Materials Science and Technology Division

Materials Theory Seminar

"Opto-Electronic and Thermoelectric Properties of Si and SiGe Nanowires"

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Monday, December 17, 2007
9:00 a.m., HTML/4515, Room 265

Abstract:

We report the results of a first principles study of the structural, electronic, and optical properties of hydrogen-passivated silicon nanowires with [001], [011], and [111] growth directions and diameters ranging from 1 to 3 nm. We show that the growth direction, diameter, and surface structure all have a significant effect on the structural stability, electronic band gap, band structure, and band edge effective masses of the nanowires. In addition, we have used a combination of density functional theory, classical molecular dynamics and cluster expansion techniques to optimize the thermoelectric figure of merit (ZT) of Si and Si_xGe_{1-x} nanowires. The electrical conductivity (σ) and Seebeck coefficient (S) were obtained using the Boltzmann transport equation with the constant relaxation time approximation, and with first principles electronic structure calculations. A range of SiGe nanowires with different Ge concentrations and distributions were investigated. We found that the transport coefficients σ, S, and thus ZT strongly depend on the wire growth direction, surface structure, as well as the concentration and distribution of Ge.

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Host: Randy Fishman