§16. Molecular Dynamics Simulation of Chemical Vapor Deposition of Amorphous Carbon

Ito, A.M., Takayama, A.,
Saito, S., Ohno, N., Kajita, S. (Nagoya Univ.),
Nakamura, H.

Deposition of amorphous carbon appears on the various scenes in the research of plasma-material interaction. In the plasma-wall interaction of nuclear fusion reactors, the deposition of amorphous carbon is especially important as the following two viewpoints. One is the re-deposition of carbon impurity on a divertor wall and the first wall. Since amorphous carbon material created by the re-deposition process includes hydrogen isotopes, the mechanisms of the re-deposition process should be understood to realize tritium recycling in future reactors. The other is the coating on plasma facing materials with the amorphous carbon. It is considered that the amorphous carbon which is rich in sp3 ratio such as diamond like carbon (DLC) has plasma resistance. However, the manufacturing of the sp3-rich amorphous carbon is difficult yet. It is desired to clarify the formation mechanism of the sp3-rich amorphous carbon.

To understand these deposition processes, we must find mechanisms from phenomena in nano-scale. Using molecular dynamics (MD) simulation that deal with atomic motion directly, it is possible to investigate phenomena in nano-scale. In the present paper, the amorphous formation due to chemical vapor deposition onto diamond and graphite is investigated by using MD simulation.

Though nano-structures of amorphous carbon is not understood well, Robartson proposed that the amorphous carbon can be classified by the sp^3/sp^2 ratio of carbon atoms and hydrogen content, in principle [1]. In the present paper, we focus on the latter point in particular, where the ratio of number of hydrogen atoms to carbon atoms (H/C) was used as measure of the hydrogen content. Moreover, we classify the H/C in source and the H/C in deposit, which are, in MD simulation, the H/C about injected atoms and molecules and the H/C about atoms composing amorphous carbon material, respectively.

We performed MD simulation in which carbon and hydrogen were simultaneously injected as isolated atoms into the surfaces at a material temperature of 600K. The ratio of incident flux of hydrogen atoms to that of carbon atoms was corresponding to the H/C in source, where the incident flux of carbon atoms was always fixed to 2.5 x $26^{.6}$ atoms/m^2s, and the incident flux of hydrogen atoms was selected to be 0.1 to 8.0 times that of the carbon atoms. In this simulation conditions, deposition rate which is defined as ratio of the number of deposited carbon atoms to the number of injected carbon atoms is determined in Fig. 1. As a result, it is shown that as the H/C in source increases, the deposition rate decreases exponentially. The fact can be confirmed from experiment by Liu et al.[2] in which the deposition rate can be fitted as a decreasing exponential function of the H/C in source gas hydrocarbons as Fig. 2.

We consider that the dependence of deposition rate on H/C in source is key point to understand the formation process of amorphous carbon material. In nuclear fusion, it is expected for the present result to bring SOL/divertor simulation new modeling for deposition of impurity.

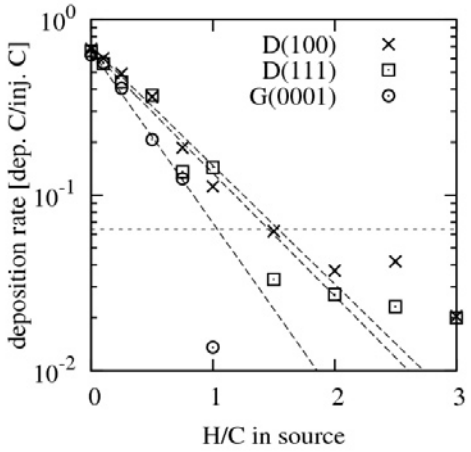

Fig. 1. the deposition rate in the MD simulation as a function of the H/C in source.

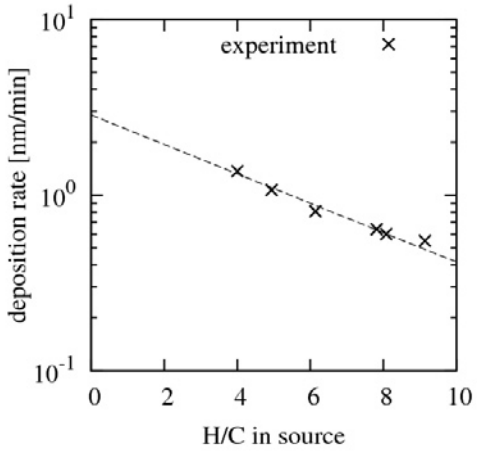

Fig. 2. deposition rate in experiment by Liu et. al.[2] as a function of the H/C in source.

1) J. Robertson: Mater. Sci. Eng. R 37 (2002) 129.
2) D. Liu, J. Zhang, Y. Liu, J. Xu, and G. Benstetter: J. Appl. Phys. 97 (2005) 104901.