§25. Graphene – Hydrogen Interaction in the Case of Oblique Injection

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In molecular dynamics (MD) simulations, the equations of motion of the atoms are solved numerically, and so it is a powerful tool to investigate these elementary processes.[1] We showed previously [2,3] that the reaction depends strongly on the incident energy of the hydrogen atom.

At the nanoscale level, the surface of the divertor plate is not flat. CFCs [4] have a structure whereby several thousand carbon fibers are twisted. The fibers have a polycrystalline structure, with clusters measuring approximately 1nm to 1μm, and the crystal axes of the clusters are not aligned. Moreover, single crystalline graphite has a structure in which many graphene sheets are layered. In this case, oblique incidence as well as vertical incidence should be taken into account to understand the reaction at the surface of the divertor plate. Here, we investigate both the energy dependence and incident angle dependence of the reactions between a hydrogen atom and a graphene sheet by using MD simulations.

The simulation model is set as described below. A single hydrogen atom is allowed to impinge on the graphene sheet. The graphene sheet consists of 160 carbon atoms, and periodic boundary conditions are used in the x and y directions. The initial temperature of the graphene sheet is set to zero Kelvin. The hydrogen atoms are injected onto the graphene sheet from a distance z_0 = 3Å. The x and y coordinates of the starting position of the hydrogen are set randomly. 2500 simulations for the same initial state, except that the x and y coordinates of the injection position has been performed to obtain statistics for three reaction types; reflection, adsorption, and penetration. The set of 2500 simulations is performed for each parameter set (E_{in}, θ, ϕ), where E_{in}, θ and ϕ are the incident energy, polar and azimuthal angle of injection.

Figure 1(a) shows the incident energy dependence of the reflection rate at different values of θ, and with ϕ = 0. The reflections are caused by the small potential barrier, and we observe that the reflection rate increases with increasing θ. In the case of θ = 80 degree, all atoms are reflected. Figure 1(b1) shows the penetration rate as a function of energy at different values of θ. As θ increases, larger incident energies are required for penetration to occur. This shift is because the vertical component of the incident energy decreases with $\cos^2\theta$. As shown in Fig. 1(b2), the penetration rates are described as a function of $E_{\mathrm{in}}\cos^2\theta$. The adsorption rates are shown in Fig. 1(c) as a function of incident energy for various values of θ. The adsorption rate cannot be written as a function of $E_{\mathrm{in}}\cos^2\theta$.

The dependence of the reaction rates on the azimuthal angle ϕ is also investigated. The adsorption rates do not depend on ϕ. This is because the graphene sheet has six-fold rotational symmetry in ϕ and the small potential barrier is almost completely symmetrical under rotations in ϕ. In the higher-incident-energy case, penetration is the dominant process, and the small potential barrier that was important for lower incident energies can be regarded as negligible. In the case of θ = 60 degree, the penetration rate is found to be dependent on ϕ. This results from the fact that the projection of the core electrons on to the plane of the graphene sheet is different at different azimuthal angles.

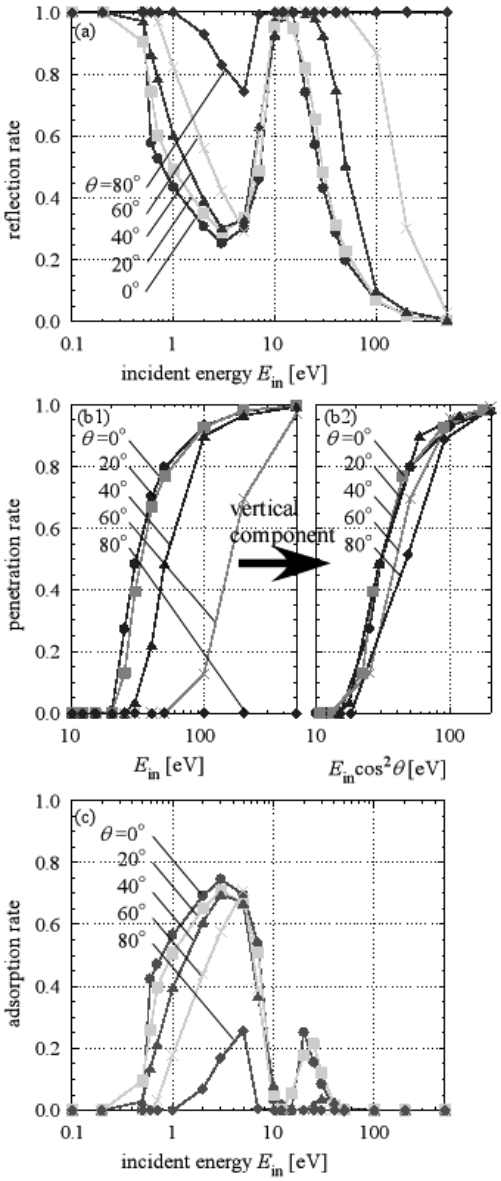

Fig. 1. Incident energy dependence of (a) reflection, (b1) penetration, and (c) adsorption rates with different values of θ. The graph (b2) shows the penetration rate against the vertical component of incident energy, i.e., $E_{\mathrm{in}}\cos^2\theta$.

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