

Heat transfer through a water layer in micro/nano-channel for cooling applications

Background

Heat transfer through micro channels is being investigated due to its importance in micro channel cooling applications. Molecular dynamics simulation is regarded as a potential tool for studying such microscopic phenomena in detail. However, the applicability of molecular dynamics method is limited due to scarcely known inter atomic interactions involved in complex fluids. In this study we want to use an empirical force field (ReaxFF), which is parameterized using accurate quantum chemical simulation results for water, to simulate heat transfer phenomena through a layer of water confined between two platinum slabs. The model for water seems to reproduce the macroscopic properties such as density, radial distribution function and diffusivity quite well. The heat transfer phenomena through a channel filled with water, which is confined by two platinum (100) surfaces are studied using ReaxFF. The model accurately predicts the formation of surface mono-layer. The heat transfer analysis shows temperature jumps near the walls which are creating significant heat transfer resistances. A low bulk density in the channel creates a multi-phase region with vapor transport in the region.

Using molecular simulations we want to study these heat fluxes in the system, accommodation and diffusion coefficients for different bulk densities and different wall properties (e.g. coatings of the wall).

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