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Modeling the phonon heat transport in semiconductor superlattices

by

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In this thesis, we present a thorough study of the cross-plane lattice thermal conductivity in superlattices. We have first developed a general Boltzmann model for cross-plane thermal conductivity in superlattice considering a heat transport by particle-like phonons. The key development presented in the developed model in that the initial Boltzmann equation is considered spatial-dependent and the anisotropy of the Brillouin zone is accounted for. The model is free of adjustable parameters and all its vibrational parameters are temperature-dependent to insure accuracy in the full temperature range. Then, in order to model the phonon heat transport in superlattices, we have classified the phonons into two categories, according to their wavelengths. Phonons of wavelengths greater than the superlattice period and root mean square interface irregularities undergo ballistic transmission through the interfaces and obey dispersion relations determined by the Brillouin zone folding effects of the superlattice, whereas phonons of wavelengths shorter than the superlattice period may experience scattering processes at the interfaces. We have assessed the assumption of mixed phonon heat transport in superlattices with reference to experimental measurements regarding the effects of period thickness and temperature on cross-plane thermal conductivity in $Si/Si_{0.7}Ge_{0.3}$ and $Si_{0.84}Ge_{0.16}/Si_{0.76}Ge_{0.3}$ superlattices. Lastly, we have employed the developed model to investigate the interplay between the alloy scattering and interface scattering and find the lower limit to the thermal conductivity of $Si_{1-x}Ge_x/Si_{1-y}Ge_y$ superlattice.

Date: Monday, September 26, 2016
Place: Rm. 215, Physics Dept.
Time: 3:00 p.m.