MOLECULAR DYNAMIC SIMULATION OF THERMAL CONDUCTIVITY OF NANOMATERIALS

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Abstract

The control of thermal transport is essential for many modern nanomaterials and necessary for the new generation microelectronics devices. The study and understanding of the heat flow across the nanomaterials is the main priority for the large spectrum of microelectronic industries. Unfortunately, quantitative measurements of thermal properties at nanoscale are still problematic, even with use of advanced techniques like Scanning Thermal Microscopy. Therefore, the molecular dynamics simulations can be helpful for the better description of thermal transport processes inside of nanomaterials.

This contribution represents the equilibrium molecular dynamics simulation (Green-Kubo relation) to predict the thermal transport properties (especially thermal conductivity) of nanomaterials. We focused on semiconductors (silicon) and insulators (diamond and polyethylene) and showed the difference between real and simulated value of thermal conductivity in dependence on temperature. Moreover, the effect of various inter atomic potentials (force fields) on the value of thermal conductivity was studied.

Keywords: Scanning thermal microscopy, molecular dynamics, thermal conductivity, Green-Kubo

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