Monte Carlo Simulation of Phonon Transport

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Silicon Nanowires – Efficient TE Materials

Thermal Conductivity in Silicon Nanowires

Thermal Conductivity in Silicon Nanowires

Confined Acoustic Phonon Spectrum

Why confined?
Due to acoustic mismatch between Si and SiO₂ – severe when confined more

SiO₂ is acoustically soft
Acoustic impedance mismatch \( \zeta = \rho v_s \) mismatch between Si & SiO₂ is \( \sim 40 \% \)

Solve elastic continuum equation with free-standing boundary conditions (FSBC):
Normal component of stress tensor vanishes at interfaces

\[ T_{ij} n_j \bigg|_s = 0 \]

M. Dutta et al., Int. J. High Speed Electronics and Systems 9, 1 (1998)
Confined Acoustic Phonons $\rightarrow$ Slower Phonons

Flattened dispersion $\rightarrow$ lower group velocity

Phonon confinement insufficient to explain two orders of magnitude reduction in thermal conductivity
Thermal Conductivity – Roughness Dependence

Bulk Si → SiNWs: Two orders of magnitude reduction in thermal conductivity

Why Monte Carlo for Phonons

- Normal (N) processes do not offer resistance because there is no change in direction
  \[ \vec{k}_1 + \vec{k}_2 \iff \vec{k}_3 \]

- Umklapp (U) processes offer resistance to phonons because they turn phonons around
  \[ \vec{k}_1 + \vec{k}_2 \iff \vec{k}_3' \pm \vec{G} \]

N processes change the phonon distribution \(\rightarrow\) indirectly affect the thermal conductivity
Why Monte Carlo for Phonons

Can treat the actual surface without using a specularity parameter.

\[ \Delta = 0.25 \text{ nm} \]
\[ \lambda = 2.5 \text{ nm} \]

A good way to capture phonon localization and the particular features of a given surface better than specularity parameter

When solving the BTE – ensemble Monte Carlo (EMC) technique is the state-of-the-art

Utilizing random numbers to determine
- how long does a particle fly between scattering events
- what scattering mechanism to choose
- how to update momentum afterwards

Very robust and versatile
Dispersion Approximation

\[ \omega_q = \omega_o + v_s q + cq^2 \]


<table>
<thead>
<tr>
<th></th>
<th>( \omega_o ) ( 10^{13} ) rad/s</th>
<th>( v_s ) ( 10^5 ) cm/s</th>
<th>( c ) ( 10^{-3} ) cm²/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>LA</td>
<td>0.00</td>
<td>9.01</td>
<td>-2.00</td>
</tr>
<tr>
<td>TA</td>
<td>0.00</td>
<td>5.23</td>
<td>-2.26</td>
</tr>
<tr>
<td>LO</td>
<td>9.88</td>
<td>0.00</td>
<td>-1.60</td>
</tr>
<tr>
<td>TO</td>
<td>10.20</td>
<td>-2.57</td>
<td>1.11</td>
</tr>
</tbody>
</table>
Dispersion Approximation

Heat one end, let phonons diffuse, wait for steady state temperature gradient to be established, and from Fourier’s law determine the thermal conductivity.

Phonon Initialization: Number of Phonons

\[ N = V \sum_{p=LA,TA} \sum_{q} \left( \langle n_{q,p,T} + \frac{1}{2} \rangle \right) \]

\[ \langle n(q,p,T) \rangle = \frac{1}{\exp\left( \frac{\hbar \omega_p, q}{k_B T} \right) - 1} \]

\[ N = V \sum_{p=LA,TA} \sum_{i=1}^{N_w} \left[ \frac{1}{\exp\left( \frac{\hbar \omega_i}{k_B T} \right) - 1} \right] \frac{q_{i,p}^2}{2\pi^2 v_{i,p}} g_p \Delta \omega \]

10 x 10 x 10 nm\(^3\) cell has \(\sim 10^5\) phonons

\[ \tilde{N} = N / W_t. \]

Phonon Initialization: Phonon Attributes

\[ N = V \sum_{p=LA,TA} \sum_{i=1}^{N_w} \frac{1}{\exp\left(\frac{\hbar \omega_i}{K_B T}\right) - 1} \frac{q_{i,p}^2}{2\pi^2\nu_{i,p}} g_p \Delta \omega \]

- Frequency
- Polarization
- Group Velocity
- Direction \((q_x, q_y, q_z)\)
- Position \((x, yz)\)
Phonon Initialization: Frequency

Frequency is found from the cumulative number density function

\[ F_i = \sum_{k=1}^{i} \frac{N_k}{\sum_{k=1}^{N_\omega} N_k} \]

- Pick a random number \( R \)

\[ F_{i-1} \leq R \leq F_i \]

- Select \( \omega \) from the \( i^{th} \) spectral interval
Phonon Initialization: Polarization

Polarization is found from the ratio of LA to TA phonons in a particular spectral interval

\[ P_i(LA/TA) = \frac{N_i(LA)}{N_i(LA) + N_i(TA)} \]

- Pick a random number \( R \)

\[ R < P_i(LA/TA) \]

*polarization* \( p = LA \) else \( p = TA \)
Phonon Initialization: Group Velocity and Wavevector

Group velocity and magnitude of wavevector can be found from the dispersion

\[ \omega_q = \omega_o + v_s q + cq^2 \]

Direction of wavevector - isotropic

\[ \hat{s} = \begin{pmatrix} \sin \theta \cdot \cos \psi \\ \sin \theta \cdot \sin \psi \\ \cos \theta \end{pmatrix} \]

\[ \psi = 2\pi R_2, \cos \theta = 2R_1 - 1 \]
Phonon Initialization: Position

Phonons in a cell are distributed isotropically

Position of $n^{th}$ phonon in $c^{th}$ cell

$$r_{n,c} = r_c + L_x R_1 i + L_y R_2 j + \frac{L_z}{n_z} R_3 k$$

$R_1$, $R_2$, and $R_3$ are random numbers
$L_x$, $L_y$, and $L_z$ are dimensions of the device
$n_z$ is the number of cells
Phonon Initialization: Energy of Cell

Energy of the cell should automatically be in accordance to the cell temperature

\[ E = V \sum_{p=LA,TA} \sum_{i=1}^{N_w} \left[ \frac{\hbar \omega_i}{\exp\left(\frac{\hbar \omega_i}{K_B T}\right) - 1} \right] \frac{q_{i,p}^2}{2 \pi^2 v_{i,p}} g_p \Delta \omega \]

- Check for consistency between \( N, E, \) and \( T \)
- Find \( T \) from *numerical inversion of \( E \) (of each cell)* and check if it corresponds to the initialization temperature
Phonon Diffusion

• Let the phonons diffuse with their initial velocities and track their position.

• If the phonon crosses a cell, delete it from that cell and assign the new cell number.

• After each time step, calculate the temperature from the net new energy of each cell.

• If a phonon reaches an end cell, delete it from the simulation domain.

• Reinitialize the phonons in the end cells after each $dt$. 
Ballistic steady state temperature is given by the Stefan-Boltzmann law of blackbody radiation:

$$T_{ss}^B = \left[\left(\frac{T_H^4}{4} + \frac{T_L^4}{4}\right)/2\right]^{1/4}$$
Phonon Monte Carlo Transient Simulation
Phonon-Boundary Diffuse Scattering

- Phonon that underwent a scattering at the boundary is deleted and a new phonon is emitted from the boundary.

Direction of wavevector – isotropic (normal to the surface)

\[
\hat{s} = \left(\begin{array}{c}
\sin \theta \cdot \cos \psi \\
\sin \theta \cdot \sin \psi \\
\cos \theta
\end{array}\right)
\]

\[\theta = \sin^{-1}(R_1)\]

\[\psi = 2\pi R_2\]

Phonon Scattering

• Phonon that underwent scattering is deleted and a new phonon is created from new distribution function weighted by the scattering rate.

• Phonons that underwent a U scattering are replaced by phonons which have a new direction.

• Phonons that underwent a N scattering are replaced by phonons with same direction but different magnitude.

• Phonon-impurity/isotope scattering is treated as isotropic.
Phonon Reinitialization

Frequency is found from the cumulative number density function weighted by scattering probability.

More LA phonons

T = 300K

Important for conserving the energy

Phonon Monte Carlo Transient Simulation

Thermal Conductivity

Flux crossing two adjacent cells in steady state

\[ \Phi = \frac{W_t}{dt} \sum_{i=1}^{N_c} \bar{h}_i \omega \frac{q_z}{|q|} \]

Thermal conductivity is calculated from Fourier’s law

\[ \kappa = \frac{1}{A} \frac{\Delta L}{\Delta T} \Phi \]
Bulk Silicon Thermal Conductivity

Limitation of Diffuse Boundary Scattering


Surface Roughness Inclusion in Monte Carlo

Can treat the actual surface without using a specularity parameter.

\[ \Delta = 0.25 \, nm \]
\[ \lambda = 2.5 \, nm \]


A good way to capture phonon localization and the particular features of a given surface \( \Rightarrow \) better than specularity parameter.
Transient Results

Thermal Conductivity: Roughness Dependence

- $\kappa_\parallel$ is more than an order of magnitude lower than that in bulk due to strong boundary scattering of phonons.
- Decreases with increase in rms.

$\kappa_\parallel_{\text{bulk}} = 148 \text{ Wm}^{-1}\text{K}^{-1}$
Thermal Transport Quasi-Balistic Phonons

![Graphs showing temperature and energy over time with notes on good saturation and length increase.]

Good saturation

Increase the length
Thermal Transport: Things to Look For

Losing phonons

Bug in the code
Thermal Transport: Things to Look For

10x phonon-phonon scattering

Losing phonons but not as much as before

Bug in the code
Thermal Transport: Things to Look For

Worse than before

Losing phonons

Only boundary scattering

Bug in the randomization after boundary scattering
Thermal Transport: Things to Look For

Losing more phonons than that are injected
By changing the dispersion, the algorithm can be easily adapted to calculate the thermal conductivity of different semiconductors.

GaN Nanowires for Thermoelectric Applications
A. Davoody 3:30 Thursday
Monte Carlo simulation of phonon transport can be used to account for the large reduction in thermal conductivity in silicon nanowires

- Roughness inclusion as in electron transport
- Can be adapted to other semiconductors


