

### §30. Molecular Dynamic Simulation of Hydrogen Isotope Injection into Graphene

Takayama, A., Nakamura, H., Ito, A. (Nagoya Univ.)

It is required for the investigation into the behavior of the impurity in the divertor region of a nuclear fusion device to clarify what kind of reactions occur, what kind of and how many particles yield, and how the carbon material become when hydrogen isotopes are injected into carbon materials. As the first step for the purpose, we performed classical molecular dynamics simulations of collision between single hydrogen isotope atom and single graphene sheet which is the basic element of carbon materials. This collision process is regarded as one of the basic processes of complex plasma-carbon interaction at the vicinity of the divertor plate. In the previous works<sup>(1-3)</sup> we investigated the case of hydrogen. The cases of deuterium and tritium injection, which are more realistic and important for an application to nuclear fusion devices, were simulated in this report.

In our classical molecular dynamics simulation the modified Brenner's reactive empirical bond order (REBO) potential<sup>(1-4)</sup>, which can deal with chemical reactions. As the simulation model, single atom of hydrogen, deuterium or tritium with various energy is injected into single graphene sheet of 1.97 nm x 2.13 nm at random incident positions.

Three kinds of reactions, that is reflection, absorption, and penetration, are observed. Figures show the rate of occurrence of each reactions as the function of the incident energy. It is apparent that reflection due to  $\pi$ -electron effect in the incident energy range of  $\leq 1$  eV and penetration in the energy range of  $> 30$  eV do not depend on the mass of incident isotope. The peak of the reflection due to nuclei shift to higher  $E_I$  as the mass of the incident isotope increase. This tendency is consistent with a simple estimation of a necessary condition to the incident energy  $E_I$  for reflection due to nucleus of carbon,

$$E_I > 0.84 \frac{m}{m_H} \frac{m_C + m_H}{m_C + m} [\text{eV}],$$

where  $m$ ,  $m_C$ ,  $m_H$  are the mass of incident atom, carbon and hydrogen, respectively.

#### References

1) Ito, A., Nakamura, H., and Takayama, A.: submitted to J. Nucl. Mater.; e-print cond-mat/0703377.

2) Ito, A. and Nakamura, H.: J. Plasma Phys. 72 (2006) 805.

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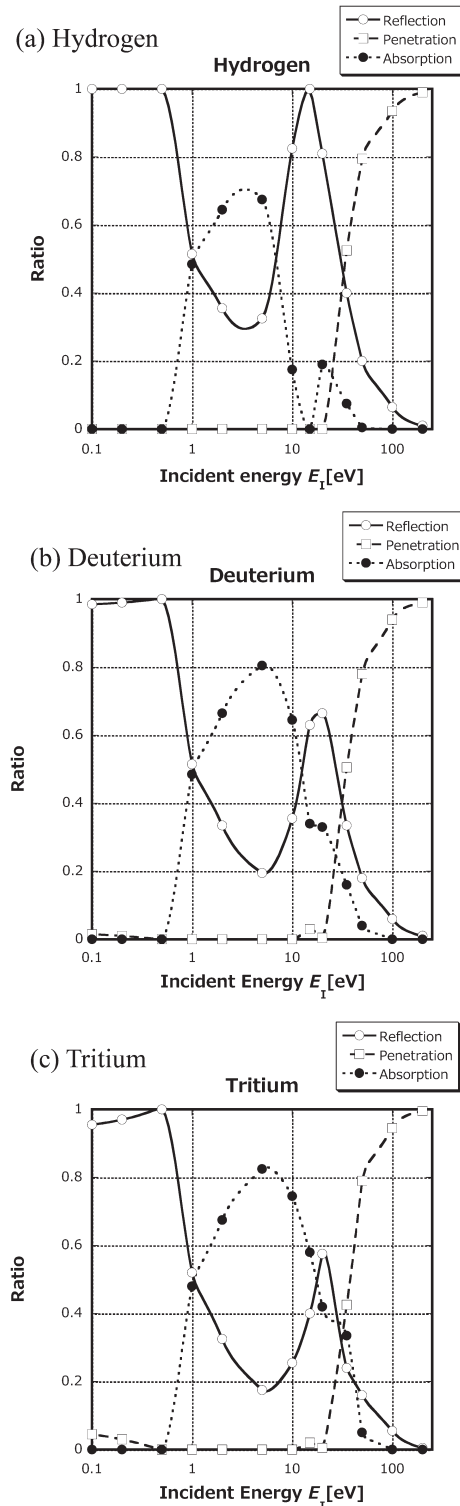


Figure: The rate of occurrence of reflection (open circle-solid line), penetration (open square-dotted line), and absorption (closed circle-dashed line) as the function of incident energy. Incident atom is (a) hydrogen, (b) deuterium, and (c) tritium, respectively.