Can we define unique effective masses in Si nanowires?

Dragica Vasileska and Gerhard Klimeck
(ASU, Purdue)

It is expected that Peltier coolers made of nanowires can be integrated with conventional devices and used to remove the heat from deep inside the device. The efficacy of the Peltier coolers is quantified with the so-called ZT factor that is proportional to the ratio of the electrical and thermal conductivities. Thus, in order to properly determine the efficacy of Peltier coolers we need to properly determine the electrical and thermal conductivities of long nanowires. The electrical conductivity is strongly affected by the carrier masses along the propagation and confinement directions. By calculating the band-structure of 2nm×2nm, 3nm×3nm and 5nm×5nm nanowire cross-sections with (100) orientation of the wafer and [010] and [011] transport orientations we can explore at what wire cross-section the bulk model for the effective masses in the confinement direction fails, which suggests that in order to properly calculate the electrical conductivity of small cross-section nanowires one has to take into consideration the full carrier dispersion.