Molecular dynamics simulation of the domain size effect on the values of thermal conductivity of long chain n-alkanes

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Abstract

Phase change materials such as n-alkanes that possess desirable characteristics such as high latent heat, chemical stability and negligible supercooling are widely used in thermal energy storage applications. However, n-alkanes have the drawback of low thermal conductivity values. Understanding the thermal transport phenomena associated with n-alkane such as n-eicosane ($C_{20}H_{42}$) and triacontane ($C_{30}H_{62}$) is crucial for improving the efficiency of thermal storage systems. In this paper, the thermal conductivity of long chain n-alkanes ($C_{20}H_{42}$, $C_{24}H_{50}$, $C_{26}H_{54}$ and $C_{30}H_{62}$) is investigated by utilizing non-equilibrium molecular dynamics (NEMD) simulations. The main challenge in this work is to remove the possible domain size effect from the existing data for solid n-alkanes. Thus, the effect of the cross section of the system is studied. We utilized three different numbers of molecules for the case of $C_{30}H_{62}$ to investigate the effect of the size effect due to the cross section area. Results confirm that the 600 number of molecules being used for the simulation box is sufficient to remove the size effect. All simulations were performed with the large-scale atomic/molecular massively parallel simulator (LAMMPS) molecular dynamics package.

Keywords: Non-Equilibrium Molecular Dynamics; n-alkanes; Phase Change Materials; Thermal Conductivity; Thermal Energy Storage.