Atomistic modeling of the phonon dispersion in free-standing $\langle 100 \rangle$ Si nanowires

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Introduction: Nano-structured semiconductor devices play a vital role in areas ranging from CMOS [1] to thermo-electricity [2]. The finite extent and increased surface to volume ratio in the nano-structured devices result in very different phonon dispersions compared to the bulk materials. This work investigates the effect of geometrical confinement on the phonon dispersion, sound velocity(V_{snd}) and lattice thermal conductivity (κ_l) in $\langle 100 \rangle$ Silicon nanowires (SiNW) using an atomistic force constant based Modified Valence Force Field (MVFF) model.

Modified VFF model: VFF is a force constant based atomic potential calculation method successfully used to model the phonon dispersion in semiconductor materials [3]–[5]. The force constants represent the various kinds of interaction between the atoms. For phonon modeling in non-polar diamond lattices we consider the following interactions (Fig.1), (a) bond-stretching(α), (b) bond-bending(β) (c) bond stretch coupling(γ) (d) bond bending-stretching coupling (δ) and (e) co-planar bond bending coupling(λ).

The dynamical matrix (DM) is assembled using the second derivative of these interactions.The bulk DM has periodic boundary condition along all the directions (Born-von Karman condition, Fig.1). For free-standing SiNW, periodic boundary conditions are applied along the length of the wire (X-dir), whereas the surface atoms (Y-Z dir) are free to vibrate (Fig.3).

Experimental benchmark: The MVFF model has been benchmarked by the calculation of phonon dispersions in different bulk zinc-blende lattices. One of the representative calculation is shown for bulk Si (Fig.2). The model reproduces the important features of the experimental phonon dispersion for Si (at 80K) [6] in the entire Brillouin zone very well. The force constant values for Si are listed in Table.I.

Nanowires phonon dispersions: The phonon dispersion is calculated in free-standing $\langle 100 \rangle$ SiNW where the surface atoms are allowed to vibrate freely (Fig.3). For comparison, the dispersion in SiNWs with cross-section size (W=H) (a) 1.08nm (for comparison purpose[1]), (b) 2.17nm and (c) 3.26nm are shown in Fig.4. The lowest two phonon bands are $\propto q^2$ (flexural modes) while next two are acoustic like ($\propto q$) [9]. The higher sub-bands have mixed acoustic and optical branch like property. The number of sub-bands increase as the wire cross-section size increases (Fig.4) due to increased number of atoms which results in a higher degree of vibrational freedom. The first four vibrational eigen modes are shown in Fig.5 (arrows show the displacement direction). The first two modes (Fig.5 a,b) are the flexural modes responsible for NW bending. The next mode (Fig.5c) is called the longitudinal mode. Mode no. 4, representing the extra degree of rotational movement, is called the torsional mode (Fig.5 d).

Sound velocity variation (V_{snd}): The sound velocity (V_{snd}) is another way to compare the vibrational modes in SiNWs. V_{snd} is obtained using the sub-bands 3 and 4 (transverse and longitudinal modes) of the phonon dispersion, similar to the way suggested for the bulk V_{snd} calculation in [8]. V_{snd} shows a reduction with decreasing wire cross-section size (acoustic mode softening) [9] since the number and the energy of vibrating modes is less for smaller wires[1] (Fig.6).

Lattice thermal conductivity (κ_l) variation: The changing phonon dispersion strongly affects the thermal properties of the ultra-scaled SiNWs. The ballistic κ_l, changes significantly with wire cross-section size[1] [10]. Smaller wires show higher κ_l at higher temperature (Fig.7a). A comparison of κ_l at 300K shows that κ_l reduces as the wire cross-section size increases. An important point to note here is that κ_l is expected to decrease in smaller wires due to the scattering of phonons [10] which has been neglected in the present study.

Conclusions: A modified atomistic force constant based model for the calculation of phonon dispersion in zinc-blende lattices has been developed. This model shows a very good agreement to the experimental bulk phonon data. An important impact of device miniaturization is the presence of surfaces which affect the phonon dispersion in SiNW. The clear demarcation of phonon bands as acoustic and optical branches become vague in SiNW. This affects the sound velocity and lattice thermal conductivity in SiNW which show a large deviation from the bulk values. The geometry dependent calculation of phonon dispersion in small nanowires is therefore important to properly understand the thermal properties.

[1]At such small dimension, bulk-like bonds are no longer satisfied [7]

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TABLE I: Force constants used for Silicon in MVFF model [4]

Sp.const(N/m)	α	β	γ	δ	λ
Silicon	49.4	4.79	0	5.2	6.99

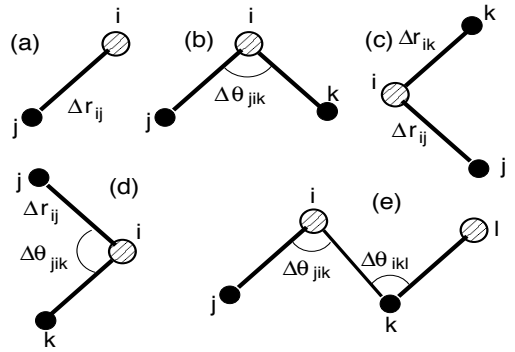

Fig. 1: The short range interactions used for Phonon dispersion calculations. The interactions are (a) Bond-stretching(α), (b) Bond-bending(β) (c) Bond stretch coupling(γ) (d) Bond bending-stretching coupling (δ) (e) Coplanar bond bending coupling(λ).

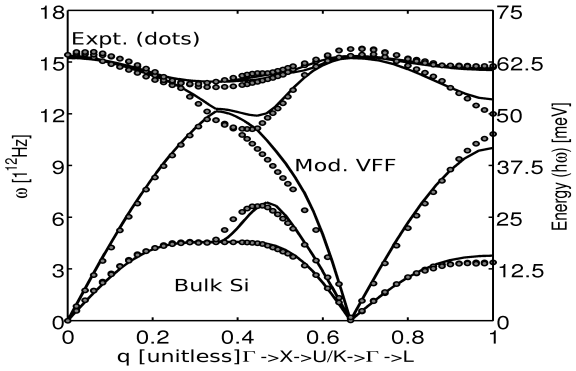

Fig. 2: Bulk Silicon phonon dispersion comparing the MVFF method (lines) and the experimental data (dots) [6] at 80K.

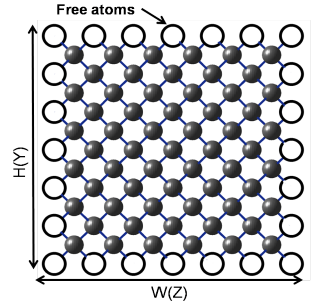

Fig. 3: Projected unitcell structure of a ⟨100⟩ oriented Silicon nanowire. The white atoms (for visual guidance) show the freely vibrating surface atoms. Grey colored atoms are inside the wire

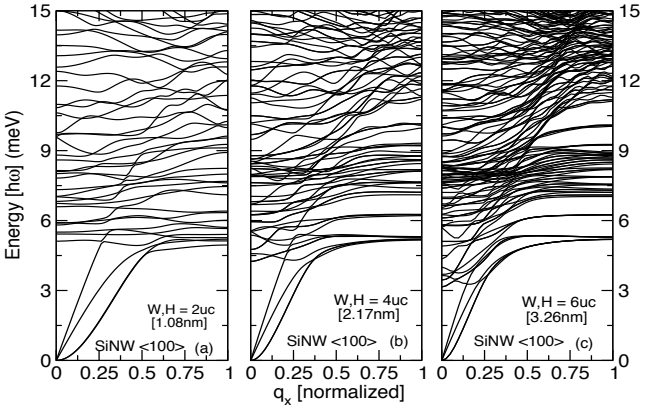

Fig. 4: Effect of cross-section size on the phonon dispersion in ⟨100⟩ SiNW. Wire dimensions are (W = H) (a) 2uc [1.08nm] (b) 4uc [2.17nm] (c) 6uc [3.26nm]. As the cross-section size increases the number of phonon modes within a given energy range increase. (uc = unitcell)

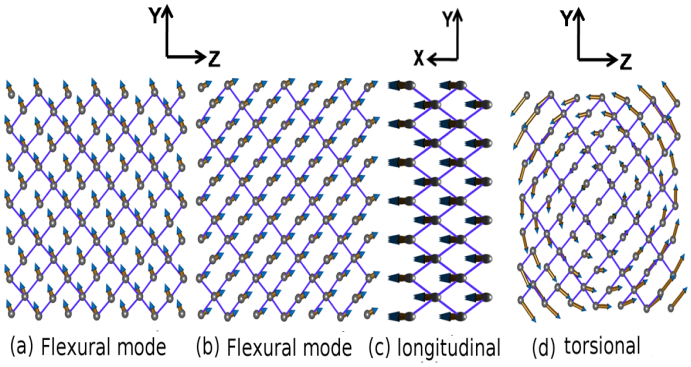

Fig. 5: Eigen modes of atomic displacement shown for a SiNW with W, H = 1.63nm. The atomic displacement shown are at q_x = 0 for (a) mode = 1, (b) mode = 2. These modes are called *flexular modes* which cause bending of the NW.(c) mode = 3, called the *longitudinal mode* causing atomic motion along the wire axis.(d) mode = 4, called the *torsional mode*, observed only in wires, which represents the extra rotational degree of freedom.

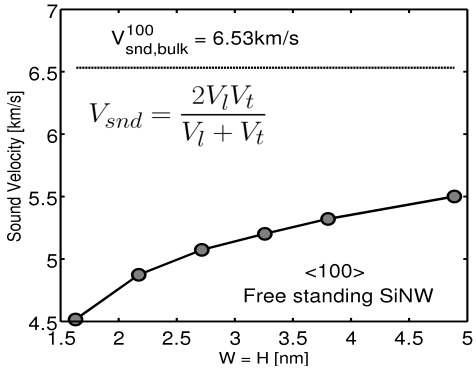

Fig. 6: Sound Velocity (V_{snd}) in ⟨100⟩ SiNW with free boundary. For comparison the bulk V_{snd} is shown along ⟨100⟩ direction [8]. Increasing wire diameter increases the V_{snd} since the vibrational degree of freedom increases.

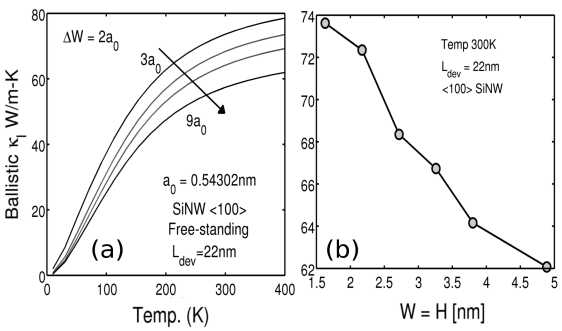

Fig. 7: Variation in the ballistic lattice thermal conductivity (κ_l) (a) with temperature for different cross-section size SiNW and (b) at room temperature (300K) for different NW size. Length of the wire (L_{dev}) is kept at 22 nm.