T4B-2 Is a constant relaxation time suitable for periodic 1D stacks of InAs/GaAs quantum dots?

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Due to the quantum confinement of electrons and phonons, semiconductor nanostructures are expected to provide an improved figure-of-merit. We investigate thermoelectric transport in a periodic 1D stack of disk-shaped InAs quantum dots (QDs) in GaAs. The electron relaxation time as a key characteristic of a periodic 1D stack of QDs is calculated using the Boltzmann equation. Electron minibands provided by the tight-binding approach are adequately represented within the Kronig-Penney model of a periodic 1D stack of QDs. Solution of the dispersion relation for acoustic phonons reveals that an effective medium approximation can be applied with a good accuracy. We find that a geometry-controlled relaxation time significantly increases at the center and at the boundaries of the first Brillouin zone. The use of a constant relaxation time is inadequate. From the numerical analysis of the electric and thermal transport coefficients, we conclude that an enhancement of the efficiency of the 1D stack of QDs as a thermoelectric convertor can be realized for the cases of one to three electronic minibands.
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T4B-3 Study on mechanical properties of single crystal bismuth telluride nanowire by molecular dynamics simulation

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In the present work, the mechanical properties of a single crystal bismuth telluride nanowire are studied by molecular dynamics methods. Bond potentials developed by B.L.Huang et al(PRB 77, 125209,2008) have been adopted in this simulation. We simulated the mechanical behavior of Bi_2Te_3 nanowire between principal axis under different strain rate at low temperature, and that of Bi_2Te_3 bulk for comparison. The simulation results show that the nanowires deform through bond-stretching and breaking in response to the axial tension. Due to its marked anisotropy, the nanowire shows quite unique failure behaviors in different direction, the failure stress for the *a*-axis (6.9 GPa) is almost five times bigger than that for the *c*-axis (1.4 GPa). The stress-strain curve of nanowire reveals a different appearance from that of Bi_2Te_3 bulk. Nanowire has much lower Young's module, as it has more free surfaces. The effect of strain rate on the mechanical properties of nanowire is also analyzed and shows a decreasing failure stress and failure strain with decreasing strain rate, however which is not obvious in the simulation of Bi_2Te_3 bulk.

T4B-4 Analysis of thermoelectric properties of scaled silicon nanostructures using an atomistic tight-binding model

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The progress in nanomaterials' synthesis allows the realization of low-dimensional thermoelectric devices based on 1D nanowires and 2D superlattices. These confined systems offer the possibility of partially engineering the electronic and phonon dispersions. Thus, the electrical and thermal conductivity, and the Seebeck coefficient can be designed to some degree independently, providing enhanced ZT values compared to their bulk material's value. The large design space demands proper modeling tools supporting material and structure parameter optimization in order to achieve highest possible ZT values.
In this work, we calculate the electrical conductivity, the Seebeck coefficient, and the electronic thermal conductivity of scaled silicon nanowires and superlattices using an atomistic $sp^3d^5s^*$-spin-orbit-coupled tight-binding model. This atomistic model provides an accurate estimate of the electronic structure and carrier velocities, while being computationally affordable. We examine n-type and p-type nanostructures of diameters/thicknesses from D = 3nm to 12 nm, in [100], [110] and [111] transport orientations, at different doping levels. The parameters of interest are calculated within the framework of the relaxation time approximation. A theoretical upper limit for the thermoelectric parameters is also given assuming ballisticity. Finally, an estimate of the lattice thermal conductivity needed to achieve high ZT values, is calculated, and compared to experimental results.

T4B-5 A non-equilibrium molecular dynamics study of in-plane thermal conductivity of silicon thin films

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We employ the non-equilibrium molecular dynamics (NEMD) simulation to calculate the in-plane thermal conductivity of a silicon thin film. To eliminate the finite-size effect, samples of various lengths are simulated and an extrapolation technique is employed. To perform the quantum correction which is necessary when MD simulation temperature is lower than Debye temperature, we manage to obtain the confined spectra via the EMD simulations. The investigation shows the thermal conductivities corrected by the bulk or the thin-film DOS are very close and agree excellently with the theoretical predictions having a similar surface roughness based on the phonon Boltzmann equation. Those uncorrected or corrected by the Debye DOS fail on the other hand. It is thus concluded that it is improper to employ the Debye DOS for the quantum correction and a use of the bulk one is sufficient for thin films, unless the temperature is very low or the film thickness is very small.