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Size Effect in Non-equilibrium Molecular Dynamics

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ABSTRACT

Direct method is commonly used to compute the thermal conductivity of a nanoscale material after molecular dynamics simulation. Direct method simply applies Fourier's Law to get the value of thermal conductivity, which requires heat flux, cross sectional area and temperature gradient. A typical structure includes one heat source, one heat sink and a device region between them. Although it is usually assumed that the temperature gradient is a constant through the entire device region, the temperature profile is not linear for a material in nanoscale because phonon mean free path is comparable to the size of the whole system. Furthermore, bath length and device length can have influence on temperature profile. In this project, two methods of temperature gradient computing and the size effect of each method are discussed. Method 1 uses the center region of the device to get temperature gradient and method 2 uses the temperature difference between hot bath and cold bath divided by the device length as temperature gradient. The thermal conductivity computed from Green-Kubo method is used as a standard to test the two calculation methods and the size effect. Argon with atomic weight 40 is used as the nanoscale material because of its moderate phonon mean free path. Result shows that both method 1 and method 2 can compute the bulk-limit thermal conductivity but the necessary size conditions are different. Method 1 requires a long device and method 2 requires a long bath region.

KEYWORDS

Thermal conductivity, nanoscale, Fourier's Law, temperature gradient, Green-Kubo, size effect

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