Title: Low dimensional nanostructures as efficient thermoelectric materials for energy conversion and generation

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Abstract

The efficiency of thermoelectric converters is measured by the dimensionless figure of merit $ZT=\sigma S^2/(\kappa_e+\kappa_l)$, where σ is the electrical conductivity, S is the Seebeck coefficient, and κ_e is electronic and κ_l the lattice part of the thermal conductivity. Large improvements in ZT have been recently reported in low-dimensional and nanostructured materials as a result of suppressed phonon conduction (κ_l). This has been even observed for traditionally poor thermoelectrics such as silicon. Other than the reduction in κ_l, further improvements in ZT could potentially originate from the power factor (σS^2). In this work we use the atomistic $sp^3d^5s^*$ tight-binding model and linearized Boltzmann transport theory to calculate the electrical conductivity, Seebeck coefficient, and thermoelectric power factor of narrow 1D silicon and germanium nanowires and ultra-thin-layers. We present a comprehensive analysis of the thermoelectric coefficients of n-type and p-type channels of diameters/widths from 12nm down to 3nm, in different transport orientations. We show that for length scales below 7nm quantum mechanical confinement can alter the bandstructure of the channels and affect the power factor. The effect of confinement and geometry on the power factor originates mostly from changes in the conductivity which is strongly affected, rather than the Seebeck coefficient. In general, enhanced scattering at these diameter scales strongly degrades the conductivity and power factor of the device. We identify cases, however, for which confinement largely improves the channel's conductivity, resulting in ~2-3X power factor improvements.

Biographies

Neophytos Neophytou received his PhD in Electrical and Computer Engineering from Purdue University, West Lafayette, IN, USA in 2008. He is currently a Post-Doctoral Researcher at the Institute of Microelectronics, Technical University of Vienna in Austria. His area of specialization is theory, computational modeling and simulation of transport in nanoelectronic devices. He has worked extensively on theoretical modeling of atomistic and quantum effects on the electronic properties of nanoscale devices, nanowires, ultra thin-body devices, carbon nanotubes, graphene nanoribbon devices and III-V HEMT devices. His current research interests include thermoelectric transport in nanostructured devices, for energy conversion and generation applications.

Hans Kosina received the Diplomingenieur degree in electrical engineering and the PhD degree from the Vienna University of Technology in 1987 and 1992, respectively. In 1998 he received the venia docendi in microelectronics from the same university. He is currently a professor at the Institute for Microelectronics. His research interests include Technology CAD, semiconductor device modeling, electronic transport in nanostructures, Monte Carlo methods for classical and quantum transport, modeling of carbon nanotube and graphene-based devices, nanostructured thermoelectric energy converters, and optoelectronic devices. Dr. Kosina is Associate Editor of the Journal of Computational Electronics and of the IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems. He authored and co-authored more than 130 publications in peer-reviewed journals and 250 contributions to conference proceedings.