Nanocomposites and nanomaterials

Thermal conductivity of Ge/Si composite quantum dots: a molecular dynamics study

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Over the past decade, there draws significant interest in the exploration of high figure of merit (*ZT*) thermoelectric (TE) materials that can efficiently convert waste heat into electricity. For a high performance TE material, the concurrent of low thermal conductivity k and high electrical conductivity σ is essential since *ZT* increases linearly with σ and is inversely proportional to k [1]**.** Many attempts have been made on the exploration of Si/Ge heterostructures with quantum dots for TE applications. These materials effectively decrease the thermal conductivity by reducing particle size, which helps to scatter the phonon at the interfaces [2,3].

In this work, we investigated the temperature dependence of the thermal conductivity of Si/Ge heterosturcutres with multifold quantum dots by equilibrium molecular dynamics simulations using the Stillinger-Weber potential. We calculated the thermal conductivity of multifold Ge/Si/Ge composite quantum dots consisting of a deliberate insertion of Si between Ge sub-dots. The result shows that the thermal conductivity of Ge/Si/Ge composite quantum dots first decreases and then increases with decreasing the volumetric ratio. The effect of number of Si insertion layers on the thermal conductivity of Ge/Si/Ge nanocomposites is also studied. An interesting finding is that the effective thermal conductivity decreases with an increase in the fold of composite quantum dots. The reduction of the thermal conductivity make such multifold Ge/Si/Ge composite quantum dots materials promising candidates for future TE applications in microelectronics.

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