Monte Carlo Modeling of Heat Generation in Silicon Nanostructures

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Project Goals

- Understanding of heat generation and transport at nanoscales, i.e. dimensions less than the phonon mean free path ($\Lambda$)
- “Granularity” of energy transport
- Study both 3D and 2D problems
- Apply in context of nano-devices and nano-thin films
Nanoscale Heat Transport

Heat diffusion equation ($D \gg \Lambda$)

$$C_s \frac{\partial T}{\partial t} = \nabla \cdot (k_s \nabla T) + Q''$$

Phonon Boltzmann Transport Equation (BTE) ($D < \Lambda$)

$$\frac{\partial e''}{\partial t} + \bar{v} \cdot \nabla e'' = \frac{e''_{eq} - e''}{\tau_{phon}} + Q'''$$

$$e'' = \text{phonon \ energy \ density}$$

$$Q''' = \text{electron} - \text{phonon \ energy \ density \ transfer \ rate}$$

<table>
<thead>
<tr>
<th>Year</th>
<th>Feature Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>1999</td>
<td>180 nm</td>
</tr>
<tr>
<td>2001</td>
<td>150 nm</td>
</tr>
<tr>
<td>2003</td>
<td>130 nm</td>
</tr>
<tr>
<td>2006</td>
<td>100 nm</td>
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</tbody>
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$\Lambda \sim 300 \text{ nm}$ in Silicon at 300 K
Sub-Continuum Heat Generation

Small heat source ($D \ll \Lambda$ phonons)

$\Lambda = 300$ nm (bulk Si)

$\Lambda \sim t_{si} < 300$ nm

Reduced number of collisions near small heat source cannot maintain equilibrium, $T \uparrow$

Not all phonons are created equal
Joule Heating Energy Transfer

High Electric Field

Hot Electrons (Energy E)

E > 60 meV
\( \tau \sim 0.1 \text{ps} \)

E < 60 meV
\( \tau \sim 0.1 \text{ps} \)

Optical Phonons

\( (v_{\text{op}} \sim 1000 \text{ m/s}) \)

Acoustic Phonons

\( (v_{\text{ac}} \sim 7000 \text{ m/s}) \)

\( \tau \sim 4 \text{ ps} \)

\( \tau \sim 1 \text{ ms}^{-1} \text{s} \)

Heat Conduction In Package

Graph showing temperature and frequency relationship with some data points.
Peak Device Temperature Scaling

- $Q' = I \cdot V$
- Simple hot spot T model ($Q' \rightarrow$ optical phonons)
- Decreasing voltage/power as devices scale down
- Expect T rise due to localization of power density

![Diagram showing temperature increase ($\Delta T$) and power ($Q'$) vs. channel length (L)].
Heat Generation with Monte Carlo

- Electrons treated as semi-classical particles, not as “fluid”
- Drift (free flight), scatter and select new state
- Full information about phonon generation (optical vs. acoustic, \( q, \omega \))
- Reasonable speed ~ 50 \( \mu \)sec CPU time per particle per psec on modern desktop
Silicon Electron Energy Bands

- May ignore impact ionization at low $V_{dd}$
- Analytic band approximation below $\sim 1$ eV
“Fixed-field” MC Implementation

- Analytic, non-parabolic bands ($V_{dd} \leq 1.1$ V)

\[ E(1 + \alpha E) = \frac{\hbar^2}{2} \left( \frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z} \right) \]

- Inelastic acoustic and optical phonon scattering

\[ \Gamma(k) = \frac{2\pi}{\hbar} |M(k)|^2 g(E_k \pm \hbar\omega_q) \]

- 20,000 simulated “super-particles”

\[ \Rightarrow 10^{20} \ (1/cm^3) \ real \ electrons \]

- Post-processor to electron device solver
MC Code Complexity

- Integrate acoustic scattering rates using FULL phonon dispersion relation
- Include both TA and LA phonons
- Include all 6 known intervalley phonons
- Use deformation potentials extracted from full-band MC
LA vs. TA Phonon Scattering

- Traditional MC lumps LA and TA scattering


\[
\Xi_{LA} = \Xi_d + \Xi_u \cos^2 \theta \quad \Xi_{TA} = \Xi_u \sin \theta \cos \theta
\]

- ... not known with much certainty

shear: \( \Xi_u \approx 10 \text{ eV} \) (also 8.8, 8.4, 9.2 eV)

dilation: \( \Xi_d \approx 1 \text{ eV} \) (also 1.2, 1.13, 5, 11.7 eV)

- Most recent values  (Fischetti & Laux, *J. Appl. Phys.* 1996)
Average LA, TA Def. Potentials

\[ D_{TA} = \sqrt{\langle \Xi_{TA}^2 \rangle} = \frac{\sqrt{\pi}}{4} \Xi_u \]

\[ D_{LA} = \sqrt{\langle \Xi_{LA}^2 \rangle} = \left[ \frac{\pi}{2} \left( \Xi_d^2 + \Xi_d \Xi_u + \frac{3}{8} \Xi_u^2 \right) \right]^{1/2} \]

 Gems  Averaged values: \( D_{LA} = 8.7 \text{ eV}, \ D_{TA} = 4.4 \text{ eV}, \)
\( v_{LA} = 9000 \text{ m/s}, \ v_{TA} = 5300 \text{ m/s} \)
**Intervalley Phonon Scattering**

\[ k' = k \pm q + G \]

- **Intravalley** ~ acoustic, \( E < 60 \text{ meV} \)
- **Intervalley** ~ optical (f and g type) inelastic
- Does g-phonon at 0.3G (LO 730 K) dominate?
Computed Phonon Generation

Near-full band MC complexity for analytic-band MC speed – towards a device designer’s MC?
Confined Electrons and Phonons

- Electro-thermal transport in ultra-thin silicon films ($t_{si} \sim 5$ nm): role of electron and phonon confinement
- Great electrostatic channel control
- 1-D electron and phonon transport along channel
- Electron (and phonon!) quantum confinement
Heat Generation in 10 nm Device

Compare $W=J \cdot E$ (from nanoMOS 2.0) with heat from net collected phonon emissions of Monte Carlo run
Conclusions

- Not all phonons created equal
  - fast: Brillouin zone-center acoustic
  - slow: optical, zone-edge acoustic

- Phonon bottleneck problem

- Fast analytic-band MC code provides complexity for future ($V_{DD} \leq 1.1$ V) nano-device technologies

- Transport properties different in 2D