Incident angle dependence of reactions between graphene and hydrogen atom by molecular dynamics simulation

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The divertor plate of nuclear fusion reactor, which consists of graphite tiles or carbon fiber composites, is bombarded with hydrogen plasma. The hydrogen plasma erodes the divertor plate, yielding H_2 and other hydrocarbon molecules such as CH_x and C_2H_x, which are undesirable impurities in plasma confinement experiments. To understand the nature of chemical and physical interactions between hydrogen plasma and the divertor plate, it is important to clarify the elementary processes of the reactions. Molecular dynamics (MD) simulation which solves the equation of motion of the atoms numerically is a powerful tool to research the elementary processes. In the previous research, we showed that the reaction strongly depends on incident energy of hydrogen atom. We also clarified its physical mechanism in the case of perpendicular injection against a graphene sheet by MD simulation[1].

The surface of the divertor plate is not flat in the nanoscale level any longer. For example, carbon fiber composite (CFC) has such a structure that several thousand carbon fibers are twisted. In this case, oblique incidence as well as vertical incidence should be taken into account. The present research investigates the incident angle dependence of the reactions between a hydrogen atom and a graphene sheet by MD simulation.

As shown in Fig.1, we inject a hydrogen atom one by one to a graphene sheet which consists of 160 carbons with periodic boundary condition, and calculate adsorption, penetration and reflection rates. Figure 2 (a) shows the penetration rate decreases as the inclination angle θ becomes larger, because the perpendicular component of incident energy decreases. The adsorption rate has more complicated θ dependence as shown in Fig.2 (b). When incident energy is 0.5eV, the adsorption rate has the maximum value at $\theta = 20$ deg. We found that there is a dome-shaped small potential barrier the height of which is 0.3-0.5eV in front of adsorption sites. Adsorbed hydrogen atoms must have larger perpendicular component of kinetic energy than the potential barrier. Incident angle dependence is never negligible to understand the physics on the divertor plate.

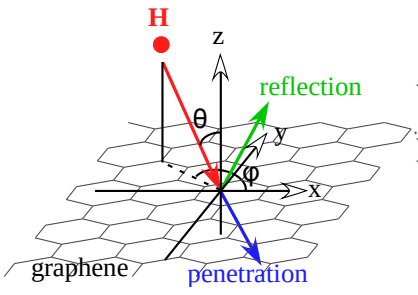

Figure 1. Experimental setup.

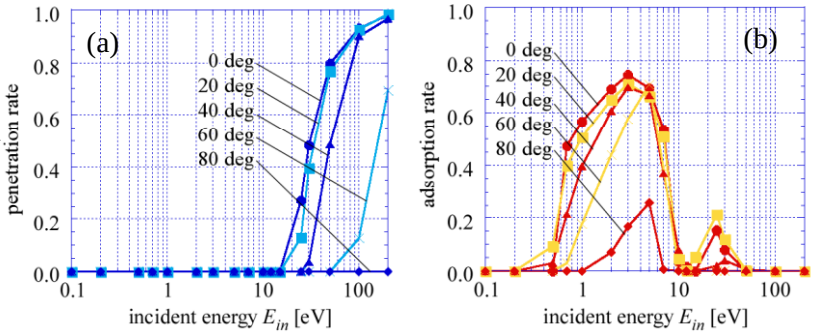

Figure 2. Graph of incident energy dependence of the (a) penetration and (b) adsorption rates with different incident

[1] A. Ito, H. Nakamura and A. Takayama, J. Phys. Soc. Jpn. **77** (2008) 114602.