Title: Atomistic simulations of the electronic properties of Si and Ge nanowires and thin-layers: Bandstructure effects

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Abstract

Ultra-narrow semiconductor nanowires (NWs) and ultra-thin-layers (UTLs) are candidates for a variety of applications such as advanced transistor devices, optoelectronics, biosensors, etc. Due to strong quantum confinement these channels exhibit different electronic properties than bulk. These properties often depend on the confinement length scale, confinement orientation, and transport orientation. In this work we calculate the electronic properties of silicon (Si) and germanium (Ge) ultra-thin NWs and UTLs up to 12nm in diameter/thickness. For the electronic structure calculation we employ the $sp^3d^5s^*$ atomistic tight-binding (TB) model. We show that the electronic properties of these low-dimensional channels such as the effective mass, the carrier velocities, and valley separations are a strong function of geometry and orientation. This geometry dependence is especially important for holes, in which case large reduction in the subband effective masses is observed in the p-type [111] and [110] NWs and p-type (110)/[110] ultra-thin-layers as the confinement length scale is reduced down to 3nm. We further calculate the transport properties of these channels in both, the ballistic and diffusive regimes. For this we use the ballistic Landauer formalism and the linearized Boltzmann transport theory, respectively. In the case of Boltzmann transport we include carrier scattering by phonons, surface roughness, and ionized impurities. We show that the anisotropy in the electronic structure of the different NW and thin-layer channels translates into different transport properties, especially in the case of carrier mobility calculations.

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.