Effect of Stacking Faults and Surface Roughness on the Thermal Conductivity of Si Nanowires

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It has been shown experimentally that the thermoelectric figure of merit (ZT) of Si nanowires (NWs) can be improved by engineering their surface roughness (SR) [1]. If the reduction of the thermal conductivity exceeds the degradation of the power factor, the conversion efficiency increases. In addition to SR, a significant decrease of the thermal conductivity can originate from stacking faults (SFs), which naturally occur in III-V materials [2]. Recent calculations of phonon relaxation times due to scattering at SR and SFs resulted in excellent agreement with measured thermal conductivities of InAs NWs [3].

In this work, the thermal conductivity of ⟨111⟩-oriented Si NWs with SFs, as already studied in optical experiments [4], and SR is simulated based on density functional theory (DFT) [5]. The linearized Boltzmann transport equation (BTE) and the SR scattering model developed in Ref. [3] are first validated on Si NWs where experimental data for detailed roughness profiles exist [6] (Fig. 1). It is found that a Gaussian autocorrelation function of SR fits the measured thermal conductivity better than an exponential one (Fig. 1 (a)). For a NW with rough surface, a more than 80% decrease of the thermal conductivity is possible for specific roughness profiles (Fig. 1 (a)). When the autocorrelation length falls below a certain value, the thermal conductivity starts to increase. This behavior can be explained by the ratio between L and wave length λ_{ph} of the most contributing phonons. Long-wavelength phonons with $\lambda_{ph} >> L$ are hardly scattered by the SR potential.

As in the case of InAs NWs, comparable reductions of the thermal conductivity of Si NWs can be obtained with SFs instead of SR. The inclusion of SF requires the phonon band structure of a diamond-wurtzite (DMWZ) super-lattice, which represents an intermediate case between diamond (DM) and wurtzite (WZ) (Fig. 2). The average energy difference (ΔV) between DM and WZ phonon band structures is about 0.51 meV (Fig. 3 (a)). Different spatial distributions of the SF distance l_{sf} result in similar values of the thermal conductivity (Fig. 3 (b)). For the shortest possible distance between SFs along the NW, the room-temperature thermal conductivity reduces to ~25% of its ideal NW value (8 vs. 30 W/Km).

Our simulations show the general possibility of engineering ZT of Si NWs. However, it still has to be clarified how the power factor changes under the same conditions.

[1] A. I. Hochbaum et al., Nature, **451**, 163 (2008). [2] S. F. Karg et al., Nanotechnology, **25**, 305702 (2014). [3] K. Vuttivorakulchai et al., J. Appl. Phys., **124**, 205101 (2018). [4] Y. Li et al., Nanoscale **7**, 1601 (2015). [5] K. Vuttivorakulchai et al., ESSDERC, (IEEE, 2018), pp. 34-37. [6] J. Lim et al., Nano Lett., **12**, 2475 (2012).

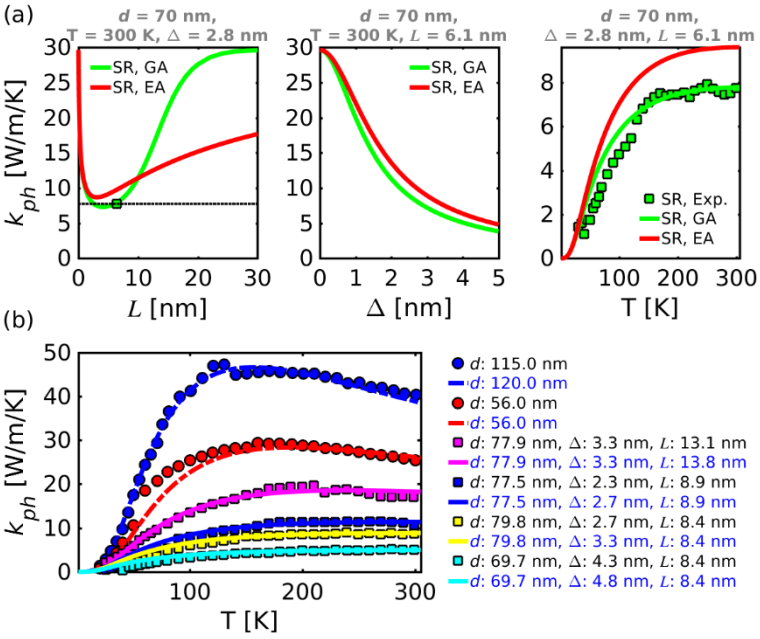

Fig.1: Thermal conductivity (k_{ph}) of Si NWs with Gaussian autocorrelation (GA) and exponential autocorrelation (EA) functions for SR. (a) k_{ph} as a function of the correlation lengths (L) (left), roughness heights (Δ) (middle), and temperature (T) (right). The green-square symbols represent measured k_{ph} of a Si NW with a diameter (d) equal to 70 nm, Δ = 2.8 nm, and L = 6.4 nm from Lim et al. [6]. The black dotted-line indicates measured k_{ph} at 300 K. (b) k_{ph} of Si NWs with different d as a function of T. *Lines or blue text in the legend represent simulated k_{ph} with GA function for SR. Symbols or black text are the experiments [1,6].*

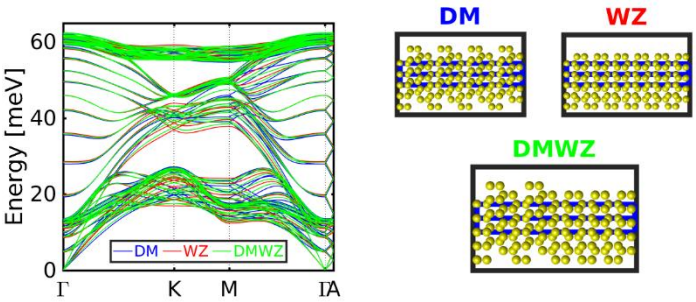

Fig.2: Left panel: DFT phonon band structures of bulk DM, WZ, and DMWZ lattices. Right panel: Hexagonal structures along the ⟨111⟩ *direction of DM and the* ⟨0001⟩ *direction of WZ. The blue solid lines are unit cells used for the computation of bulk phonon band structures with the same number of atoms in each cell.*

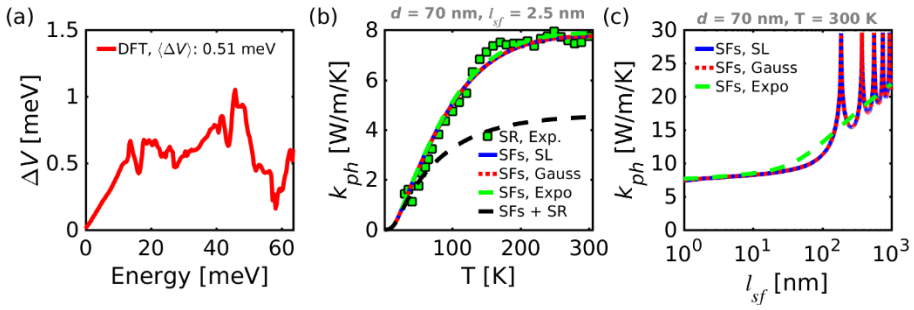

Fig.3: (a) Energy difference between DM and WZ phonon band structures as a function of phonon energy. The two (three) smallest cubic unit cells of DM (WZ) in ⟨111⟩ *(*⟨0001⟩*) direction are chosen with* 401×101×101 ***q****-point sampling. (b) k_{ph} of Si NWs with different l_{sf}-distributions, i.e. super-lattice (SL), Gaussian (Gauss) with standard deviation (σ) equal to 0.5 nm, exponential (Expo) as function of* T. *The black-dashed line is simulated k_{ph} of Si NW with SFs (exponential distribution of l_{sf}) and SR (d = 70 nm, Δ = 2.8 nm, and L = 6.1 nm). The green-square symbols are measured k_{ph} of a Si NW with d = 70 nm, Δ = 2.8 nm, and L = 6.4 nm from Lim et al. [6]. (c) k_{ph} of Si NWs with different distributions of SFs as function of l_{sf} at room temperature.*