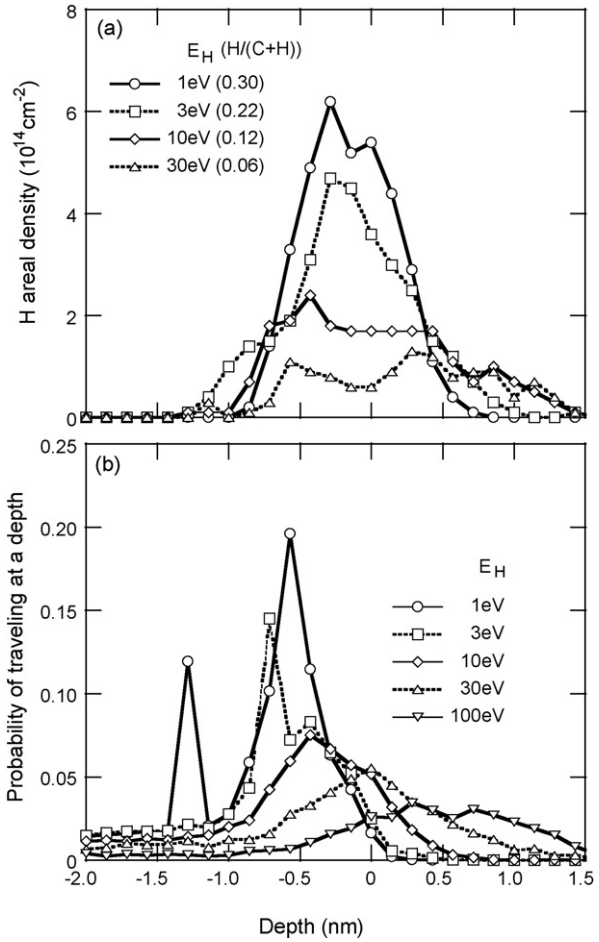

Fig. 2. (a) Depth profile of H in an amorphous C layer as a function of the impact energy, along with the H/(C + H) ratio averaged between −0.43 and 0.14 nm in depth. (b) Probability distribution that a projectile (H) travels at a depth of a hydrogenated amorphous C layer with the averaged H/(C + H) ratio of 0.3, as a function of the impact energy.