

Predictive calculation of the lattice thermal conductivity with Temperature-dependent vibrational parameters

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Abstract:

This paper presents a predictive model for the lattice thermal conductivity. The model is based on Callaway's solution to the Boltzmann equation for phonons which discriminates between the natures of the resistive and non-resistive phonon processes. However, the present model uses temperature-dependent lattice vibrational parameters and sound group velocities calculated on the basis of a dynamical matrix. No adjustment to thermal conductivity measurements is required. The model requires only the material mechanical properties as inputs to yield the material thermal conductivity as a function of temperature. A precise transmission probability function is introduced in the model in order to widen its application for the cases where interfaces are present. The importance of all the features of the developed model is demonstrated clearly with reference to reported data regarding the effects of surface orientation and isotope composition in single crystals, the effect of alloy composition in alloys, and the effect of grains boundaries in polycrystals. Namely, the developed model accounts for (i) the effects of surface orientation and isotope composition on the thermal conductivity of silicon and germanium single crystals, (ii) the effect of alloy composition on the thermal conductivity of silicon-germanium alloys, and (iii) the effect of phonon scattering at grains boundaries on the thermal conductivity of polycrystalline silicon. VC 2012 American Institute of Physics.

[<http://dx.doi.org/10.1063/1.4769429>]