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Comparison of hydrogen atom and hydrogen ion injection onto a tungsten surface using time-dependent density functional theory

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In atomic-scale simulations of plasma–wall interactions, simulation methods such as the binary collision approximation, molecular dynamics, and density functional theory were traditionally employed. However, these methods made it difficult to treat incident particles from plasma as ions, and instead, neutral atoms were used as substitutes. In reality, however, the particles incident from the plasma were ions, and the validity of substituting them with neutral atoms remained unclear. To address this issue, we performed simulations in which the incident particles from plasma were treated either as ions or as neutral atoms, and then the difference between these two cases was explained.

When dealing with ion incidence, it is necessary to consider the neutralization process of the ions where the ions are neutralized by capturing electrons during interaction with the surface of a wall. To implement ion incidence simulations that incorporate this neutralization process, we employed the Ehrenfest molecular dynamics (Ehrenfest MD) method. In this method, the motion of electrons is described quantum mechanically by the time-dependent Kohn–Sham equation based on time-dependent density functional theory[1], while the motion of nuclei is described classically by Newtonian equations of motion.

In this study, we performed Ehrenfest-MD simulations in which a hydrogen ion or hydrogen atom was vertically incident onto the {110} surface of a tungsten thin film composed of 48 atoms. The simulation box size was $17.9 \times 16.9 \times 50.7$ Bohr³, with a grid of $60 \times 60 \times 176$. This grid corresponds to cutoff energies of 110.7, 124.5, and 119.1 Ry along the x-, y-, and z-directions, respectively, in terms of plane-wave representation. The k-point sampling was $1 \times 1 \times 1$. ONCV[2] pseudopotentials were used in the calculations. All simulations were performed using the QUMASUN[3] code.

The simulation result of the Ehrenfest MD is obtained as a superposition of states. Namely, by the interaction with the surface, the injected ion particle changed to the superposition of ion state and neutral state. We recently proposed a method to quantitatively evaluate the neutralization probability of the ion from a wave function[4]. In the evaluation, we defined a small region V surrounding the hydrogen nucleus (see Fig. 1), and the probability of detecting m electrons within a small region V was estimated. The probability of detecting electrons was interpreted as the ion neutralization probability. For example, in the case of hydrogen, if exactly one electron is present in the region V, the hydrogen is interpreted as being neutral; if no electrons are present, it is interpreted as a positive ion.

Figure 1 shows the initial and final states of a simulation in which a hydrogen ion with a kinetic energy of 100 eV collides head-on with a tungsten atom. In the initial state, no electrons were present around the hydrogen nucleus, whereas in the final state, electrons were observed around the nucleus.

Analysis of the simulation results suggested that, under the conditions shown in Figure 1, the incident hydrogen ion was reflected as an ion with a probability of approximately 25%, and was neutralized with a probability of about 50%. Interestingly, the results also suggested that it became a negative ion with a probability of around 25%.

In this way, by using Ehrenfest MD, which simultaneously calculates the quantum mechanical motion of electrons and the classical mechanical motion of nuclei, we were able to represent the ion neutralization process that occurs during hydrogen ion incidence. In this presentation, we will report on the comparison between hydrogen ion and hydrogen atom incidence.

References

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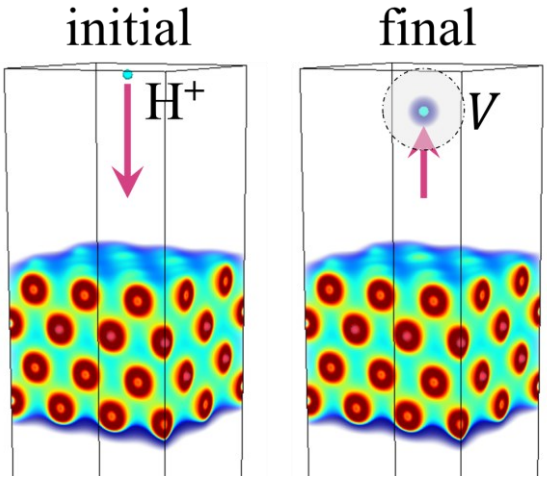

Figure 1. Initial and final states in the simulation. Spheres represent atomic nuclei, and the 3D heat map shows the electron density distribution.