Elastic-Wave Modeling of Long-Wavelength Phonon Dynamics in Superlattice Nanowires With Rough Interfaces

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To differentiate the effect of phonon-phonon scattering and phonon-interface scattering on the thermal conductivity in silicon nanowires (SiNW), long wavelength phonon dynamics has been considered, as phonon-phonon interactions are infrequent for long wavelength (low-energy) phonons. Experimental measurements on SiNWs have shown that, their thermal conductivity below the Casimir limit can be explained with phonon-surface scattering [1]. Using the elastic-medium finite-difference time-domain (FDTD) technique, we can accurately model the dynamics of long wavelength lattice waves and their interaction with interfaces. Previously we presented the application of this model to calculate thermal conductivity in III-V superlattice (e.g. InGaAs/InAlAs) and in rough SiNW. The calculated cross plane thermal conductivity showed good agreement with experimental data at low temperature. For this work we propose to apply our model to extract long wavelength phonon lifetime for a rough superlattice nanowire, which will provide valuable insight on the effect of surface and interlayer roughness in the thermal transport of such superlattice nanowires.

To model the phonon dynamics in the rough interfaces, we start from our previously developed FDTD code [2]. Here, the elastic-wave equation is solved with the velocity-stress formulation using FDTD technique. To generate the rough superlattice interfaces and boundaries with a particular RMS roughness and correlation length, two types of autocorrelation functions (ACF) will be considered, namely gaussian and exponential. For the superlattice structure, AlGaAs/GaAs superlattice will be constructed with rough interfaces, but the general formulation and code can be used to simulate any structure with appropriate parameters.

To simulate the transport in the nanowires, we will use a Gaussian wave-packet as the excitation, which will be launched from the central region of the superlattice and will propagate through the rough interfaces toward the boundaries. Depending on the roughness properties used (i.e., rms roughness and correlation length), the Fourier transform of this wave, which peaks around the launch frequency and its harmonics, will experience significant broadening. Then, we will use Lorentzian fitting for each prominent peak to obtain the full-width half max (FWHM) of the peaks which contains the information about the phonon scattering lifetime. We can run the simulation for various launch frequencies to determine the lifetime versus frequency characteristics as indicated in Fig. 1(b) for the case of rough silicon nanowire.

In conclusion, we use our FDTD code to solve the elastic-wave equation to investigate the long wavelength phonon dynamics in rough superlattice nanowires and extract phonon lifetime versus frequency power law dependance.

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References

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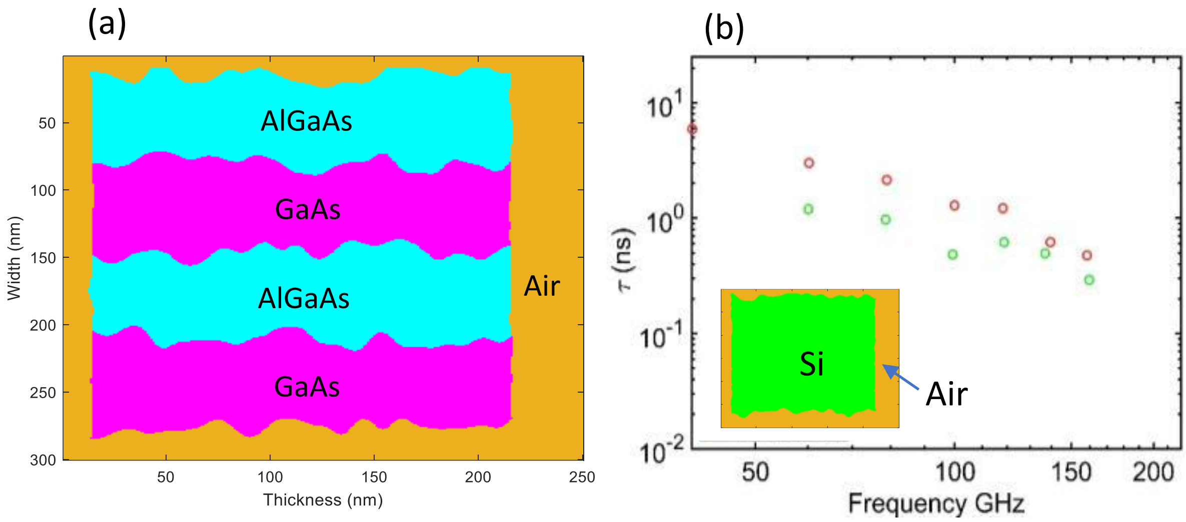

Fig. 1. (a) 2D cross section of the rough superlattice nanowire to be simulated. The RMS roughness and correlation length parameters are 5 and 10 nm respectively. (b) Representative plot of phonon lifetime versus frequency for a rough silicon nanowire. The green open dots represent RMS roughness of 1 nm and the red open circles represent RMS roughness of 5 nm. For both the cases, correlation length was 20 nm.