

On the interplay between phonon-boundary scattering and phonon-point-defect scattering in SiGe thin films

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Abstract:

This paper provides theoretical understanding of the interplay between the scattering of phonons by the boundaries and point-defects in SiGe thin films. It also provides a tool for the design of SiGe-based high-efficiency thermoelectric devices. The contributions of the alloy composition, grain size, and film thickness to the phonon scattering rate are described by a model for the thermal conductivity based on the single-mode relaxation time approximation. The exact Boltzmann equation including spatial dependence of phonon distribution function is solved to yield an expression for the rate at which phonons scatter by the thin film boundaries in the presence of the other phonon scattering mechanisms. The rates at which phonons scatter via normal and resistive three-phonon processes are calculated by using perturbation theories with taking into account dispersion of confined acoustic phonons in a two dimensional structure. The vibrational parameters of the model are deduced from the dispersion of confined acoustic phonons as functions of temperature and crystallographic direction. The accuracy of the model is demonstrated with reference to recent experimental investigations regarding the thermal conductivity of single-crystal and polycrystalline SiGe films. The paper describes the strength of each of the phonon scattering mechanisms in the full temperature range. Furthermore, it predicts the alloy composition and film thickness that lead to minimum thermal conductivity in a single-crystal SiGe film, and the alloy composition and grain size that lead to minimum thermal conductivity in a polycrystalline SiGe film. VC 2015 AIP Publishing LLC.
[<http://dx.doi.org/10.1063/1.4915948>]