Molecular Transport of Liquids in the Confined Space: A Fundamental Study and Applications to Device Process

G. Kikugawa[1]

[1] *Institute of Fluid Science, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai, Japan*

Molecular transport of liquid inside nanoscale structures have the significant relation with cutting-edge semiconductor processes. Recently, the process rule of device manufacturing is going down to several nanometers, and thus it is of great importance to understand mass transport in the nanoscopic scale in association with wet processes, particularly.

In this study, we examined mass transport of confined liquids by using molecular dynamics (MD) simulation. We discussed the diffusion property inside the nanoscale liquid film between substrates. The local diffusivity of liquid in the direction parallel to the substrate interface can be evaluated in the vicinity of the interface via the mean square displacement [1]. On the other hand, in the normal to the interface, there inherently exists heterogeneity in liquid due to the surface–fluid interaction. In this situation, it is questionable if phenomenological diffusion picture can be applied. Therefore, we developed the molecular transport model which utilizes the kinetic process for molecular migration [2]. In the nanoscopic space, molecular diffusion properties are also influenced by the hydrodynamic effect induced by molecular motion itself. We elucidated the diffusivity of liquid, which is significantly affected by the geometry of confinement by periodic boundaries from MD simulations [3] and theoretical analyses [4] (see **Fig. 1**). Through these studies, we aim to establish the microscopic picture of mass transport properties in confined liquid and bridge microscopic picture to the macroscopic fluid flow.

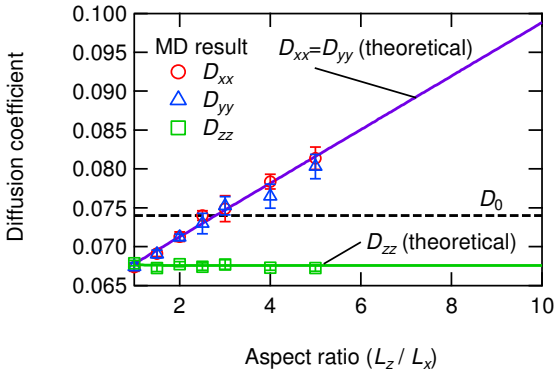

Fig. 1: Diffusion coefficients in each spatial direction as a function of the aspect ratio of the rectangular simulation box. Copyright 2015, AIP Publishing LLC.

[1] Y. Naruke, S. Kosaka, T. Nakano, G. Kikugawa, and T. Ohara, *Int. J. Heat. Mass. Trans.*, 84 (2015), 584–591.
[2] J. Suzuki, G. Kikugawa, T. Nakano, and T. Ohara, *JSME Mech. Eng. Lett.*, 1 (2015), 15-00353.
[3] G. Kikugawa, S. Ando, J. Suzuki, Y. Naruke, and T. Ohara, *J. Chem. Phys.*, 142 (2015), 024503.
[4] G. Kikugawa, T. Nakano, and T. Ohara, *J. Chem. Phys.*, 143 (2015), 024507.