Thermal Conductivity of Ge Embeded with Si Nanowire

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In this paper, a systematic study is carried out to investigate the thermal transport in Si/Ge nanocomposites by use of molecular dynamics simulation. Emphasis is placed on the effect of nanowire size, heat flux, Si/Ge interface, atomic ratio, and defects (voids). The results show that the thermal conductivity of nanowire composites is much lower than that of alloy, which accounts mainly for *ZT* enhancement and owes a great deal to the effect of interface thermal resistance. A "reflecting effect" in temperature distribution is observed at the Si/Ge interface, which is largely due to the lack of right quantum temperature correction in the region adjacent to the interface. The thermal conductivity of the nanocomposite is found to have weak dependence on the bulk temperature (200~900 K) and the heat flux in the range of $0.5\sim3.5\times10^{10}$ W/m^2. Simulation results reveal that for a constant Si wire dimension, the thermal conductivity of the $Si_{1-x}Ge_x$ nanocomposites increases with x. Our study on the influence of the defects (voids) has the same order of relative thermal conductivity reduction with increasing void density in comparison with the experimental data. Due to the small size (10 nm) of Si nanowires in our nanocomposites, the voids show less effect on thermal conductivity reduction in comparison with the experimental data with 100 nm Si wires.