A Molecular Dynamics Study on the Effects of Wall-Fluid Interaction Strength and Fluid Density on Thermal Resistance of Graphene/Argon Interface

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ABSTRACT

Molecular dynamics simulations of Argon flow confined between two parallel graphene sheets are carried out to investigate the effects of some parameters on heat transfer and thermal properties. These parameters include wall-fluid interaction strength and fluid density where for constant wall temperature simulations, we show that these two parameters have influence on near-wall fluid density. As a result, the heat transfer at wall-fluid interfaces and thus through Argon molecules across the domain will change. To analyse the results, the density and temperature profiles and two other parameters including temperature gradient of the bulk of Argon molecules and the Kapitza length are considered. The Kapitza length represents the thermal resistance at liquid-solid interface. According to the results, the increase of wall-fluid interaction strength leads to greater number of Argon molecules near the walls and consequently, the Kapitza length decreases and an enhancement is observed in temperature gradient and the slope of temperature profile. Furthermore, higher values of fluid density cause that the thermal resistance at wall-fluid interactions increases. Therefore, greater temperature jumps are observed in temperature profiles.

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