Introduction to Thermal Transport

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Objectives

• Identify reasons that heat transport is important

• Describe fundamental processes of heat transport, particularly conduction

• Apply fundamental ideas and computer simulation methods to address significant issues in thermal conduction in solids
Many Thanks to ...

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Part 1: Fundamentals
Thermal Transport: Why Do We Care?
Heat Shield: Disposable space vehicles

Apollo 10 Heat Shield

Cross-section of Mercury Heat Shield

Ablation of polymeric system
Heat Shield: Space Shuttle

Heat Resistant Tiles
- Layer of powdered tetrasilicide and borosilicate glass
- Can withstand heat of 1260 degrees Celsius
- More than 20,000 tiles coat the shuttle's surfaces
- Made of low density, high purity silica fibre
Thermal Barrier Coatings for Turbines
Heat Generation in NanoFETs

- Scaling → Localized heating → Phonon hotspot
- Impact on ESD, parasitic resistances?

Y-K. Choi et al., EECS, U.C. Berkeley

D ~ 20 nm
Q'' ~ $10^{10}$ eV/nm$^3$/s
Thermoelectrics

cold junction

<p-type> p-type

<n-type> n-type

hot junctions

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Heat Transfer Mechanisms

Three fundamental mechanisms of heat transfer:

• Convection
• Conduction
• Radiation

- Convection is a mass movement of fluids (liquid or gas) rather than a real heat transfer mechanism (heat transfer is with convection rather than by convection)

- Radiative heat transfer is important at high temperature

- Conduction is heat transfer by molecular or atomic motion
  Heat conduction dominates in solids
Radiation

Planck's Law

\[ E(\lambda, T) = \frac{2hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda kT}} - 1} \]

\[ h = 6.625 \times 10^{-27} \text{ erg-sec} \] (Planck Constant)

\[ k = 1.38 \times 10^{-16} \text{ erg/K} \] (Boltzmann Constant)

\[ c = 3 \times 10^{10} \text{ cm/sec} \] (Speed of Light)

Stefan-Boltzmann Law

\[ E = \sigma T^4 \]

\[ \sigma = 5.67 \times 10^{-8} \text{ Watts m}^{-2} \text{ K}^{-4} \]

Stefan-Boltzmann constant

Wien's Law

\[ \lambda_{\text{max}} = 3 \times 10^6 /T \]

Convection

Transport of energy by motion of atoms

Liquids and Gases

(a)
Thermal Conduction

Why does his tongue stick to a metal pole?

Would it stick to a wooden pole?

*Dumb and Dumber*
What is “Ice”?

The Hot Ice Caper

with

Sam Spade
Diamond vs. Cubic Zirconia

Which is which?

Diamond

Cubic Zirconia

http://wholesale-scales.com
Tools

http://www.sei.co.jp/RandD/itami/e-tool/gif/variety.gif
**Phenomenology of Thermal Conductivity**

Fourier’s Law

\[ J = - \kappa \frac{dT}{dx} \]

- Heat current
- Thermal conductivity

[Image: Diagram showing temperature gradient and heat source]
Thermal Conductivity of Solids

The graph shows the thermal conductivity ($\kappa$, W/mK) of various materials as a function of temperature ($T$, K). Different materials and conditions are represented by distinct lines:

- Tin (c)
- Aluminum
- Diamond
- $\alpha$-Alumina
- Iron
- Graphite (|| to layers)
- Graphite (\perp to layers)
- Uranium
- Pyroceram Glass
- Polycrystalline Sulfur
- Black Phosphorus
- Amorphous Silicon
- Amorphous Selenium
- PVC

The y-axis represents the thermal conductivity, while the x-axis represents temperature in Kelvin (K).
Mechanisms of Thermal Conductivity

Electrical conductivity

\[ \sigma(\text{Cu}) \sim 5 \times 10^5 (\Omega \text{ cm})^{-1} \]

\[ \sigma(\text{diamond}) \sim 10^{-10} (\Omega \text{ cm})^{-1} \]
**Electronic Conductivity and Wiedemann-Franz Law**

Electrons carry energy as they move → transport of heat

\[ \frac{k}{\sigma T} = L_0 \]

- \(k\) – thermal conductivity
- \(\sigma\) – electrical conductivity
- \(T\) – temperature
- \(L_0\) – Lorentz constant

Element | \(k\) (W/mK) | \(\frac{k}{\sigma T}\) (W/mK)
--- | --- | ---
Li | 71 | 2.22 10-8
Na | 138 | 2.23
In | 88 | 2.58
Bi | 9 | 3.53
Al | 238 | 2.14

\[ L_0 = \frac{\pi^2}{3} \left( \frac{k}{e} \right)^2 \]

\(L_0 = 2.45 \times 10^{-8} \text{ W}\Omega/\text{K}^2\)
Heat transport from atomic vibrations

Vibration of spring system similar to vibrations in solids
Harmonic Model

\[ E = \frac{1}{2} kx^2 \]

Simple harmonic solid with one and two atoms in the basis → acoustic and optical phonons
Long Wavelength Longitudinal Acoustic Phonon
Short Wavelength Longitudinal Acoustic Phonon
Longitudinal Optical Phonon
Acoustic vs. Optical

Which has lower energy? Why?
Transverse Phonons

\[ n = 1 \]

\[ n = 2 \]

\[ n = 3 \]

\[ n = N^{1/3} \]
Longitudinal vs. Transverse Phonons

Which has lower energy? Why?
Phonons

http://physics.ucsc.edu/groups/condensed/moseley/simulations

Schematic dispersion curves for diamond
Phonons and Thermal Conductivity

Dominant phonon – Debye solid

\[ f_D = 2.82 \ \text{kT/h} \]
Why is the Thermal Conductivity Finite?

If phonons did not scatter the thermal conductivity would be infinite?
Phonon Scattering Mechanisms

Phonon-phonon
Phonon-defect
Phonon-boundary
Phonon-electron

Macroscale

*****
***
*
Phonon-phonon Scattering

Diamond at 300K
\[ \Lambda \sim 300\text{nm} \]
\[ \lambda_D \sim 30\text{nm} \]

- Usually \( l < \Lambda < L \)
- New physics arises when \( L \) is reduced to nanometers

Sample-size dependent thermal conductivity of single crystal LiF

Blakemore, Solid State Physics
Temperature Dependence

\[ \kappa \sim 1/3 \, c_v \, v \, \lambda \]

Low T
Quantum Solid

\[ C_v \sim T^3 \]

\[ \kappa \sim T^3 \]

High T:
Phonon-phonon scattering

\[ \lambda \sim T^{-\alpha} \]

\[ \alpha \sim 1 \]

\[ \kappa \sim T^{-\alpha} \]
Thermal Conductivity of Solids
Thermal Conductivity and Thermal Diffusivity

\[ k = \rho \ c_p \ \alpha_T \]

- \( \rho \) – density
- \( C_p \) – heat capacity
- \( \alpha_T \) – thermal diffusivity
Thermal Expansion and Thermal Conductivity

• Thermal expansion
  - $\alpha = 0$ for a harmonic solid
    - Thermal expansion is a measure of anharmonicity

• Thermal Conductivity
  - $\kappa = \infty$ for harmonic solid
    - Anharmonicity $\rightarrow$ finite $\kappa$
Anharmonicity: Thermal Expansion and Thermal Conductivity

- Thermal expansion: increases with anharmonicity.
- Thermal conductivity: decreases with anharmonicity.

As anharmonicity increases from low to high:
- Thermal expansion increases.
- Thermal conductivity decreases.

The graph shows a linear relationship between anharmonicity and the properties, with a higher anharmonicity leading to a more pronounced effect on both thermal expansion and thermal conductivity.

The inset diagram illustrates the potential energy function $E(r)$, where $r_0$ represents a critical point. The curve shows different behaviors for smaller and larger values of $\alpha$. For smaller $\alpha$, the potential energy function is steeper, indicating a higher thermal conductivity. For larger $\alpha$, the function is flatter, suggesting a lower thermal conductivity.
Thermal Conductivity and Thermal Expansion

Reasonable correlation between thermal conductivity and thermal expansion.
What About Glasses?

No long-ranged order $\rightarrow$ no phonons $\rightarrow$ How is heat transported?

We will look at amorphous materials later.
Solids have much higher thermal conductivities than liquids.

Low k materials W/mK

- Water 0.6
- Ethylene Glycol 0.25
- PTFE 0.2
- Wood 0.2 – 0.4
- Engine Oil 0.15
- Fiberglass 0.04
- Air 0.03
- Snow 0.05 – 0.25 (T < 0°C)
- Silica Aerogel 0.003

Liquid Na - 72 W/mK
Why Nanoparticles Are Better Than Microparticles

Nanoparticles have about 20 percent of their atoms near the surface, allowing them to absorb and transfer heat efficiently.

Microparticles have most of their atoms far beneath the surface, where they cannot participate in heat transfer.

The relatively large mass of the microparticles can damage the pipe’s wall.

http://www.anl.gov/Media_Center/News/2004/nanofluidsbibg.html
Summary

• Radiation vs. Convection vs. Conduction
• Electronic vs. Phonon Conduction
• Physics of Phonons
• Basic Phenomenology of Thermal Conductivity
Part 2: Case Studies in Thermal Conductivity
Preamble: Introduction to Molecular-Dynamics Simulation
• Treat atoms as structureless spheres

• Write down a form by which the atoms interact, \( V(r) \)

• Solve Newton’s Second Law:
  
  • \( F = ma \)

  • Where \( F = -\nabla V(r) \)
Case Study #1: Thermal Barrier Coatings
Thermal Conductivity of Oxides

[Graph showing the thermal conductivity of various oxides as a function of temperature.]
Approach to determination $\kappa$

- Non-equilibrium: Add and remove heat

$$J = -\kappa \frac{dT}{dz}$$
Steady-State Temperature Profile

\[ J = -\kappa \frac{\partial T}{\partial N} \]

- 20mol% YSZ
- Pure ZrO₂
Temperature and Concentration Dependence of $\kappa$

<table>
<thead>
<tr>
<th></th>
<th>Sim. (W/mK)</th>
<th>Expt. (W/mK)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZrO$_2$</td>
<td>$\kappa=8.92$</td>
<td>$\kappa=8.22$</td>
</tr>
<tr>
<td>(300K)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>YSZ</td>
<td>$\kappa=3.0$</td>
<td>$\kappa=2.3$</td>
</tr>
<tr>
<td>(&gt;500K)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Temperature (K)
- Thermal Conductivity (W/mK)

ZrO$_2$ 4 mol%, 8 mol%, 12, 16, 20 mol%
Phonon Polarization

Energy (meV)

LO, TO, LA, TA

x-polarization

y-polarization

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$f = 1.6 \text{THz}$

Highly polarized - propagon

$\quad f = 3 \text{THz}$

Random polarization - diffusion
Normal Modes in Amorphous Materials

- Propagons transport heat efficiently

- Diffusons less efficient, no directionality

- Energy in locon mode remains localized unless scattered. True insulating state.

Feldman and Allen (PRB 48, 1993)
Chemical vs. Structural Disorder

Si Single crystal

(001) Si GB Superlattice

Amorphous Si

A. Bodapati et al., APL 88 141908 (2006)
New Materials for Thermal Barrier Coatings

Objective
Identify candidate materials for new thermal barrier coatings

Current
Yttria-stabilized zirconia (κ~2 W/m-K)

Performance criteria
Low thermal conductivity
high thermal expansion coefficient (match alloy substrate)
Elastically soft / mechanically compliant (match alloy)
Chemical compatibility
Mechanical integrity
**Fluorite vs. Pyrochlore**

**Fluorite**
- Complete unit cell

MO₂

ZrO₂

**Pyrochlore**
- 1/8 unit cell

A₂B₂O₇

A₂O₃-(BO₂)₂

Unoccupied 8a site

Gd₂Zr₂O₇

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## Comparison with Experiment - Thermal Conductivity

<table>
<thead>
<tr>
<th></th>
<th>$\kappa_{\text{expt}}$ (W/mK)</th>
<th>$\kappa_{\text{simul}}$ (W/mK)</th>
<th>$\kappa_{\text{simul}}/\kappa_{\text{expt}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{La}_2\text{Zr}_2\text{O}_7$</td>
<td>1.56</td>
<td>1.98</td>
<td>1.27-1.32</td>
</tr>
<tr>
<td></td>
<td>1.5</td>
<td>1.5</td>
<td>1.5</td>
</tr>
<tr>
<td>$\text{Nd}_2\text{Zr}_2\text{O}_7$</td>
<td>1.6</td>
<td>1.83</td>
<td>1.14-1.38</td>
</tr>
<tr>
<td></td>
<td>1.33</td>
<td>1.33</td>
<td>1.33</td>
</tr>
<tr>
<td>$\text{Sm}_2\text{Zr}_2\text{O}_7$</td>
<td>1.5</td>
<td>2.09</td>
<td>1.39</td>
</tr>
<tr>
<td></td>
<td>1.5</td>
<td>1.5</td>
<td>1.5</td>
</tr>
<tr>
<td>$\text{Eu}_2\text{Zr}_2\text{O}_7$</td>
<td>1.6</td>
<td>1.99</td>
<td>1.24</td>
</tr>
<tr>
<td></td>
<td>1.6</td>
<td>1.6</td>
<td>1.6</td>
</tr>
<tr>
<td>$\text{Gd}_2\text{Zr}_2\text{O}_7$</td>
<td>1.6</td>
<td>1.91</td>
<td>1.19-1.91</td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>1.1-1.4</td>
<td>1.1-1.4</td>
<td>1.1-1.4</td>
</tr>
</tbody>
</table>
Thermal Conductivity @ 1500K

- varies by factor of 2.2
Analysis

\[ \kappa = \frac{1}{3} C_v \nu \lambda \]

\( \kappa \) - thermal conductivity

\( C_v \) - specific heat = \( 3k_B/a^3 \)

\( \nu \) - speed of sound

\( \lambda \) - mean free path

\[ \lambda/a = \kappa a^2/88k_B \nu \]
Inverse Speed of Sound

A Cation Radius (Å) vs B Cation Radius (Å)

Temperature vs Inverse Speed of Sound (v\(^{-1}\) x 10\(^4\) s/m)

Elements: Ti, R, Mo, Sn, Zr, Pb, La, Pr, Nd, Sm, Eu, Gd, Y, Er, Lu

Temperature Dependence of Inverse Speed of Sound

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Mean Free Path

- varies by ~30%

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Effect of Cation and Oxygen Disorder

Pyrochlore  
No disorder  
$Y_2Zr_2O_7$  
$\kappa = 2.27 \text{ W/m-K}$

YSZ  
Anion and cation disorder  
$(\text{ZrO}_2)_2 - Y_2\text{O}_3$  
$\kappa = 1.96 \text{ W/m-K}$

Disorder decreases thermal conductivity by $\sim 10\%$
• B ion radius largely determine \( \kappa \)
  A ion radius not as important

- Use B ion to determine thermal conductivity

- Use A ion to tune to other design criteria
  - chemical compatibility
  - mechanical stability
**Engineering Better Thermal Barriers?**

Large B is good for
- lower thermal conductivity
- lower bulk modulus
- higher thermal expansion

Large B is bad for
- phase stability

**Thermal expansion coefficient**

**Bulk modulus**
Pyrochlores for Inert Matrix Fuel

Zirconates have low antisite energies $\Rightarrow$ good radiation tolerance


However, zirconates have low thermal conductivity

$\Rightarrow$ composite with higher k material

Can Pyrochlores Be Made Even Better Thermal Barriers?

• How low can thermal conductivity go?

- $\kappa = \frac{1}{3} \ C \nu \ \lambda$
- $\lambda \sim 0.31 - 0.45 \ a$
- nearest neighbor distance $\sim 0.22a$
- further reduction of $\kappa$ by $1/3 - 1/2$ possible

• How can this be accomplished?

- alloying to increase cation and oxygen disorder
- graded compositions, composites
- microstructural control (interfacial resistance)
Case Study #2:  
*Interfacial Thermal Conductivity*
Phonon Scattering Mechanisms

Phonon-phonon  Phonon-defect  Phonon-boundary  Phonon-electron

Macroscale: *****  ***  *
Nanoscale: *  ***  *****
Interfacial (Kapitza) Thermal Resistance

Temperature

J = G_K \Delta T

Three grain boundaries:

• (001) \( \theta = 43.6° \Sigma 29 \)
  – high angle, high energy

• (001) \( \theta = 11.4° \Sigma 101 \)
  – high angle, high energy

• (111) \( \theta = 42.1° \Sigma 31 \)
  – high angle, high energy

Kapitza resistance results in temperature discontinuities at interfaces
Kapitza Conductance in YSZ

\[ k = \frac{k_o}{1 + \frac{k_o R_k}{d}} \]

- \( R_k \) and \( k_o \) are obtained by a 2-parameter fit to \( k(d) \)

- \( G_k = 1/R_k \)

Kapitza Conductance

Kapitza Resistance

**Kapitza Conductance**

YSZ Yang et al. (2002)

Three Si grain boundaries:

- (001) $\theta=43.6^\circ \Sigma 29$
  - high angle, high energy
- (001) $\theta=11.4^\circ \Sigma 101$
  - high angle, high energy
- (111) $\theta=42.1^\circ \Sigma 31$
  - high angle, high energy


- data for nanocrystalline YSZ similar to that for several heterophase systems
Low-Energy, High-Angle GB: (111) $\theta = 42.10^\circ \ \Sigma 31$

$E_{gb} = 0.64 \text{ J/m}^2$

Coordination at GB
$C_3$: 0%
$C_4$: 94%
$C_5$: 6%

$J = G_K \Delta T$

$G_K = 1.53 \text{ GW/m}^2\text{K}$
**Typical High-Energy GB: (001) θ=43.60° (Σ29)**

- $E_{gb} = 1.32 \text{ J/m}^2$
- Coordination at GB:
  - $C_3$: 8%
  - $C_4$: 82%
  - $C_5$: 10%
- $G_K = 0.85 \text{ GW/m}^2\text{K}$
Interface Conductance

\[ J = G_K \Delta T \]

(001) \( \Sigma 29 \), \( \theta = 43.60° \)
- \( E_{gb} = 1.32 \text{ J/m}^2 \)
- \( G_K = 0.85 \text{ GW/m}^2\text{K} \)

(001) \( \theta = 11.42° \), \( \Sigma 101 \)
- \( E_{gb} = 0.91 \text{ J/m}^2 \)
- \( G_K = 1.71 \text{ GW/m}^2\text{K} \)

(111) \( \Sigma 31 \), \( \theta = 42.10° \)
- \( E_{gb} = 0.64 \text{ J/m}^2 \)
- \( G_K = 1.53 \text{ GW/m}^2\text{K} \)

Maiti et al:
- (310) STGB
  - \( G_K = 0.9 \text{ GW/m}^2\text{K} \) @ 575K
- (510) STGB
  - \( G_K = 0.8 \text{ GW/m}^2\text{K} \) @ 575K
High-Frequency LA mode

Acoustic scattering

Diffuse scattering

θ = 43°

Σ

LA

kz = 0.35
Frequency Dependence of Phonon Scattering

Acoustic Mismatch Model

Diffuse Mismatch Model

Transmission

Reflection

Frequency (THz)
Kapitza conductance using MD results for $\alpha(\omega)$

$$\sigma_K (T) = \frac{1}{\Omega} \sum \hbar \omega_{\lambda k} \frac{\partial n(\omega_{\lambda k}, T)}{\partial T} \frac{\partial \omega_{\lambda k}}{\partial k_z} \alpha_{\lambda k}$$

<table>
<thead>
<tr>
<th>$\Sigma K$ (MD)</th>
<th>$\sigma_K$ (computed)</th>
<th>computed/MD</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma 29$</td>
<td>0.855</td>
<td>0.457</td>
</tr>
<tr>
<td>$\Sigma 101$</td>
<td>1.710</td>
<td>0.904</td>
</tr>
</tbody>
</table>

1. Computed results only includes LA, TA modes

2. The $\Sigma 101$ computed result assumes $\alpha(\omega)$ same for TA modes as LA

3. Effects of non-normal incidence not included
**Ultrananocrystalline Diamond (Experiment)**

Measured $\kappa = 12 \text{ W/mK}$

for grain size 3~5 nm at 310K

$\rightarrow G_K = 3 \text{ GW/m}^2\text{K}$

Angadi et al. JAP 99, 114301 (2006)
A Typical Temperature Profile

Tersoff potential: 3-body interactions and naturally incorporates sp³, sp² hybridization

Σ29(001) \( \theta = 43.6^\circ \)
46400 atoms
\(<T>=1000K\)

\( \Delta T = 22.5K \)
\( G_K = 9.7 \text{ GW/m}^2\text{K} \)
Ultrananocrystalline Diamond
(Simulation)

- Average grain size, 3 nm, thickness $2a_0$, mean temperature 300K
- Thermal conductivity 13.8 W/mK

Using $d = 3 \text{nm}$,

\[ \therefore G_K = 4.6 \text{GW/m}^2\text{K} \]
Comparison of Experiment and Simulation

<table>
<thead>
<tr>
<th></th>
<th>$\kappa$ [W/mK]</th>
<th>$G_K$ [GW/m²K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experiment</td>
<td>1-12</td>
<td>3</td>
</tr>
<tr>
<td>Simulation (Polycrystalline)</td>
<td>14</td>
<td>4.6</td>
</tr>
<tr>
<td>Simulation (Grain Boundary)</td>
<td>26</td>
<td>8.5</td>
</tr>
</tbody>
</table>

Note: $d = 3 \text{ nm}$, $\kappa_0 = 2200 \text{ W/mK}$ at room temperature

- Experimental and simulation results compare within the factor of 2.
- $\kappa/\kappa_0 \sim 1\%$
- $G_K$ of diamond is much higher than that of any other materials.
• $G_K$ remains fairly constant over a wide range of angle ($\sim 20^\circ$ to $70^\circ$)

→ Coordination of atoms in the GBs is very similar

• Higher conductance at low angle ($<15^\circ$) because of the sparse distribution of dislocation

• Slight increase near $90^\circ$ because of the symmetry of diamond structure
**Bonding and Interfacial Conductance: Diamond vs. Si**

\[(001) \theta = 43.60^\circ \ (\Sigma 29)\]

Better bonding across the silicon GB should lead to better thermal transport.
Diamond vs. Silicon

(001) \( \Sigma 29 \) Grain Boundary

Si: (001) \( E_{gb} = 1.32 \) J/m\(^2\) \hspace{1cm} G_K = 0.85 \text{GW/m}^2\text{K}

C: (001) \( E_{gb} = 6.09 \) J/m\(^2\) \hspace{1cm} G_K = 8.85 \text{GW/m}^2\text{K}

Conclude: Diamond GBs 10X better conductors of heat than Si GBs

But: \( \kappa \) (diamond) = 2000 W/m-K
\( \kappa \) (Si) = 150 W/m-K

Kapitza length (equivalent thickness of perfect crystal):

\[ \lambda_K = \frac{k}{G_K} \]
Normalize Kapitza Length to Lattice Parameter

Final conclusion: Silicon GBs are better conductors of heat than diamond GBs!
Kapitza length proportional to GB energy

Extended Read-Shockley fit to Kapitza length
Case Study #3
Point Defects
Motivation

- **Phonons** play a dominant role in thermal transport of electric insulators e.g. silicon and many oxides

- Two most important processes:
  - Phonon-phonon scattering
  - Phonon-point defect scattering

- We focus on the phonon scattering from point defects
Classic formula-isotopic effect

\[
[t(f)]^{-1} = A \cdot \left(\frac{\Delta m}{m}\right)^2 \cdot C \cdot f^4
\]

\[
1/t \sim c
\]

\[
1/t \sim f^4
\]

t^{-1} – phonon scattering rate
A – material constant
\(\Delta m\) – mass difference
\(c\) - isotope concentration
\(f\) – frequency

The formula was derived from weak scattering.

Question:
- in what range of frequency
- at what concentration of dopant
the formula is applicable?

Simulation system

Simulation cell:
- Maximum used: $2 \times 2 \times 6000$ unit cells
- $L_z = 6000$ unit cells
  (3.268 µm)
- Diamond-structured Si
- Stillinger-Weber potential

Thickness of doped region $\Delta z$

$\Delta z = z_2 - z_1$ (20 - 300 unit cell)

Dopant concentration $c$

0.078 - 1.56 atom%

Phonon wave packet frequency $f$

1.5 - 13 THz
Simulation system

- Dopants randomly distributed in doped region
- Differ from Si in mass
  \[ M_{\text{dop}} = 4M_{\text{Si}} = 112 \text{ amu (atomic mass unit)} \]
  larger than \( M_{\text{Ge}} \) (72.59 amu)
  - To understand the effects of mass defect
  - To compare with previous simulations of superlattices
Calculation procedure

Four steps:

• structure creation
• initial phonon wave packet generation
  – well-defined longitudinal acoustic phonon
• MD simulation
• energy analysis
Phonon propagation and scattering description at atomic scale

- Incident phonon frequency: 2.96THz
- 1.56% dopants in doped region
- $\Delta z = 200$ unit cell
Energy trapped in the defect region becomes negligible by ~200 ps
Energy analysis

coefficient of reflected energy
\[ R = \frac{E_{\text{reflect}}}{E_{\text{total}}} \]

coefficient of trapped energy
\[ L = \frac{(E_{\text{total}} - E_{\text{reflect}} - E_{\text{tran}})}{E_{\text{total}}} \]

coefficient of transmitted energy
\[ T = \frac{E_{\text{tran}}}{E_{\text{total}}} \]

\[ R + L + T = 1 \]
Time evolution of trapped energy

The higher concentration, the longer time to scatter out.

Physically reasonable results
**Concentration effect**

Basically linear in concentration, but unexplained peak in reflection at 1% - old description

well linear when the concentration is less than 0.3%.

2.96THz
Δz = 200 unit cell

\[1/t \sim c\]

\[\left[ t(f) \right]^{-1} = A \cdot \left( \frac{\Delta m}{m} \right)^2 \cdot C \cdot f^4\]
Mass effect

\[
\left[ t(f) \right]^{-1} = A \cdot \left( \frac{\Delta m}{m} \right)^2 \cdot C \cdot f^4
\]
Frequency effect

T drops quickly with f decreasing. (f < 3.5 THZ)
T reaches minimum around 3.5 THz
Frequency effect

\[ \frac{1}{t} \sim f^\alpha \]

\[ [t(f)]^{-1} = A \cdot \left( \frac{\Delta m}{m} \right)^2 \cdot C \cdot f^4 \]

\( \alpha = 3.82 \) for \( \Delta z = 200 \)

\( \alpha = 5.23 \) for \( \Delta z = 40 \)

compared with classic result

\( \alpha = 4 \)

(assumes Debye DOS)
Phonon density of state for pure Si

0.78% dopant in 2x2x200 unit cell

Transmission coefficient, T

Frequency, THz

DOS

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

0 0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4

total  LAKxy  Lzero  LO  TA  TO
Conclusions

• Combining phonon wave-packet dynamics and MD simulation can provide an effective approach to develop atomic-level view of the scattering of phonons from point defects.

• The energy transmission and reflection coefficients are approximately linear in the dopant concentration.

• The transmission (reflection) coefficient is strongly affected by phonon frequency. At low frequency the order of power is around 4.

\[
[t(f)]^{-1} = A \cdot \left(\frac{\Delta m}{m}\right)^2 \cdot C \cdot f^4
\]
Summary

• Radiation vs. Convection vs. Conduction

• Electronic vs. Phonon Conduction

• Physics of Phonons

• Basic Phenomenology of Thermal Conductivity

• Use of Simulation to Develop Understanding of Phonon-mediated Thermal transport