Thermal Transport Properties of Low Dimensional Si, Ge, and SI-GE Superlattice Structures

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Potential low dimensional thermoelectric materials have captured considerable attention of researchers due to their possible adaptation in power generation, energy conversion, and solid-state cooling applications. Due to enhanced electrical conductivity of these systems, researchers mainly focused on to find a way of reducing thermal conductivity of these systems to enhance their thermoelectric performance. With this intention a number of theoretical and experimental studies have been carried out. Due to their extraordinary transport properties carbon based nano materials have been studied intensively and several different researchers have pointed out their highly efficient thermoelectric properties. Furthermore, as another nanostructure material family Si, Ge, and Si-Ge based nano systems have attracted attention and ZT values larger than 2.0 have been reported for some Si nanostructures. Considering the potential of these materials, we systematically investigate the thermal transport properties of bulk and nano superlattice structures of Si, Ge and SiGe by equilibrium molecular dynamics simulations. We predicted quite low lattice thermal conductivity for some specific structures of these materials. Our results show that the thermal conductivity of these structures can be suppressed up to %75 percent of bulk superlattice or pure nanowire structures.

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