nanosystems initiative munich

SONDERSEMINAR

Donnerstag, 26. Mai 2011

16:00 Uhr

WSI, Seminarraum S 101

„Non-equilibrium dynamics of localized phonons in semiconductors: Isotope effects”

Impurities in crystalline materials introduce localized vibrational modes. The coupling of these modes to each other and to the host crystal phonons sometimes exhibits an unexpectedly large isotope dependence. For example, the lifetime of the asymmetric stretch of interstitial O in Si nearly doubles upon substitution of one of its Si nearest neighbors from 28Si to 29Si, while the frequency of the mode shifts by only 0.1%! Ab-initio non-equilibrium molecular-dynamics simulations in carefully ‘prepared’ supercells reproduce and explain this isotope effect. The same theoretical approach, applied to the calculation of thermal conductivities in Si nanostructures as a function of the impurity content, also shows large isotope effects. These have yet to be measured.

This talk will begin with the discussion of the temperature- and isotope-dependence of vibrational lifetimes, and the subsequent experimental challenge to theorists. Then, I will discuss supercell preparation in (or slightly away from) thermal equilibrium and temperature control for non-equilibrium MD simulations. The method can be used to calculate the thermal conductivity of Si nanostructures containing impurities. The predictions include surprisingly large impurity isotope effects which appear to be related to the issue of vibrational lifetime. The results lead to a theoretical challenge to experimentalists. A great bottle of wine awaits the experimentalist who can measure the predicted isotope effects.

Prof. Stefan K. Estreicher
Physics Department, Texas Tech University
USA