MOLECULAR DYNAMICS SIMULATION STUDY ON SPUTTERING OF GRAPHITE OR AMORPHOUS CARBON BY LOW-ENERGY HYDROGEN OR ITS ISOTOPE ION BEAMS*

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Low energy ion impact (with injection energy less than 50 eV or so) on the carbon-based plasma facing wall materials such as graphite of a magnetic confinement fusion device can generate a significant number of sputtered species that may enter the fusion plasma as impurities. In this work sputtering properties of graphite and amorphous carbon substrates due to hydrogen (H), deuterium (D), and tritium (T) ion bombardment at low incident energies have been studied with the use of classical molecular dynamics (MD) simulations. [1,2] The classical interatomic potentials that we have used in this work are Brenner-type multi-body potential functions[3] with weak Van der Waals interactions.

In the earlier study,[4] we have shown that a high level of H/D/T dose accumulation on the top surface is prerequisite for the formation of relatively large-sized sputtered hydrocarbon species and also there is significant isotopic dependence of sputtering yields. The latter observation is qualitatively consistent with experimental yield data given in Ref. 5.

In the present study, we have extended simulation periods for beam surface interactions in an attempt to obtain more accurate yield data for the sputtering processed discussed above. In addition, we have obtained distributions of sputtered products and their kinetic energies in these processes. Details of newly obtained data will be discussed in the presentation.

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