Temperature dependence of chemical erosion of graphene by hydrogen atom bombardment

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Divertor plates bombarded with hydrogen plasma in a nuclear fusion device are shielded by plasma facing materials (PFM) composed of carbon, beryllium and tungsten. Carbon PFM, which is low-Z material, contributed to achieve high temperature of core plasma. Since carbon interacts chemically with a hydrogen (isotope) atom and ion, the problems which are tritium retention, hydrocarbon generation by chemical erosion and its re-deposition, are caused. Especially, microscopic mechanism of chemical erosion of carbon PFM by hydrogen ion and atom are less well understood. A recent trend in a divertor research is to shift PFM from carbon into tungsten with an expectation of reduction of the tritium retention. However, it is also expected that the carbon PFM will be used in the next generation device ITER under capably controls based on a lot of researches of plasma-wall interaction (PWI). Our purpose is to understand the microscopic mechanism of chemical erosion on a graphite surface. Using molecular dynamics (MD) simulation, we clarified that adsorption, reflection and penetration rates of hydrogen atom on a graphene sheet, which is an elemental molecule of graphite, depends on incident energy sensitively [1] and that different structures of graphite surfaces, which have flat (0 0 0 1), armchair (1 1 $\bar{2}$ 0) and zigzag (1 0 $\bar{1}$ 0) surfaces typically, cause different processes of chemical erosion [2].

A hard problem of MD in PWI is to research temperature dependence. The MD which treats nano-meter and pico-seconds scale has no other option to set the incident flux of hydrogen atom to 10^{28}-10^{30} atom/m^{2}s, which is extremely higher than experimental values. Little is known about the optimal control method of material temperature against strong influx of heat due to the high incident flux of hydrogen atom. In the present paper, the famous temperature control methods, which are Langevin, Nosé-Hoover and Berendsen thermostats, are compared in the chemical erosion processes of a graphite (0 0 0 1) surface. Although all of them are established by setting temperature and thermal relaxation time theoretically, their different equations of motions lead to different erosion processes. Under the Langevin thermostat, the chemical erosion process depended on the thermal relaxation time strongly than the setting temperature. We found that CH_4 is created from CH_3 radical mainly and temperature dependence of CH_4 yield agreed with experimental results.

[1] A. Ito, H. Nakamura and A. Takayama, J. Phys. Soc. Jpn., **77**, (2008) 114602.
[2] A. Ito, Y. Wang, S. Irle, K. Morokuma and H. Nakamura, proceedings The 22nd IAEA Fusion Energy Conference, Geneva, Switzerland, 2008, TH/7-1.