Molecular dynamics study on influence of nanostructures on energy transfer mechanism over a fluid-solid interface

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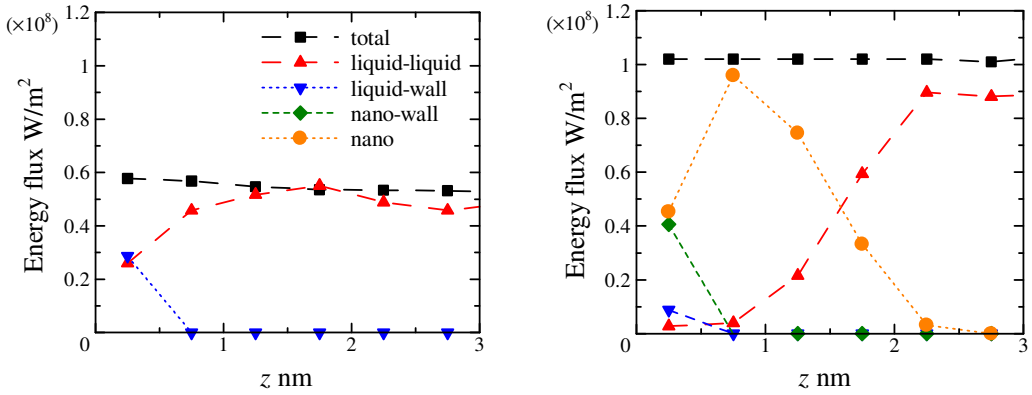
Adhesions of nanoparticles to the heat transfer surface are frequently observed when a liquid containing suspended nanoparticles is employed as the working fluid for heat transfer experiments. The interfacial thermal resistance can vary when contaminants such as nanoparticles are adherent to the surface, although the mechanism of the thermal resistance variations has not been clarified yet. In the present study the influences of slit structure[1] or carbon nanoparticle[2] adhered to a surface on the thermal resistance over liquid-solid interfaces were investigated directly by non-equilibrium classical molecular dynamics simulations with changing the interaction parameters between the liquid molecules and the atoms of slit structures or carbon nanoparticles, that between the liquid molecules and the wall atoms and the liquid pressure as calculation parameters. Also, the influences of structures at nanometer scales on the time resolved interfacial thermal resistance were calculated during condensation. The influences of the structures at nanometer scales were discussed based on the energy transfer formula at molecular scale calculated by the non-equilibrium molecular dynamics simulations.

Figures 1 (a) and (b) show the profiles of energy flux components caused by the inter-particle interactions along the heat conduction direction (z-direction) in the cases of a flat surface and a surface with carbon nanoparticles, respectively, when the calculation model system consists of an argon liquid molecular region confined between a flat platinum solid wall and a platinum solid wall on which carbon nanoparticles were adherent. The thermal resistances over the liquid-solid interfaces were calculated by the nonequilibrium molecular dynamics simulations, which were $4.71*10^{-8}$ and $2.45*10^{-7}$Km^2/W, respectively. In the vicinity of the liquid-solid interface (z = 0), the energy flux between carbon atoms and wall atoms (denoted as 'nano-wall') and that between carbon atoms (denoted as 'nano') were observed, which caused the reduction of interfacial thermal resistance in comparison with the flat surface.



(1) flat surface (2) surface with nanoparticles

Figs. 1: Influence of nanoparticles on the profiles of energy flux components in the vicinity of a liquid-solid interface.

[1] M. Shibahara, et al., *Proc. of 1st Pacific Rim Thermal Engineering Conference*, (2016) PRTEC-14385.
[2] T. Matsumoto, et al., *the Progress in Computational Fluid Dynamics*, 13, 3/4, (2013), 162-171.