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Phonons in Si Nanowires and Si/SiGe Quantum Dot Superlattices

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In this presentation we will review our recent results of the theoretical and experimental investigation of the phonon dispersion, phonon scattering rates and phonon thermal transport in Si nanowires and Si/SiGe quantum dot superlattices [1-3]. Spatial confinement of the acoustic phonons in nanostructures can strongly affect the phonon dispersion and modify phonon properties such as group velocity, polarization, density of states as well as affect phonon interaction with electrons, point defects and other phonons. Modification of the acoustic phonon dispersion is particularly strong in the free-standing nanowires or nanostructures embedded into elastically dissimilar materials, i.e. materials with large acoustic impedance mismatch (see Figures 1-2). The acoustic impedance is defined as a product of the mass density and the sound velocity in a given material. Thus, acoustically mismatched nanostructures offer a new way for controlling phonon transport via tuning its dispersion relation, i.e., phonon engineering.

Specifically, we will consider two types of nanostructures: a Si nanowire with the acoustically soft coating (such as plastic or polymer), and Si nanotube with the acoustically soft enclosure. If the acoustic impedance mismatch at the interface between Si and the soft material is large, and the diameter of the nanowire and coating thickness are in the right range (much smaller than the phonon mean free path), the phonon spectrum undergoes significant modification. This confined-induced phonon spectrum modification results in a characteristic branching and changing density of states. The latter, in its turn, leads to the electron – phonon scattering modification.

The data to be presented in this talk also include the results of the experimental investigation of the phonon thermal conduction in Si/SiGe quantum dot superlattices, and the phonon-hopping interpretation of the thermal transport in this type of Si nanostructures (see Figure 3).

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Figure 1: Calculated confined acoustic phonon dispersion for a Si nanowire with 8 nm in diameter coated with a layer of polystyrene with 2 nm thickness. Shown are the lowest axially symmetric phonons with $m = 0$ for the polystyrene coated Si nanowire (solid curves) and for the uncapped Si nanowire (dashed curves). One can see that the soft polystyrene shell, which has the sound velocity four times lower than that of the Si nanowire, makes the confined phonon spectrum denser and decreases the slope of the dispersion branches.

Figure 2: Low-temperature electron mobility in the Si nanowire coated with the “acoustically soft” material is about 50% larger than the mobility of an uncapped Si nanowire for the temperature up to 3 K. A smart choice of the coating material and its thickness allows one to engineer the spectrum of the acoustic phonons and modify the electrical and thermal conductivity.

Figure 3: Measured and calculated phonon thermal conductivity as a function of the temperature for three Ge/Si quantum dot superlattices (QDS) with different dot size. Note a good agreement over the wide temperature range of the experimental data and simulations performed based on the phonon-hopping model. The measurements were carried out using the differential 3ω method.