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Strain effects on the phonon thermal properties of ultra-scaled Si nanowires

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The impact of uniaxial and hydrostatic stress on the ballistic thermal conductance ($\kappa_B$) and the specific heat ($C_v$) of [100] and [110] Si nanowires is explored using a Modified Valence Force Field phonon model. An anisotropic behavior of $\kappa_B$ and isotropic nature of $C_v$ under strain are predicted for the two wire orientations. Compressive (tensile) strain decreases (increases) $C_v$. The $C_v$ trend with strain is controlled by the high energy phonon sub-bands. Dominant contribution of the low/mid (low/high) energy bands in [100] ([110]) wire and their variation under strain governs the behavior of $\kappa_B$, © 2011 American Institute of Physics [doi:10.1063/1.3630228]

The wide application of silicon nanowires (SiNWs) in areas ranging from complementary-metal-oxide-semiconductor transistors,\textsuperscript{1,2} to thermoelectric (TE) devices,\textsuperscript{3} nonvolatile memories,\textsuperscript{4} and solar cells\textsuperscript{5} has made SiNWs an extremely useful nano-electronics device concept. Device properties can be engineered\textsuperscript{6,7} through the introduction of built-in stress by process engineering and by external forces like wafer bending.\textsuperscript{8} Tuning lattice thermal properties using strain can be beneficial for cooling and increasing gain of lasers\textsuperscript{9,10} or improving the efficiency of TE devices.\textsuperscript{11}

Prior work: Strain/stress effects on the thermal conductivity of doped bulk zinc-blende (ZB) semiconductors at low temperatures has been well studied.\textsuperscript{12,13} Most of the bulk studies in ZB semiconductors found decrease in thermal conductivity with tensile strain which is qualitatively attributed to (1) a decrease in the phonon mean free path, (2) an increase in the Debye temperature, and (3) a change in the material stiffness.\textsuperscript{14} The few experimental\textsuperscript{15,16} and theoretical\textsuperscript{17,18,19} efforts that have focused on the strain effects on the thermal properties in nanostructures are either limited to single crystal orientation (mostly [100]) or diffusive phonon transport even in small nanostructures. This work investigates the external strain effects on the thermal properties in ultra-scaled SiNWs in the coherent phonon transport regime where the wire cross-section sizes are comparable to the phonon wavelengths.\textsuperscript{20} ($\lambda_{ph} = h \nu_{phon}/k_B T_{300K} \approx 1$ nm at $V_{sound} = 6.5$ km/s for a 3 nm $\times$ 3 nm [100] SiNW,\textsuperscript{21} where $k_B$ and h are the Boltzmann constant and Planck’s constant, respectively). The thermal properties in this work refer to the phonon dominated lattice properties. The correlation of the thermal properties to the electronic properties are not addressed as they are outside the scope of the present work.

Free-standing SiNWs’ phonon dispersion are studied using the modified valence force (MVFF) model.\textsuperscript{21,22} The MVFF model has been shown to correctly reproduce the strain effects like the Gruneisen parameters\textsuperscript{8,16} and third order elastic constants in bulk Si and Ge.\textsuperscript{18} The same set of Si MVFF parameters\textsuperscript{16,18} are used in this work to model the SiNW phonon dispersion under hydrostatic and uniaxial stress.

The ballistic thermal conductance ($\kappa_B$) across a semiconductor wire maintained under a small temperature gradient $\Delta T$ can be calculated from the calculated phonon dispersion, using the Landauer’s formula\textsuperscript{19} using Eq. (1)\textsuperscript{20,21,22}

$$\kappa_B(\tau, T) = \frac{e^2}{h} \sum_{\epsilon \in [\Delta \epsilon]} \kappa_B^\prime(\epsilon, T),$$

where

$$\kappa_B^\prime(\epsilon, T) = \int_{E_{i,\min}}^{E_{i,\max}} M(\epsilon, E_i) \cdot E_i \cdot \frac{\partial}{\partial T} \left( \frac{1}{e^{|E_i|/k_B T} - 1} \right) dE_i,$$

where $N$ is the number of energy bins in the entire phonon dispersion energy range. The terms $\epsilon$, $M(E)$, $T$, and $e$ are the strain percentage, the number of modes at phonon energy $E$, the temperature, and the electronic charge, respectively. The term $\kappa_B^\prime(\epsilon, T)$ is the contribution to the total $\kappa_B$ of SiNW for $E_{i,\min} \leq E < E_{i,\max}$. This energy resolved representation in Eq. (1) allows for better understanding of the variation in $\kappa_B$ due to strain.

From the calculated phonon dispersion, the constant volume specific heat ($C_v$) at a given $T$ can be calculated as

$$C_v(T) = \left( \frac{k_B}{m_{uc}} \right) \cdot \sum_{n,q} \left[ \frac{E_{n,q}^2}{C_{\nu,n,q}} \cdot \exp \left( \frac{-E_{n,q}^2}{C_{\nu,n,q} k_B T} \right) \right] \cdot \left[ 1 - \exp \left( \frac{-E_{n,q}^2}{C_{\nu,n,q} k_B T} \right) \right] [\text{J/kgK}],$$

where $m_{uc}$ is the mass of the SiNW unitcell in kg. The quantity $E_{n,q}$ is the phonon eigen energy associated with the branch “n” and crystal momentum vector “q”.

SiNW details: Square NWs with width (W) and height (H) = 3 nm with two channel orientations of [100] and [110] are studied (inset of Figs. 1(a) and 1(b)). Hydrostatic deformation (equal deformation along all the directions) and uniaxial deformation (along the wire axis) are applied to these wires varying up to $\pm 2\%$. The outer surface atoms in these NWs are allowed to vibrate freely. Extremely small SiNWs may show significant surface and internal atomic reconstruction\textsuperscript{9,24} or phase change\textsuperscript{25} under strain leading to larger changes in $C_v$ and $\kappa_B$, which are outside the scope of the present study.

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Ballistic thermal conductance $\kappa_I$: In all the SiNWs, $\kappa_I$ is calculated using Eq. (1) at 300 K. $\kappa_I$ increases (decreases) under uniaxial compression (tension) for both the wire orientations. Similar variations in $\kappa_I$ for [100] SiNWs are also observed by Li et al. using non-equilibrium molecular dynamics calculations. The [100] SiNW shows larger variation in $\kappa_I$ under tensile uniaxial deformation compared to the [110] SiNW (Figs. 1(a) and 1(b)). $\kappa_I$ shows a weak hydrostatic stress dependence in [100] SiNW in contrast to the [110] SiNW which shows a decrease (increase) of 2.9% (1.98%) in $\kappa_I$ under 2% compressive (tensile) strain from the unstrained value (Figs. 1(a) and 1(b)). Thus, ultra-scaled SiNWs show an anisotropic variation in $\kappa_I$ under hydrostatic deformation.

Specific heat ($C_v$): Variation in the phonon dispersion under strain also changes the $C_v$ of SiNWs. Compressive (tensile) strain decreases (increases) the $C_v$ in both types of SiNWs (Figs. 2(a) and 2(b)). This variation in $C_v$ is similar to the bulk Si behavior as reported in Refs. 13 and 15. Under hydrostatic stress, the $C_v$ decreases by $\approx 2.7\%$ at 2% compression and increases to $\approx 2.6\%$ at 2% expansion compared to the unstrained $C_v$ value for both the SiNW orientations. Under uniaxial deformation, the variation is $\leq 1\%$ for $\pm 2\%$ strain for both wire orientations (Figs. 2(a) and 2(b)). Hence, $C_v$ variation is isotropic under strain in ultra-scaled SiNWs.

Reason for the variation in $\kappa_I$: To understand the variation in $\kappa_I$ with strain, the energy dependent contributions are analyzed using Eq. (1). The entire phonon spectrum is grouped into three energy ranges: (1) $E_L$ ("low" bands), (2) $E_M$ ("mid" bands), and (3) $E_H$ ("high" bands) (see Fig. 3(a)). These bands show variable contributions under strain which determine the overall effect on $\kappa_I$ (Table I).

Under uniaxial strain, in [100] SiNW, the contribution to $\kappa_I$ is mainly from $E_L + E_M$, which decreases from $\approx 88\%$ under compression (Cm) to $\approx 84\%$ under tension (Tn) (Fig. 3(b)), whereas in [110] SiNW, the contribution to $\kappa_I$ is mainly from $E_L + E_H$, which reduces from $\approx 59\%$ (Cm) to $\approx 54\%$ (Tn) (Fig. 3(d)). Under hydrostatic strain, in [100] SiNW, main contribution to $\kappa_I$ is from $E_M$, which reduces from $\approx 56\%$ (Cm) to $\approx 45\%$ (Tn) (Fig. 3(e)), while in [110] SiNW, main contribution to $\kappa_I$ is from $E_L + E_H$, which...
Sake of brevity. The observed trends in the lattice thermal and [110] SiNWs show almost no variation in the energy bands decide the strain behavior of C. Under strain; however, C shows an isotropic behavior. Similar contribution for [100] SiNW and low/high energy contributions (Figs. 4(b) and 4(c)). The contribution increases from Cm to Tn in the E range varies considerably as shown in Fig. 4. Under uniaxial stress, both [100] and [110] SiNWs show almost no variation in the E range and minute variation in the E range(Figs. 4(a) and 4(c)). The contribution increases from Cm to Tn in the E range which governs the C trend under uniaxial strain (Fig. 2). Under hydrostatic stress, contribution from the E range increases from Cm to Tn, but in a much larger magnitude compared to uniaxial stress, for both the wire orientations (Figs. 4(b) and 4(d)). This explains the larger variation in C under hydrostatic stress (Fig. 2). Thus, the higher energy bands decide the strain behavior of C under strain, for ultra-scaled SiNWs.

Conclusions and outlook: The impact of strain on the thermal properties of ultra-scaled SiNWs has been provided. The ballistic thermal conductance behaves an-isotropically under strain; however, C shows an isotropic behavior. Similar strain behavior for lattice thermal properties are obtained in SiNWs with W = H up to 6 nm, which are not shown for the sake of brevity. The observed trends in the lattice thermal properties can be understood by the different types of contribution of phonon modes in different energy ranges. The behavior of C in SiNWs is similar to bulk Si; however, C variation is very different from bulk Si. Under the low stress condition, hydrostatic strain can be beneficial in engineering C and uniaxial stress for engineering C for cooling lasers. However, high external strain (|< 2%|) field may be needed to engineer C to improve the efficiency of TE devices. The presence of surface roughness, phonon-phonon and phonon-electron scattering may reduce the values of C; however, the trend with strain is expected to remain the same.

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TABLE I. Value of band contribution to C under strain (Fig. 3). Variation shown from compression (Cm) to tension (Tn) for uniaxial (Un) and hydrostatic (Hy) strain for both SiNW orientations (Or).

<table>
<thead>
<tr>
<th>Strain, (Or)</th>
<th>Ei (meV)</th>
<th>k(L) (0-22)</th>
<th>k(M) (22-44)</th>
<th>k(H) (44-65)</th>
<th>Dominant band</th>
<th>Cm to Tn</th>
</tr>
</thead>
<tbody>
<tr>
<td>Un, [100]</td>
<td>36%–34%</td>
<td>52%–50%</td>
<td>13%–13%</td>
<td>L,M</td>
<td>↓</td>
<td></td>
</tr>
<tr>
<td>Hy, [100]</td>
<td>32%–37%</td>
<td>56%–45%</td>
<td>11%–16%</td>
<td>M</td>
<td>↓</td>
<td></td>
</tr>
<tr>
<td>Un, [110]</td>
<td>49%–46%</td>
<td>42%–46%</td>
<td>10%–8%</td>
<td>L,H</td>
<td>↓</td>
<td></td>
</tr>
<tr>
<td>Hy, [110]</td>
<td>45%–48%</td>
<td>45%–44%</td>
<td>7%–10%</td>
<td>L,H</td>
<td>↑</td>
<td></td>
</tr>
</tbody>
</table>

FIG. 4. (Color online) Variation in CV with phonon energy bands under various conditions. 3 nm x 3 nm [100] SiNW with (a) uniaxial stress, (b) hydrostatic pressure. 3 nm x 3 nm [110] SiNW with (c) uniaxial stress, (d) hydrostatic pressure. The higher sub-bands show larger variation in CV contribution compared to the lower energy sub-bands.

Increases from ~52% (Cm) to ~58% (Cm). These details are also summarized in Table I. Thus, low/mid energy contribution for [100] SiNW and low/high energy contribution for [110] SiNW explains the anisotropic nature of C.

Reason for C variation: Under the action of strain the contribution of the phonon bands in E range varies considerably as shown in Fig. 4. Under uniaxial stress, both [100] and [110] SiNWs show almost no variation in the E and E range and minute variation in the E range (Figs. 4(a) and 4(c)). The contribution increases from Cm to Tn in the E range which governs the C trend under uniaxial strain (Fig. 2). Under hydrostatic stress, contribution from the E range increases from Cm to Tn, but in a much larger magnitude compared to uniaxial stress, for both the wire orientations (Figs. 4(b) and 4(d)). This explains the larger variation in C under hydrostatic stress (Fig. 2). Thus, the higher energy bands decide the strain behavior of C under strain, for ultra-scaled SiNWs.

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