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H, He, Ne, Ar-bombardment of amorphous hydrocarbon structures

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Abstract

Amorphous hydrogenated carbon films have found various applications due to the unique combination of properties of this material. In tokamak-like fusion reactors, this material is subject to bombardment primarily by H, but also to smaller amounts of noble gas ions. The effect of these low energy noble gas ions on the erosion of carbon is however not known. In this work, both cumulative and non-cumulative bombardment simulations were performed of hydrogen, helium, neon, and argon ions impinging onto a-C:H surfaces at energies ranging from 2 to 10 eV, employing a reactive hydrocarbon potential model. At noble gas/hydrogen ratios of 1/10 we saw no significant difference between the sputtering yields obtained from the bombardment simulations of different noble gas ions. A marked difference in the surface morphology was, however, observed between the final simulation cells from the 5 eV and the 10 eV ion bombardment simulations.

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1. Introduction

The interest in amorphous hydrogenated carbon (a-C:H) layers has been continuously increasing during the last decades. One of the most technically and scientifically challenging applications of these materials is the use of carbon-based coatings as a protective surface for the first wall structures in tokamak fusion devices. Due to the excellent plasma facing properties, carbon-based materials are promising candidates for coating the divertor plates, and hydrogenated carbon-based materials will most probably be produced at the surface in ITER through interaction with the boundary plasma [1]. The main drawback of using carbon as a first wall material has, however, proven to be the co-deposition of tritium and the chemical erosion caused by the impacts of low-energy (1–100 eV) hydrogen ions and neutrals escaping from the core plasma. This is an important application of energetic particle-surface interaction theory in the prediction of the erosion of tokamak fusion reactor walls.

The erosion mechanisms of carbon at low plasma temperatures, that is, low ion impact energies, can principally be classified as chemical sputtering. This denotes the ejection of molecular species from the

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surface as a result of formation and breaking of chemical bonds. Carbon based plasma facing components are also very efficiently eroded by oxygen with the formation of carbon oxides. With a selection of good gettering materials in the first wall, the effect of oxygen can, however, be suppressed, in contrast to the intense flux of low-energy hydrogen which always is present.

Another major issue to be dealt with in the design of plasma facing components is the erosion of carbon surfaces by impurity ions, i.e., ions which are not the main plasma constituents, hydrogen, deuterium or tritium. These ions, the most important ones being argon, neon and helium, will not only erode the carbon surface but also penetrate it. Mixed layers which are formed with different carbon/ion ratios could be re-eroded by incoming hydrogen ions. Therefore, the erosion behavior of these layers should be studied during the deposition of hydrogen.

The aim of the current work is to obtain an understanding of whether and how the noble gas ions affect the buildup of hydrogen and carbon erosion from a-C:H plasma facing materials.

In our previous works of hydrogen bombardment onto a-C:H surfaces [2–5], we have shown that carbon molecules can erode from a-C:H by the swift chemical sputtering mechanism, where low-energy ($\geqslant 2$ eV) hydrogen ions penetrate between two carbon atoms, which can cause chemical bonds to break and thus lead to erosion of hydrocarbon molecules. In simulations of prolonged H bombardment, the predominant hydrogen erosion mechanism for low H fluences was ion reflection from the surface [4,5]. When the dose increased, the ion reflection decreased and the sputtering of hydrogen molecules became more and more frequent. The number of hydrogen atoms in the a-C:H cell increased rapidly during the first 500–1000 impact events, and eventually reached a steady-state. Due to replacement collisions, driving surface hydrogen deeper into the cell, small increments occurred after ~2000 impact events. Since the H/C ratios in the simulation cells were clearly higher than the bulk saturation value of ~0.4, the concentration due to the high-flux bombardment was designated the term *supersaturated*. The high hydrogen content lead to the shielding of carbon atoms from new incoming hydrogen ions, and thus a decrease of roughly an order of magnitude in the carbon erosion yield.

Reduced carbon erosion yields at extremely high flux densities ($\sim 10^{22}$–10^{23} m^{-2} s^{-1}) have been reported both in tokamaks [6–9] and in plasma simulators [10]. The data for the flux dependence were recently reviewed by Roth et al. [11]. The assumption that the carbon erosion yield Y_C is dependent on the ion flux density Γ as $Y_C = \Gamma^{-\alpha}$, has given α values of ~0.4–1.25. Since the ion fluxes onto the divertor plates in ITER are estimated to be as high as 10^{24} m^{-2} s^{-1} this effect could be favorable to the use of carbon in these plates. The supersaturated hydrogen concentration at the surface is a reasonable explanation for this flux dependence of the C erosion yield in tokamak and plasma simulator experiments.

2. Simulation method

The bombardment of hydrogen and noble gas ions onto a-C:H surfaces was performed by means of MD simulations. We employed the reactive bond-order potential energy function due to Brenner–Beardmore in its second parameterization [12] in order to model the hydrogen and carbon interactions in our simulations. This potential provides a reasonable description of the bulk phases of carbon and the changes in atomic hybridization due to chemical reactions. Many studies involving interactions of hydrocarbons with carbon surfaces have therefore been carried out using this potential [13–17]. Moreover, a large advantage in using an empirical force model such as this one is that it is computationally much more efficient than quantum mechanical force models. This enables us to deal with system sizes and time scales relevant in the present study. Although this model is not as accurate as quantum-mechanical methods, it retains the essential characteristics of the chemical bond. In our simulations the equations of motion were solved using a fifth-order predictor–corrector Gear algorithm, and the scaling methods of Berendsen et al. [18] were used for the temperature and pressure control.

The creation of a-C:H cells to be used in our bombardment simulations consisted basically of four different phases: construction of random cells, annealing of the cells in order to find stable structures, attaining desired carbon coordination fractions, and creation of surfaces. A total of 4 simulation cell samples with slightly different compositions were created in order to improve the statistical significance of our results.

In the initial sample manufacturing phase 1000 atoms were randomly distributed in a box with the