Introduction to Thermal Transport

Simon Phillpot
Department of Materials Science and Engineering
University of Florida
Gainesville FL 32611

sphil@mse.ufl.edu

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 …

- Patrick Schelling (Argonne National Lab → U. Central Florida)
- Pawel Keblinski (Rensselaer Polytechnic Institute)
- Robin Grimes (Imperial College London)
- Taku Watanabe (University of Florida)
- Priyank Shukla (U. Florida)
- Marina Yao (Dalian University / U. Florida)

Part 1: Fundamentals

Thermal Transport: Why Do We Care?

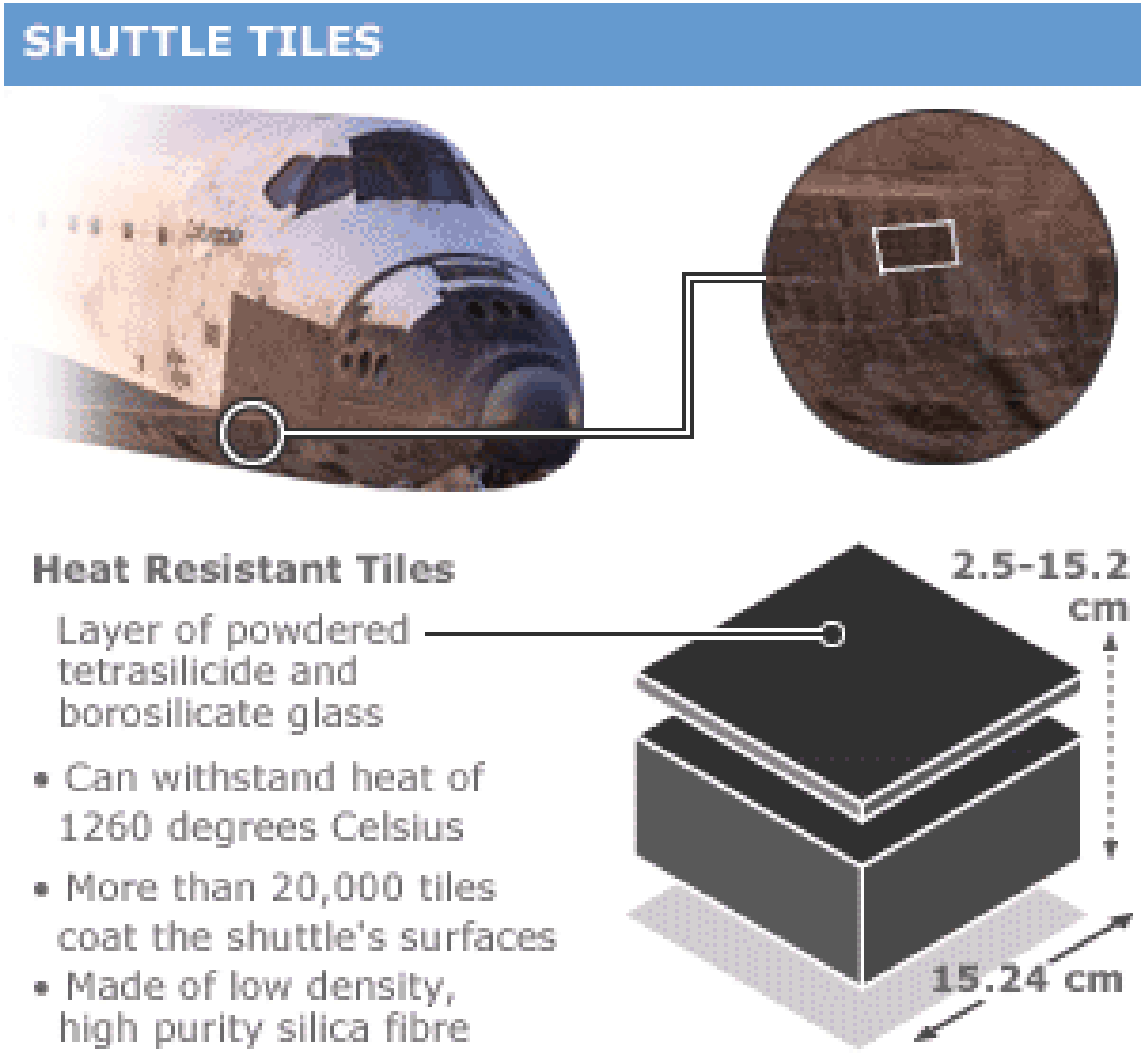
Heat Shield: Disposable space vehicles

Apollo 10 Heat Shield

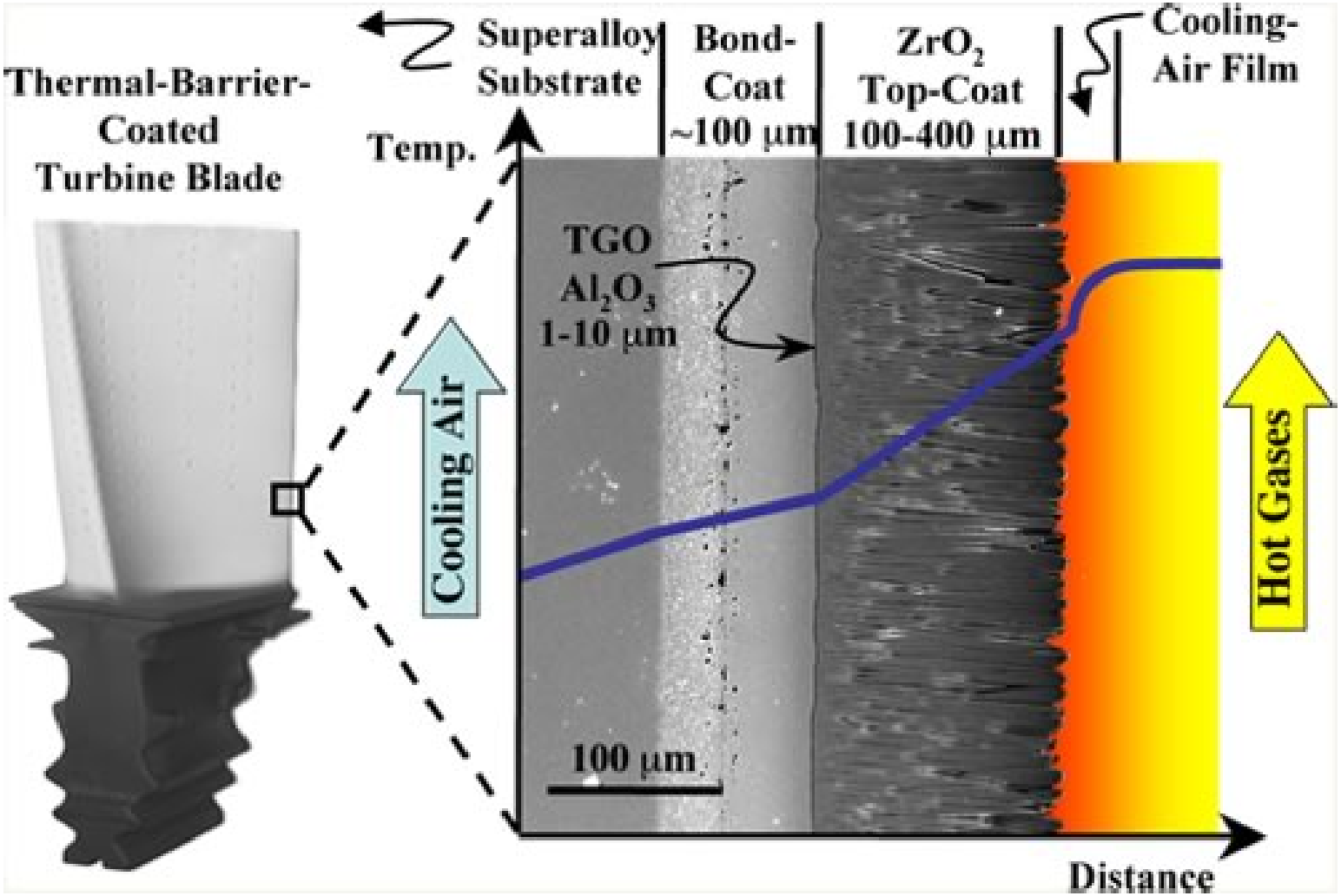
Cross-section of Mercury Heat Shield

Ablation of polymeric system

Heat Shield: Space Shuttle

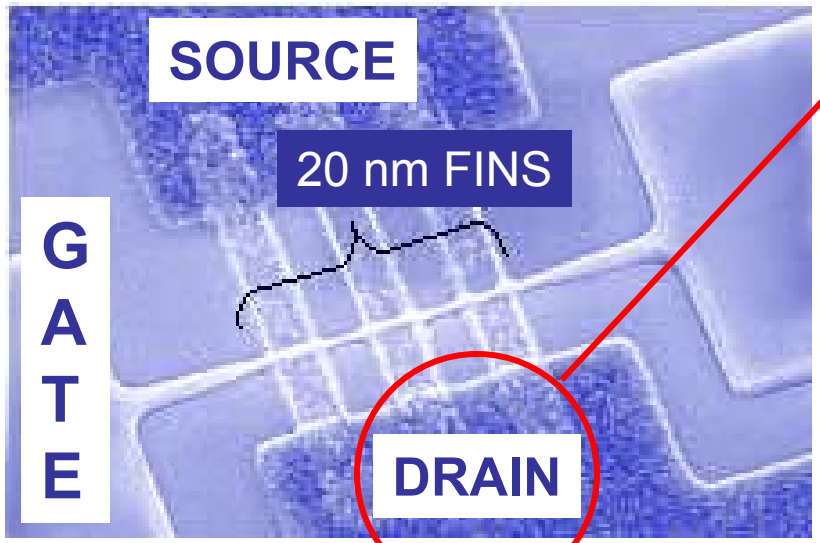


Thermal Barrier Coatings for Turbines

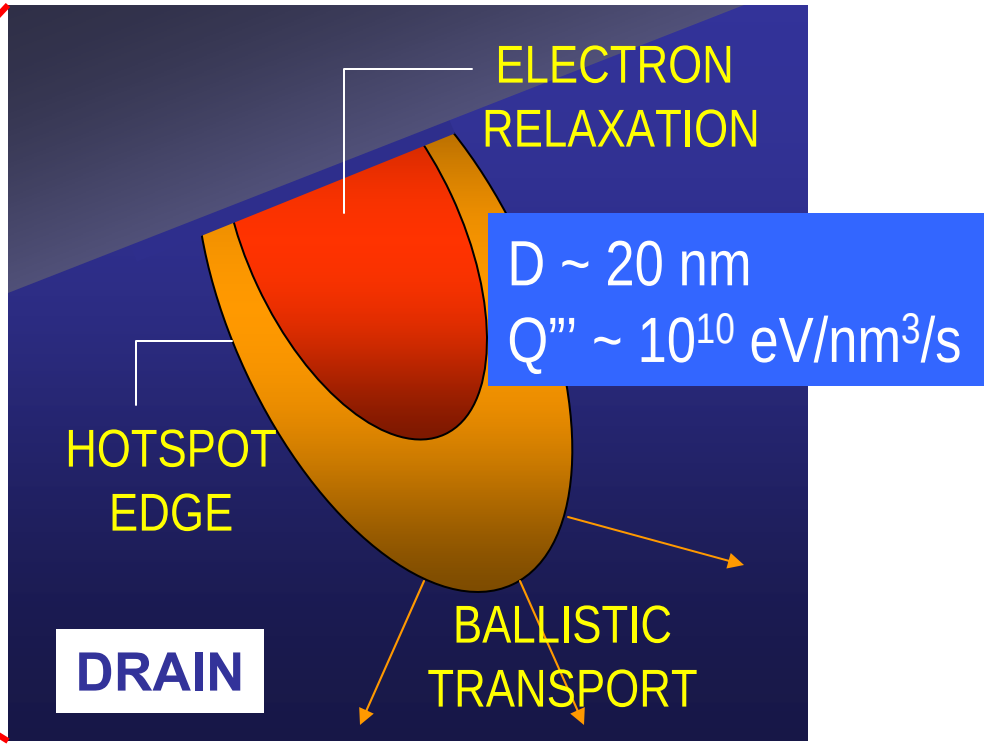


http://www.mse.eng.ohio-state.edu/fac_staff/faculty/padture/padturewebpage/padture/turbine_blade.jpg

Heat Generation in NanoFETs

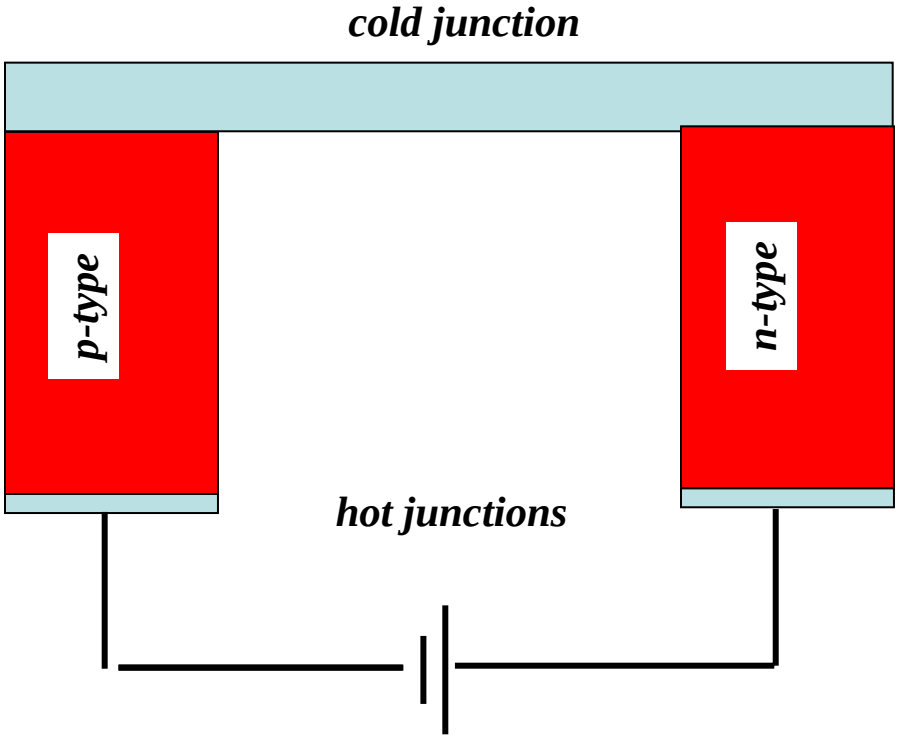


Y-K. Choi et al., EECS, U.C. Berkeley



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

Thermoelectrics



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

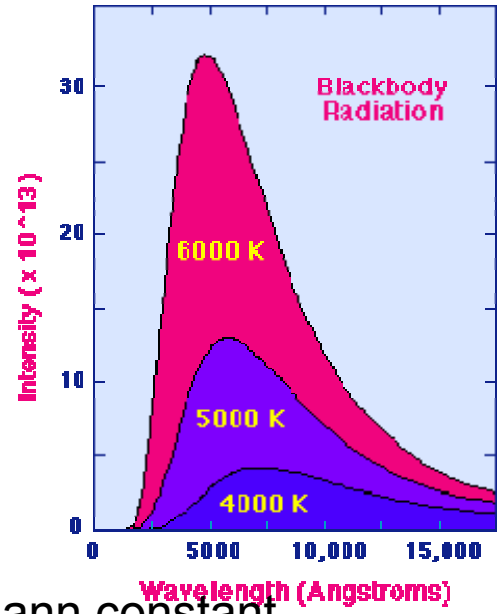
Planck's Law

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

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

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

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



Stefan-Boltzmann Law

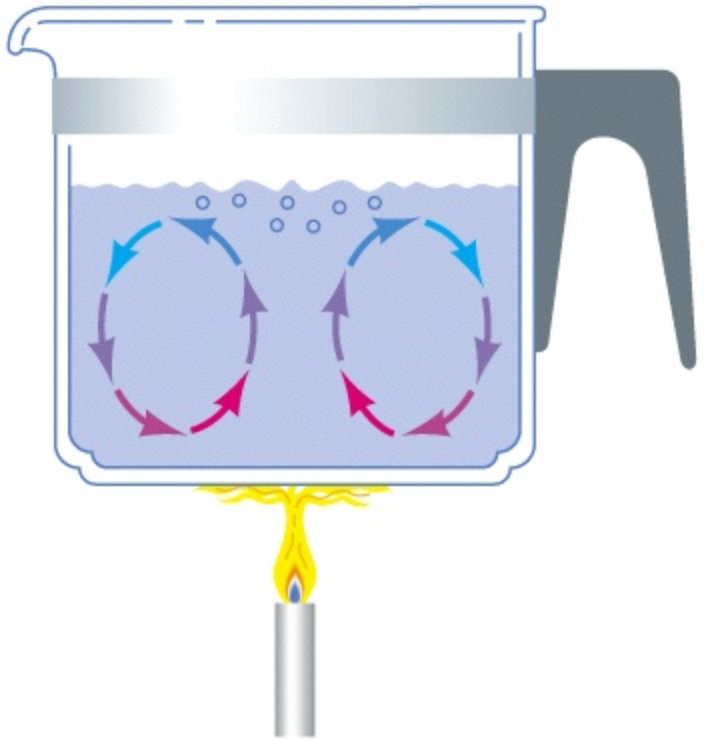
$E = \sigma T^4$ $\sigma = 5.67 \times 10^{-8}$ Watts m^{-2} K^{-4} Stefan-Boltzmann constant

Wien's Law

$\lambda_{max} = 3 \times 10^6 / T$

http://csep10.phys.utk.edu/astr162/lect/light/radiation.html

Convection



(a)

Transport of energy by motion of atoms

Liquids and Gases

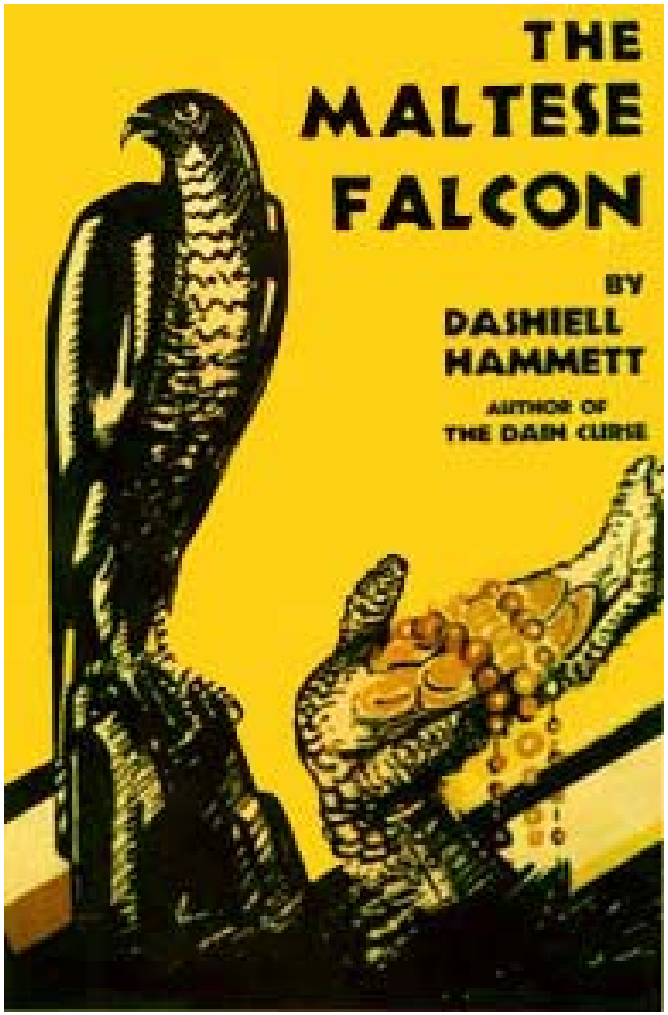
Thermal Conduction

Dumb and Dumber

Why does his tongue stick to a metal pole?

Would it stick to a wooden pole?

What is "Ice"?



The Hot Ice Caper

with

Sam Spade

Diamond vs. Cubic Zirconia

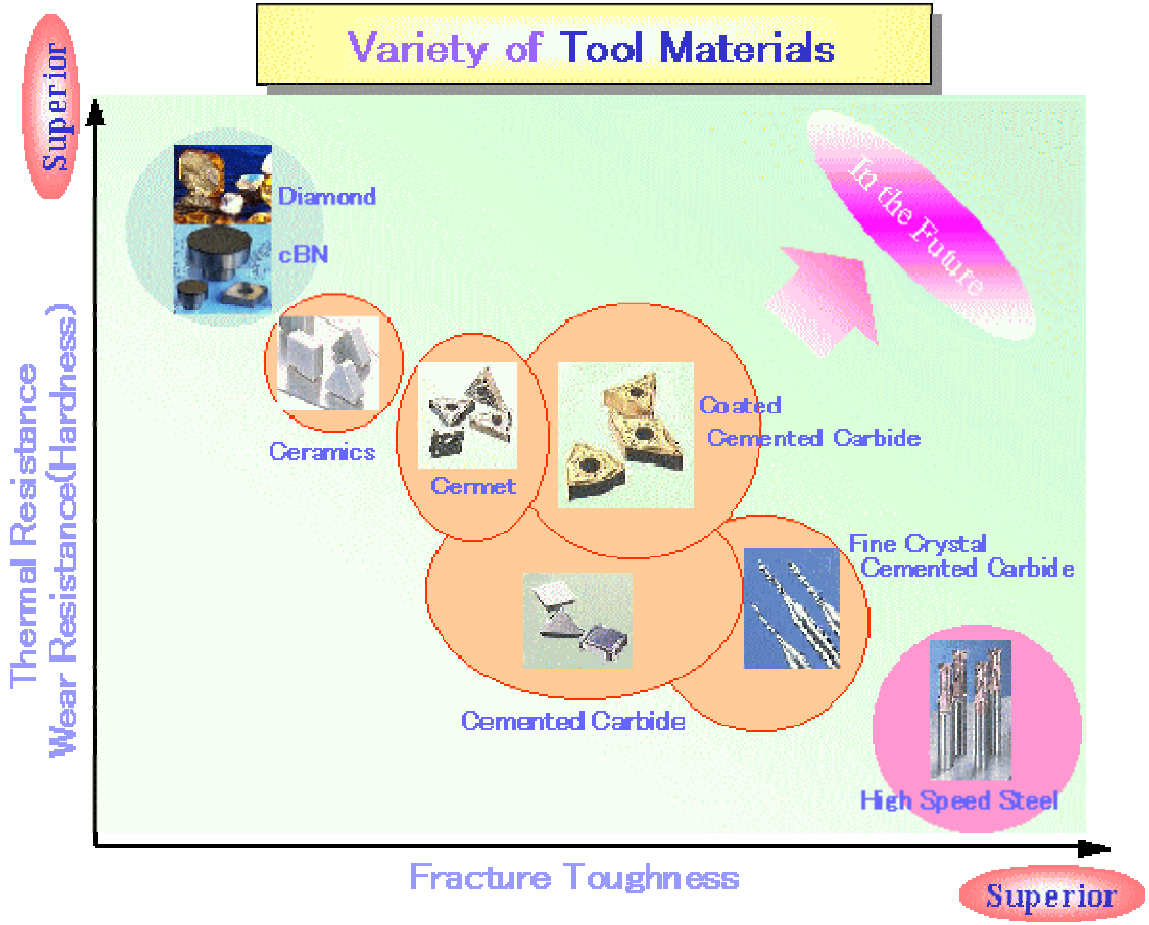
Diamond

Which is which?

Cubic Zirconia

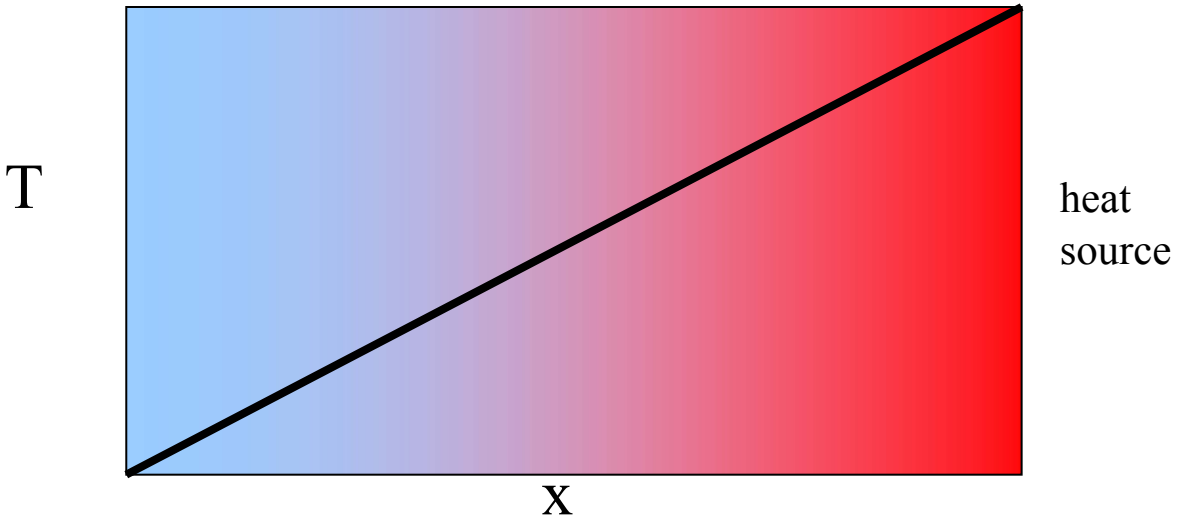
http://wholesale-scales.com

Tools



http://www.sei.co.jp/RandD/itami/e-tool/gif/variety.gif

Phenomenology of Thermal Conductivity



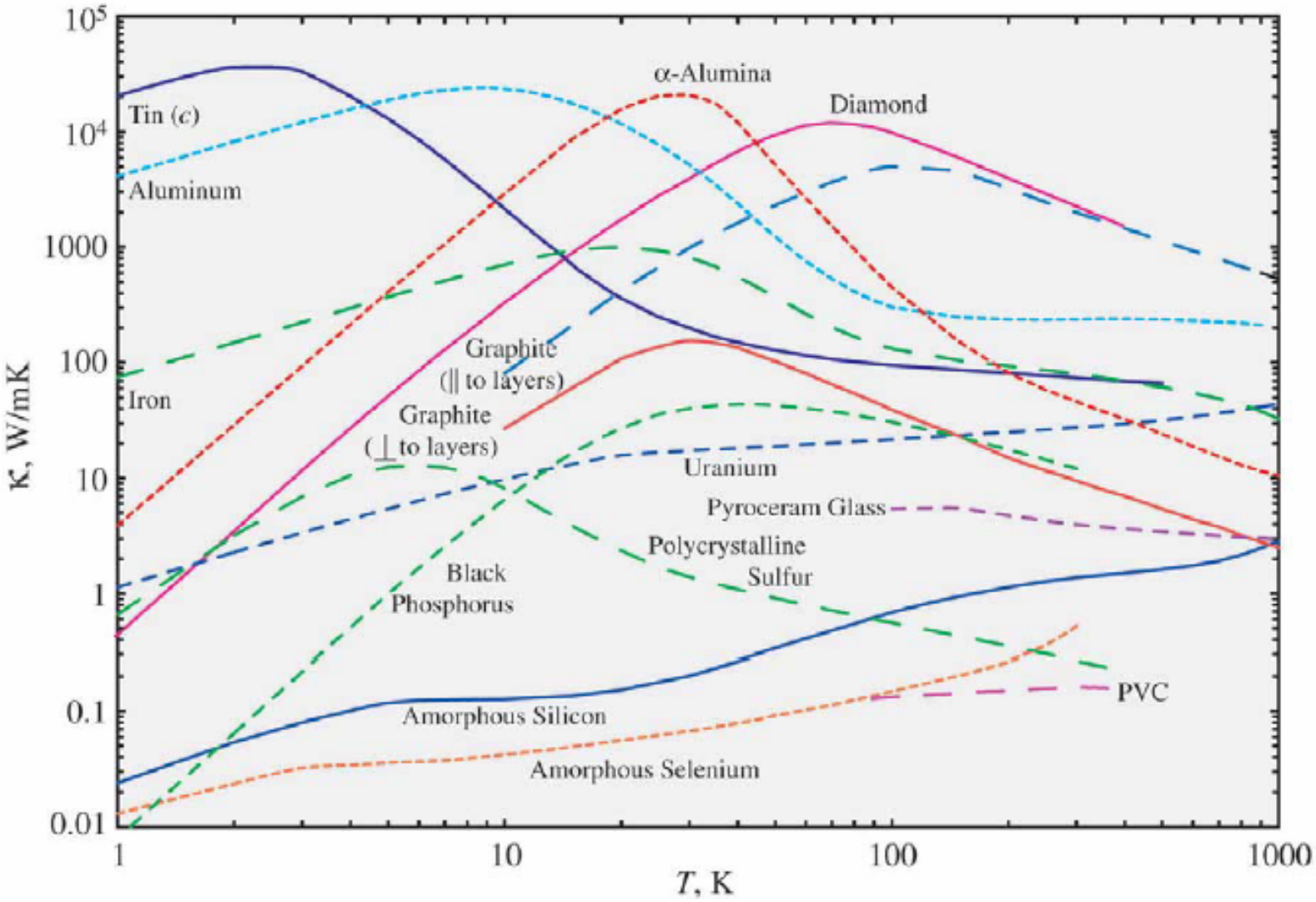
Fourier's Law

$$J = - \kappa \, dT/dx$$

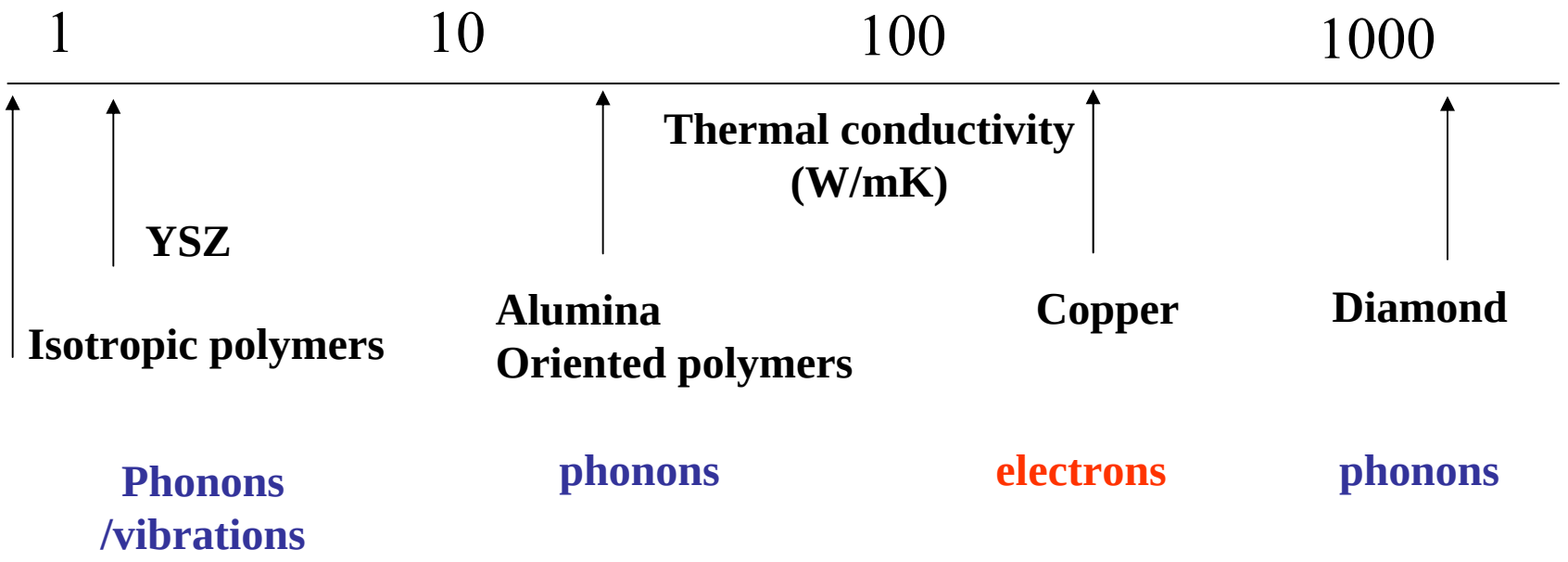
Heat current

Thermal conductivity

Thermal Conductivity of Solids



Mechanisms of Thermal Conductivity



Electrical conductivity

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

$\sigma(\text{diamond}) \sim 10^{-10}\ (\Omega\ \text{cm})^{-1}$

Electronic Conductivity and Wiedemann-Franz Law

Electrons carry energy as they move → transport of heat

$$k/\sigma T = L_0$$

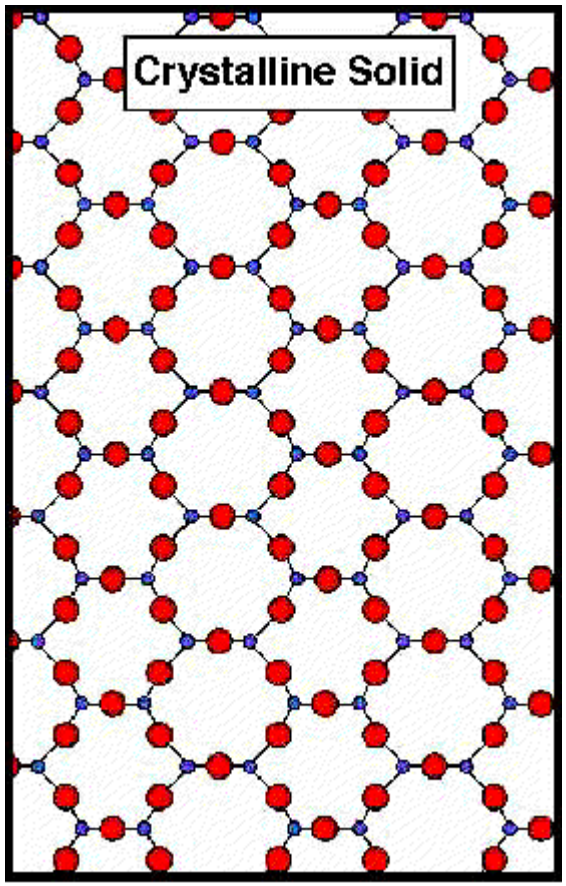
k – thermal conductivity
σ – electrical conductivity
T – temperature
L_0 – Lorentz constant

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

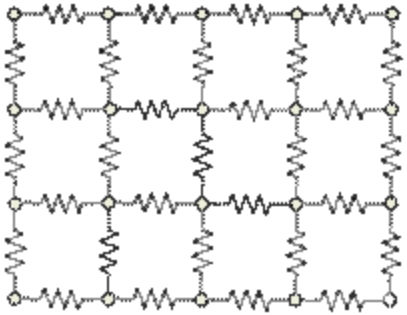
$L_0 = 2.45\ 10^{-8}\ W\Omega/K^2$

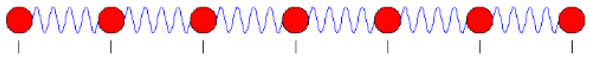
Element	k (W/mK)	k/σT
Li	71	2.22 10-8
Na	138	2.23
In	88	2.58
Bi	9	3.53
Al	238	2.14

Crystalline Materials: From Solids to Springs



Heat transport from atomic vibrations





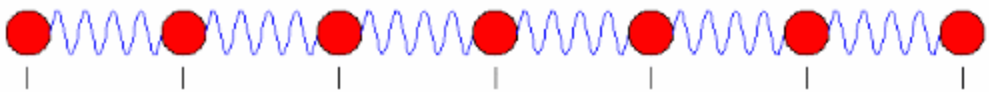
Vibration of spring system similar to vibrations in solids

Harmonic Model

$$E = \tfrac{1}{2} kx^2$$

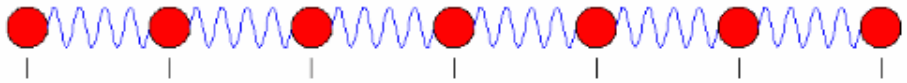
Simple harmonic solid with one and two atoms in the basis → acoustic and optical phonons

Long Wavelength Longitudinal Acoustic Phonon



Short Wavelength Longitudinal Acoustic Phonon

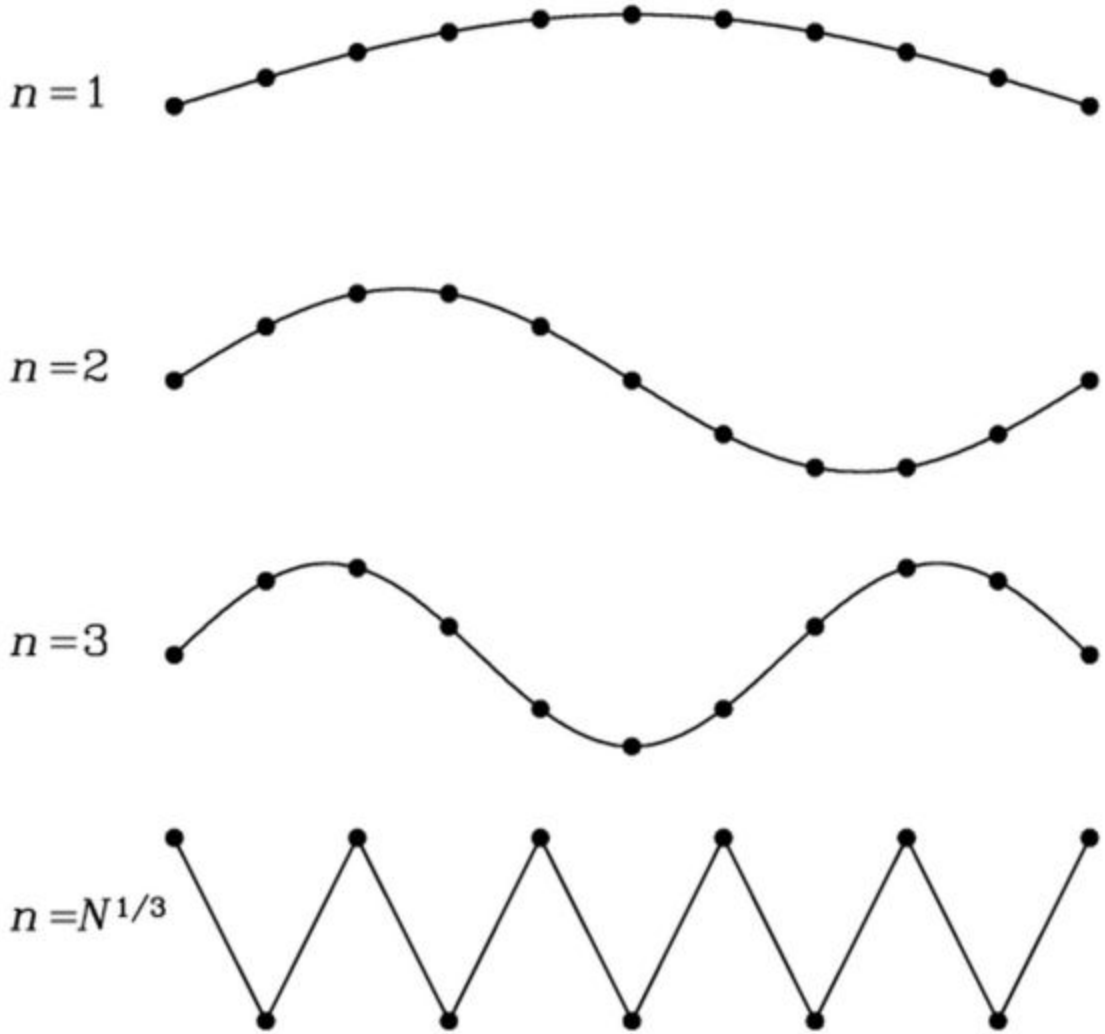
Longitudinal Optical Phonon



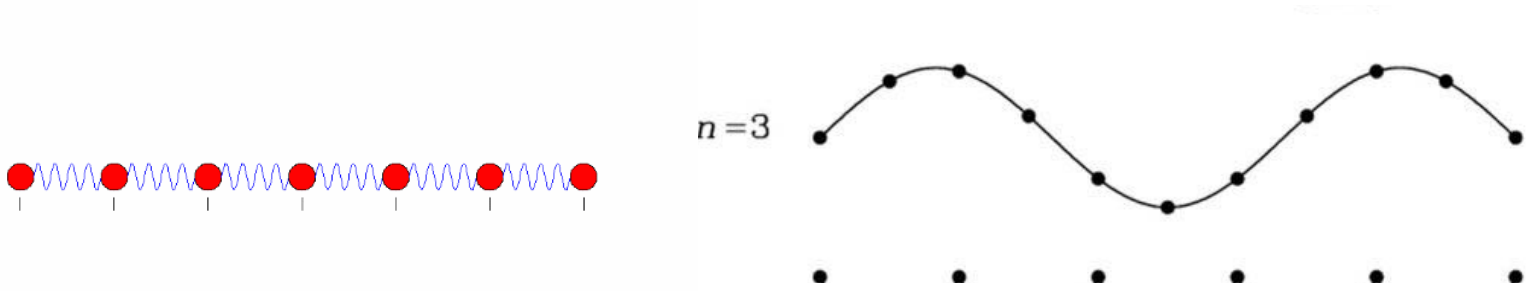
Acoustic vs. Optical

Which has lower energy?
Why?

Transverse Phonons



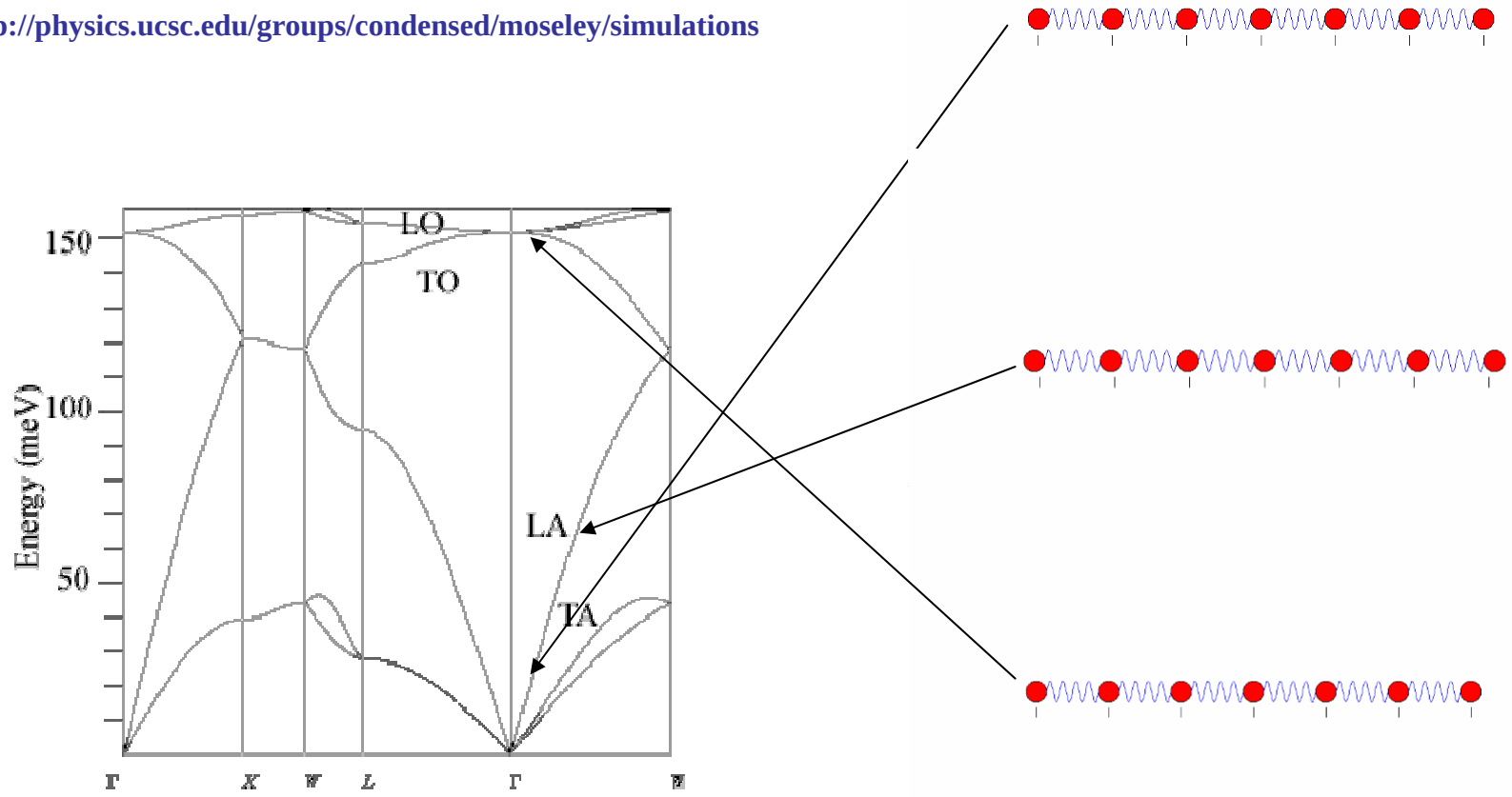
Longitudinal vs. Transverse Phonons



Which has lower energy?
Why?

Phonons

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

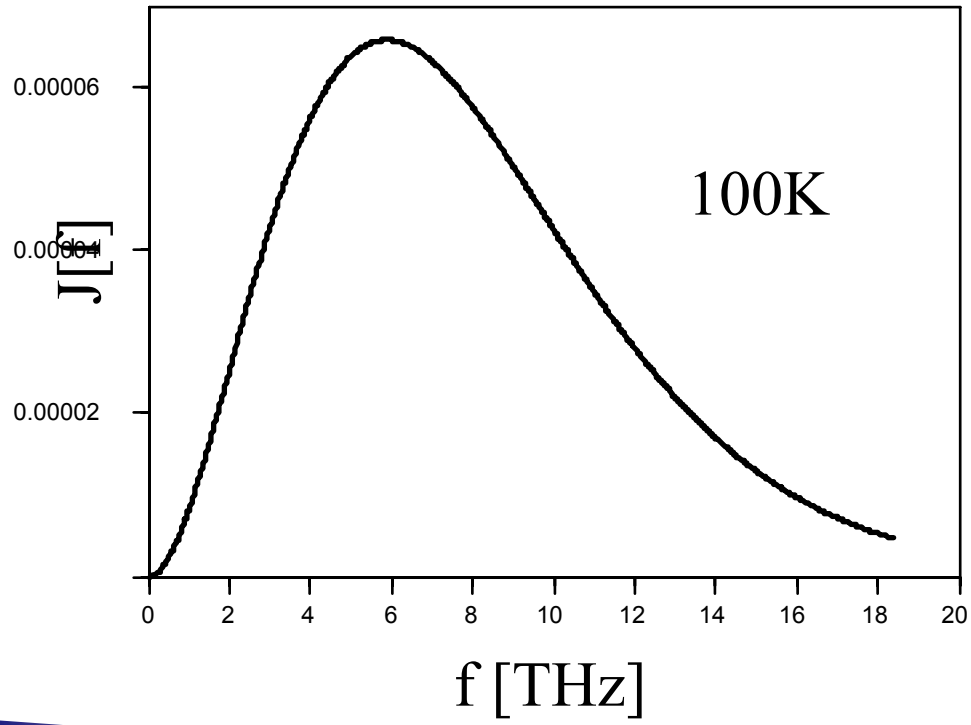


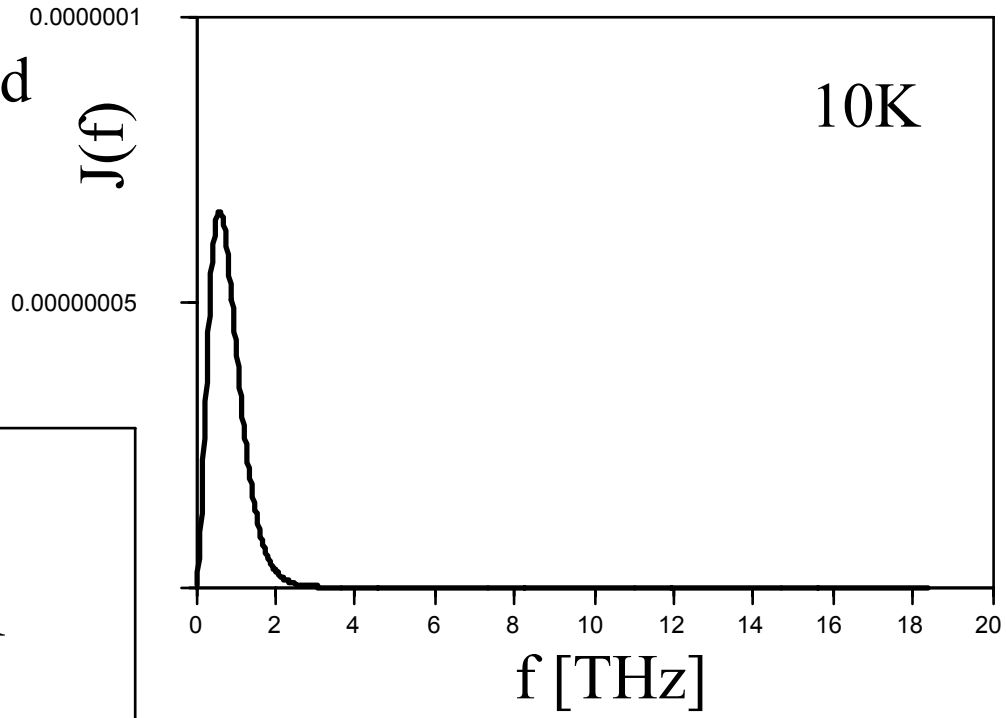
Schematic dispersion curves for diamond

Phonons and Thermal Conductivity

Dominant phonon – Debye solid

$f_D = 2.82\ kT/h$

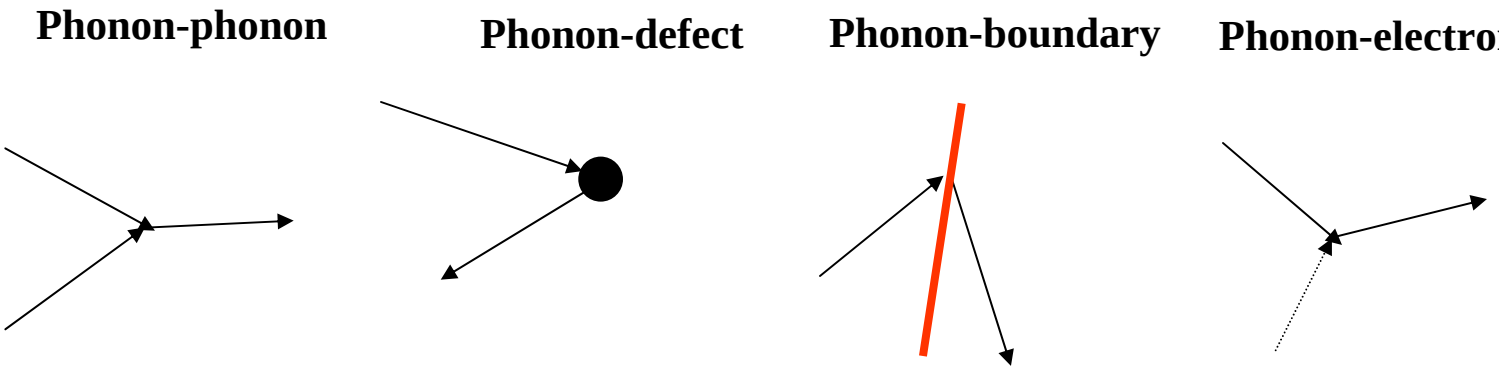




Why is the Thermal Conductivity Finite?

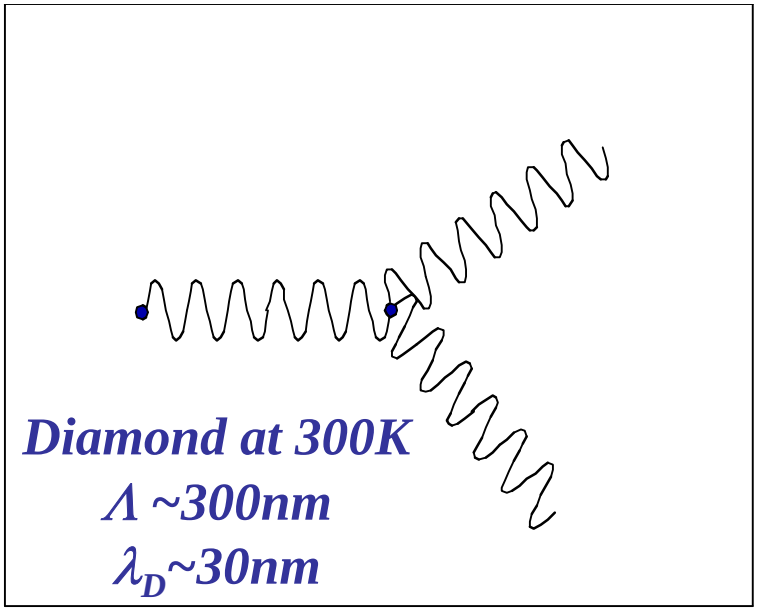
If phonons did not scatter the thermal conductivity would be infinite?

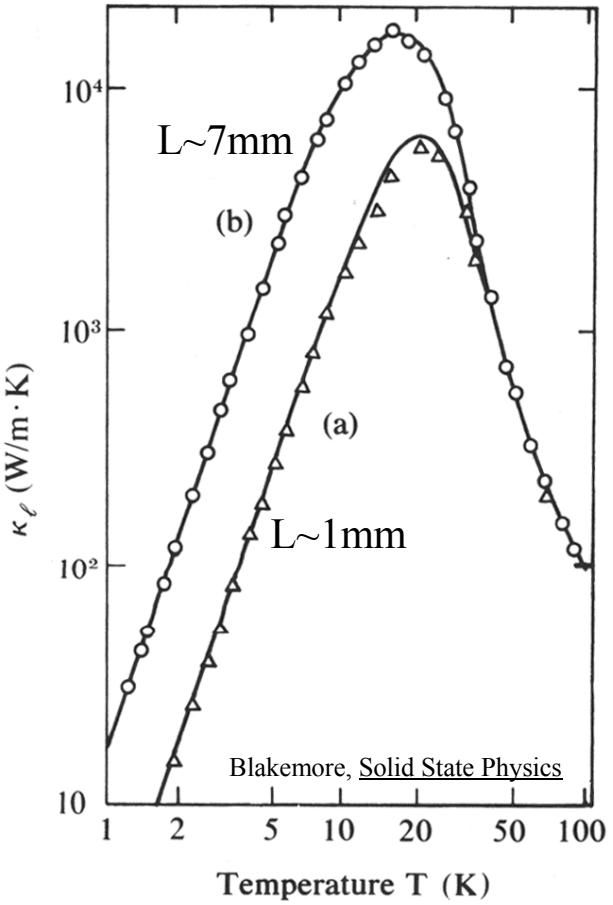
Phonon Scattering Mechanisms



Macroscale	*****	***	*	

Phonon-phonon Scattering





Sample-size dependent thermal conductivity of single crystal LiF

- Usually l < Λ < L
- New physics arises when L is reduced to nanometers

Temperature Dependence

$\kappa \sim 1/3\ c_v\ v\ \lambda$

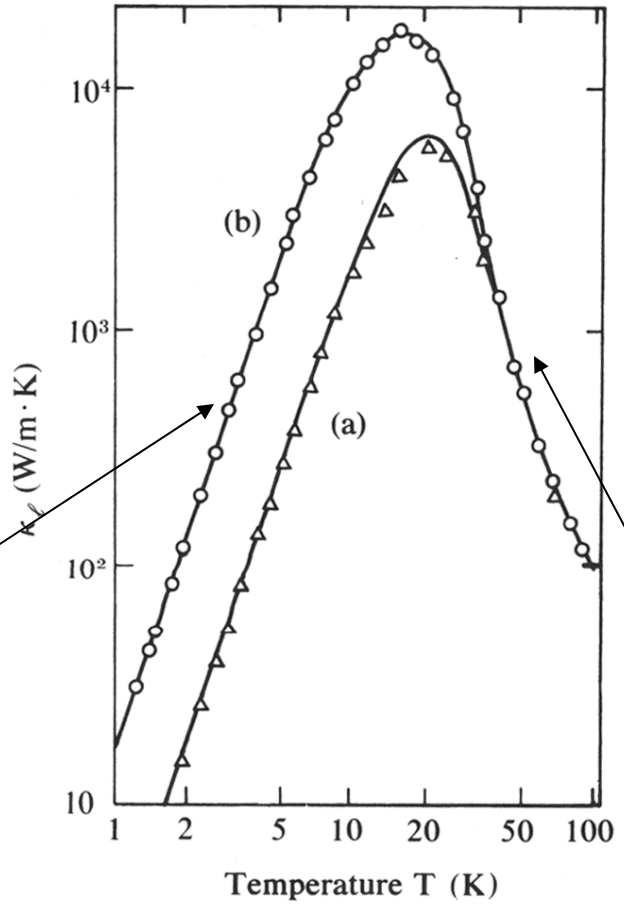
Low T

Quantum Solid

$C_v \sim T^3$

→

$\kappa \sim T^3$



High T:

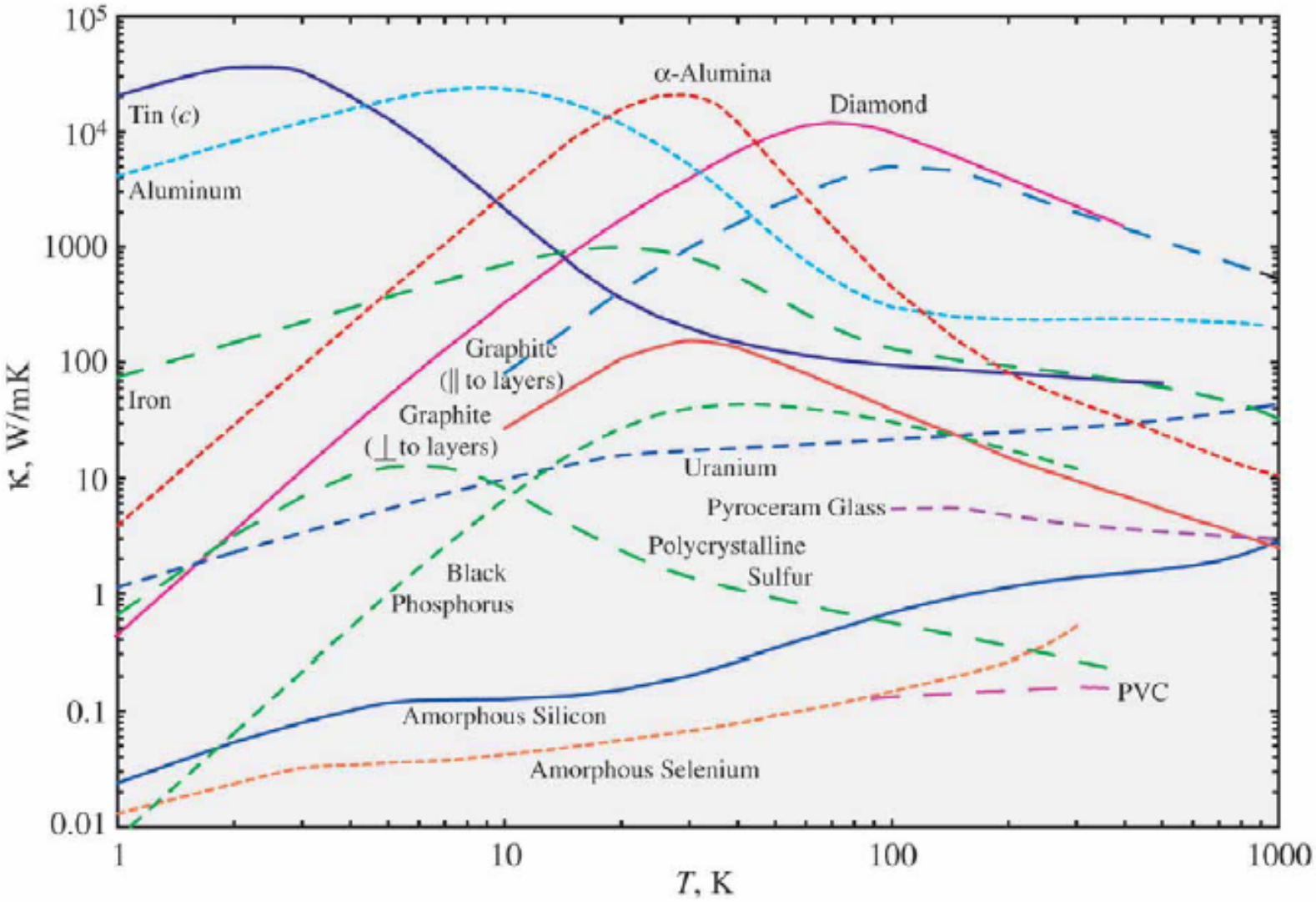
Phonon-phonon scattering

$\lambda \sim T^{-\alpha}$

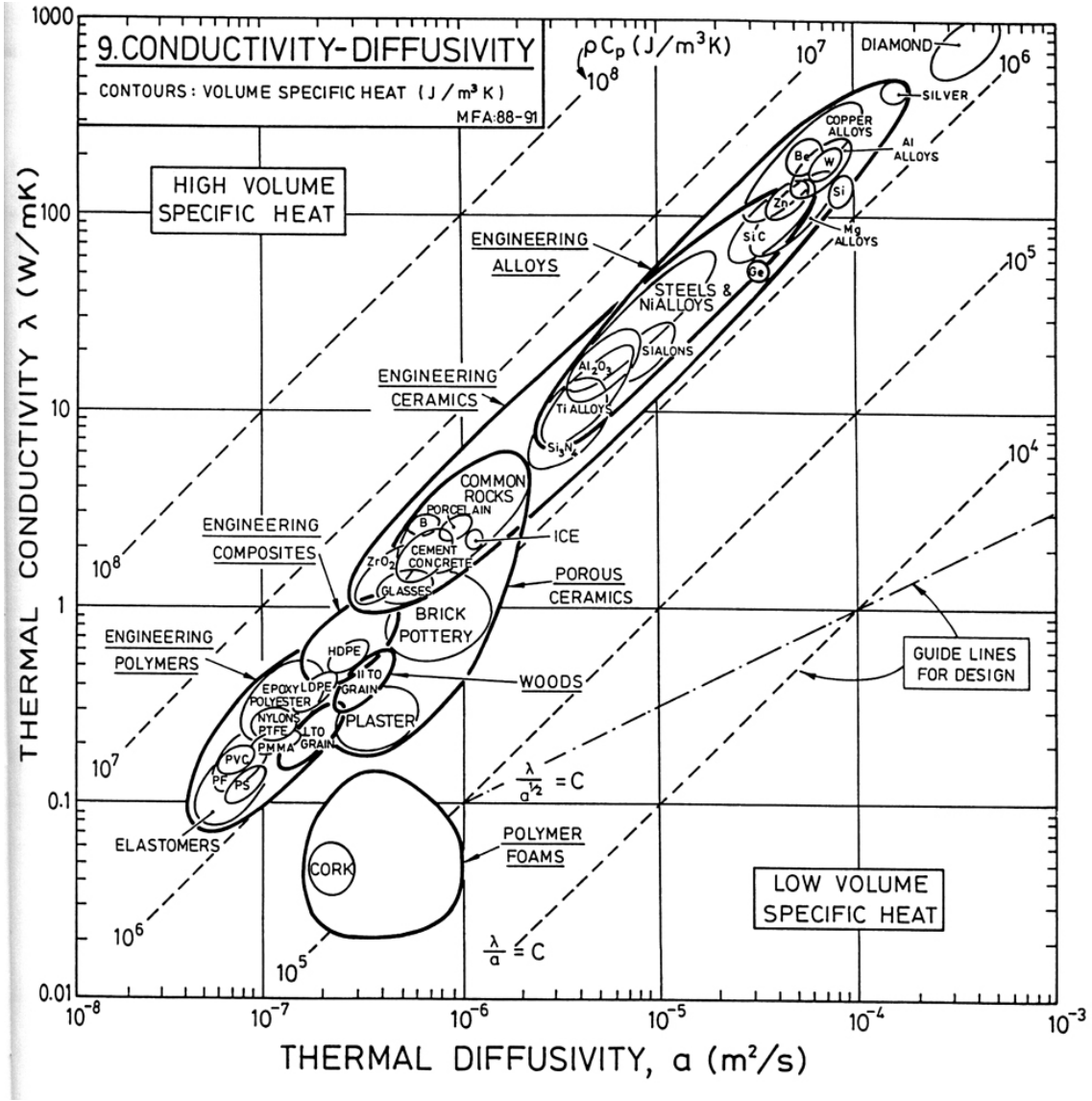
$\alpha \sim 1$

$\kappa \sim T^{-\alpha}$

Thermal Conductivity of Solids



Thermal Conductivity and Thermal Diffusivity



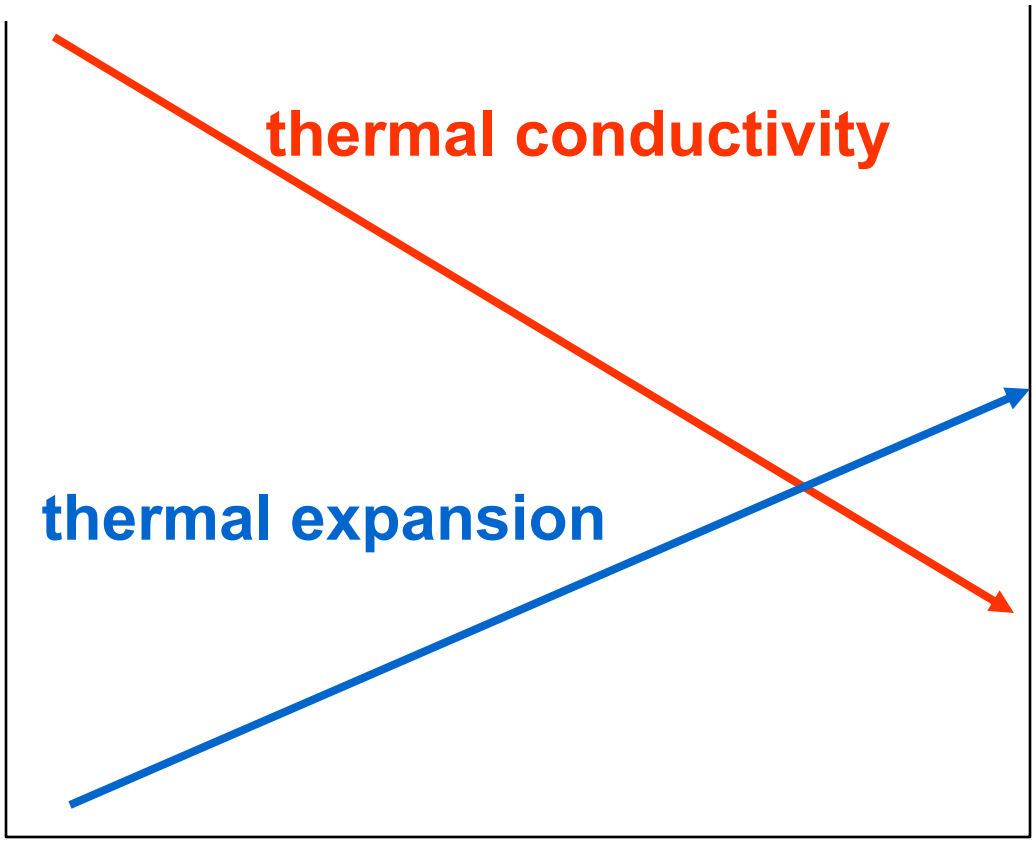
$$k = \rho\, c_p\, D_T$$

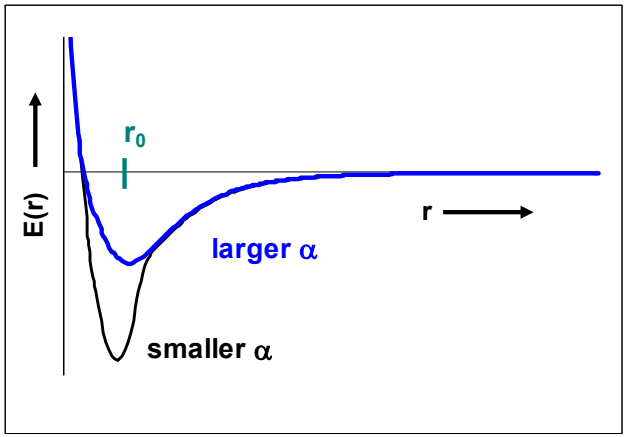
ρ – density
C_p – heat capacity
D_T – thermal diffusivity

Thermal Expansion and Thermal Conductivity

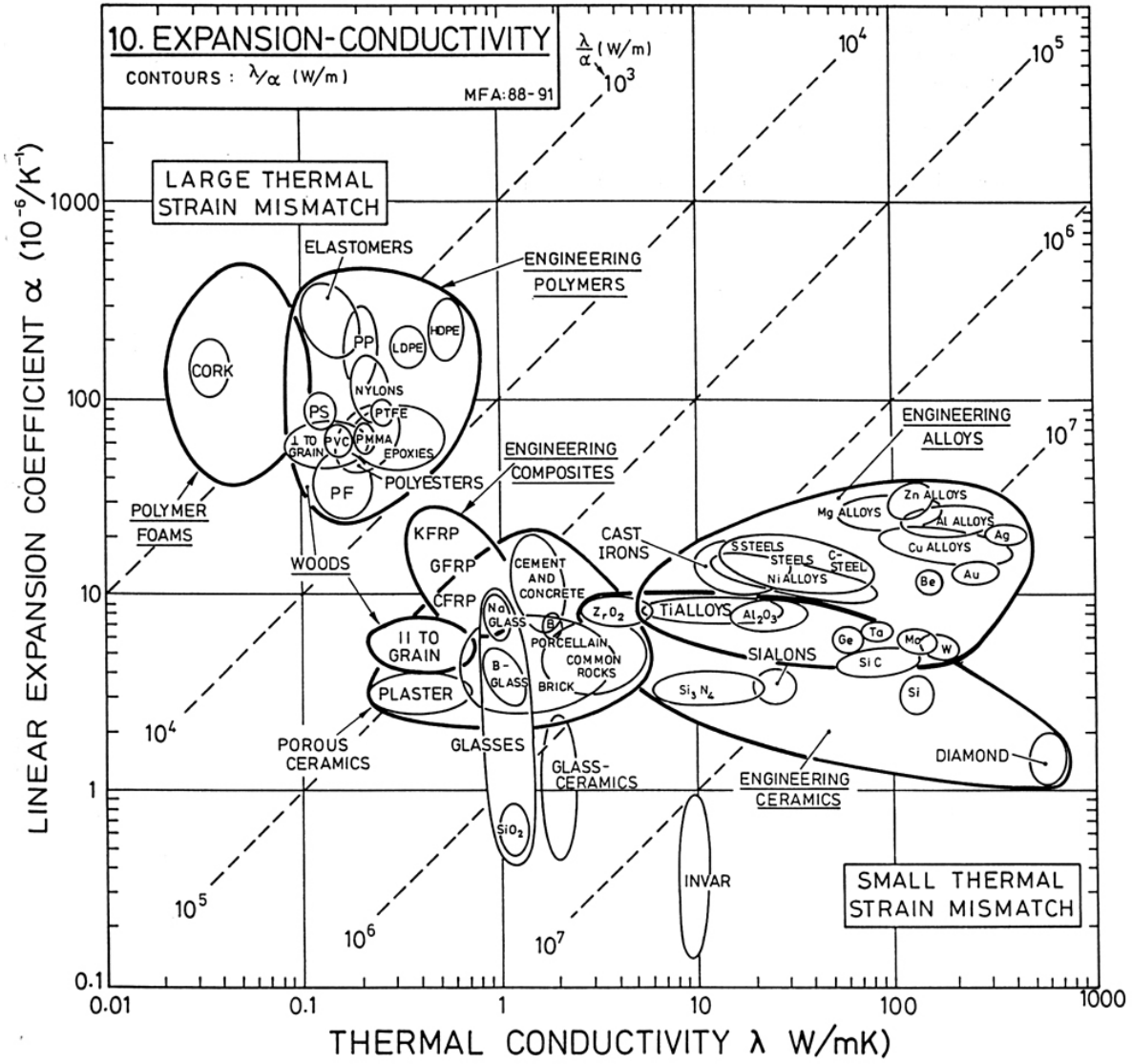
- Thermal expansion
  - α =0 for a harmonic solid
  - – Thermal expansion ismeasure of anharmonicity
- Thermal Conductivity
  - $\kappa = \infty$ for harmonic solid
  - – Anharmonicity → finite κ

Anharmonicity: Thermal Expansion and Thermal Conductivity



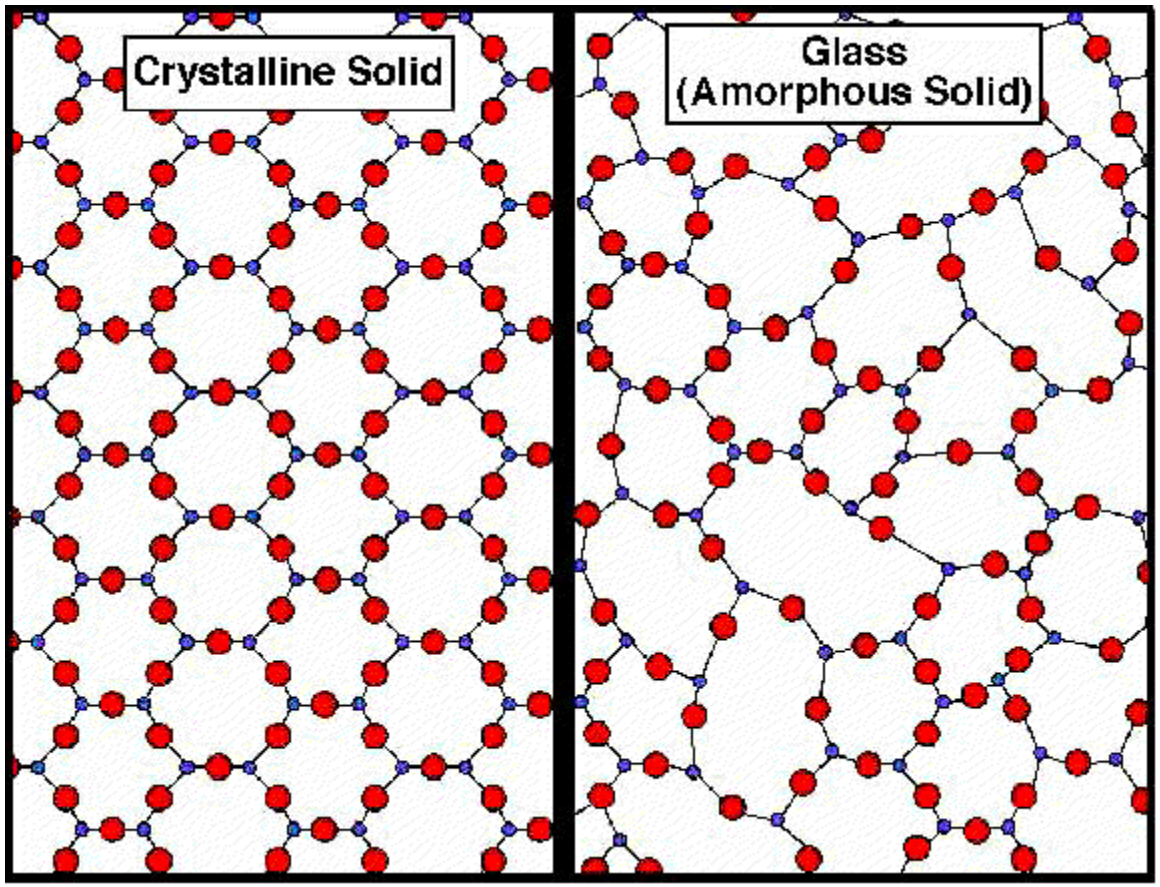


Thermal Conductivity and Thermal Expansion



Reasonable correlation between thermal conductivity and thermal expansion

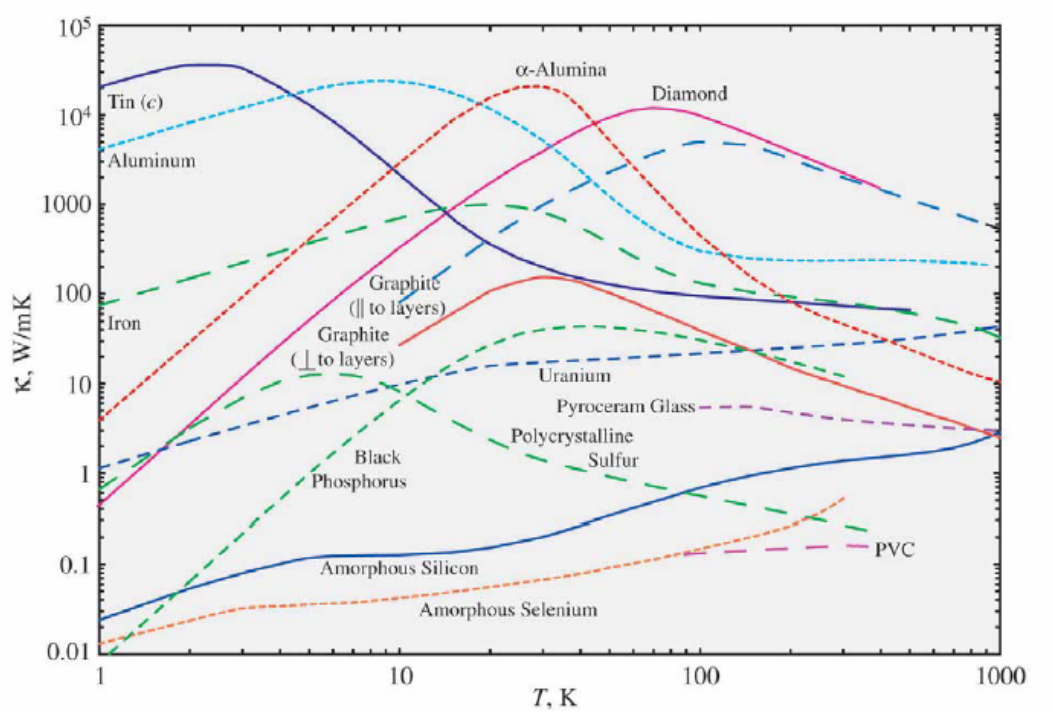
What About Glasses?



No long-ranged order → no phonons → How is heat transported?

We will look at amorphous materials later

Solids have Much High Thermal Conductivities than Liquids

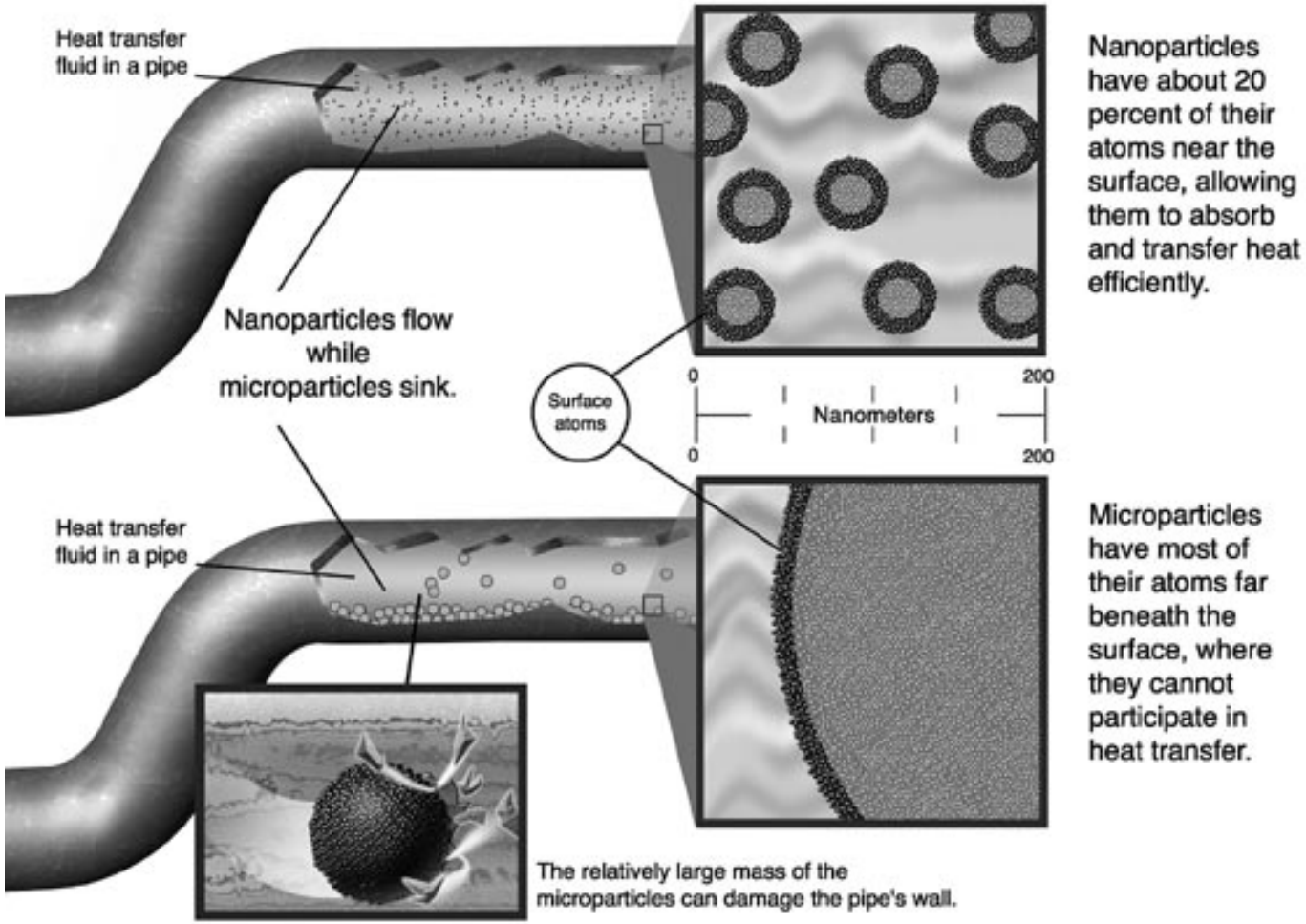


Low k materials	W/mK
Water	0.6
Ethylene Glycol	0.25
PTFE	0.2
Wood	0.2 – 0.4
Engine Oil	0.15
Fiberglass	0.04
Air	0.03
Snow	0.05 – 0.25 (T < 0C)
Silica Aerogel	0.003

Liquid Na - 72 W/mK

Nanofluids

Why Nanoparticles Are Better Than Microparticles



http://www.anl.gov/Media_Center/News/2004/nanofluidsbig.html

Summary

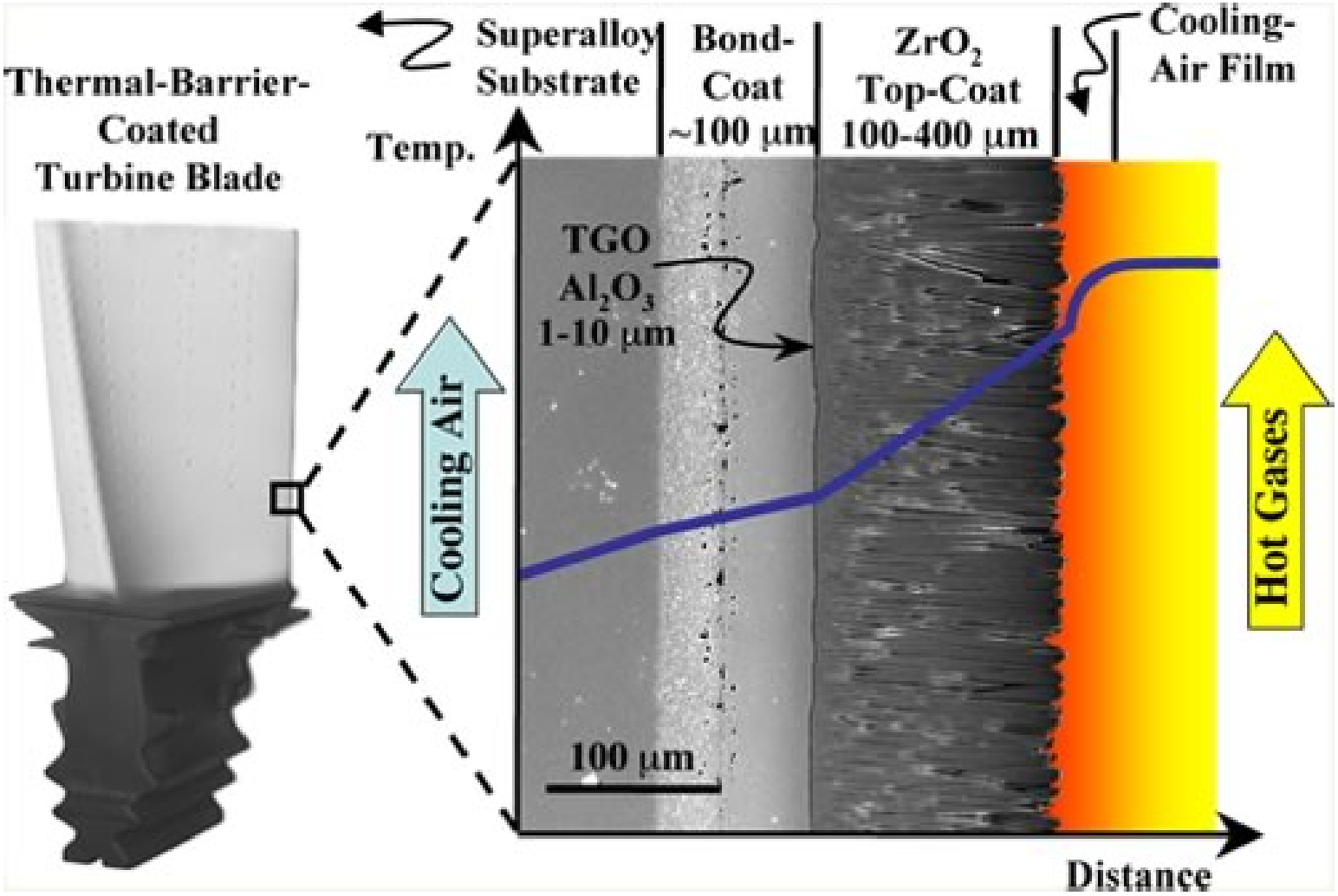
- Radiation vs. Convection vs. Conduction
- Electronic vs. Phonon Conduction
- Physics of Phonons
- Basic Phenomenology of Thermal Conductivity

Part 2: Case Studies in Thermal Conductivity

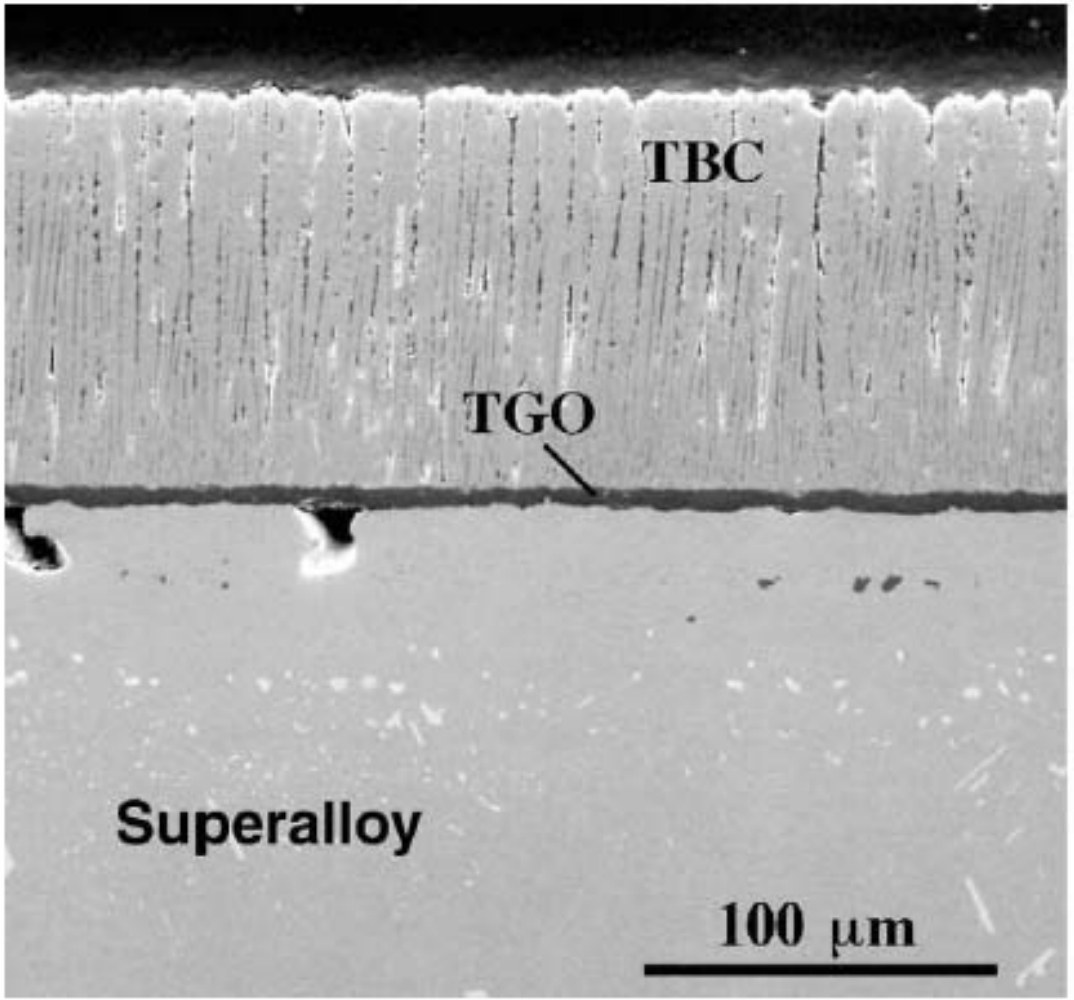
Preamble: Introduction to Molecular-Dynamics Simulation

- 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

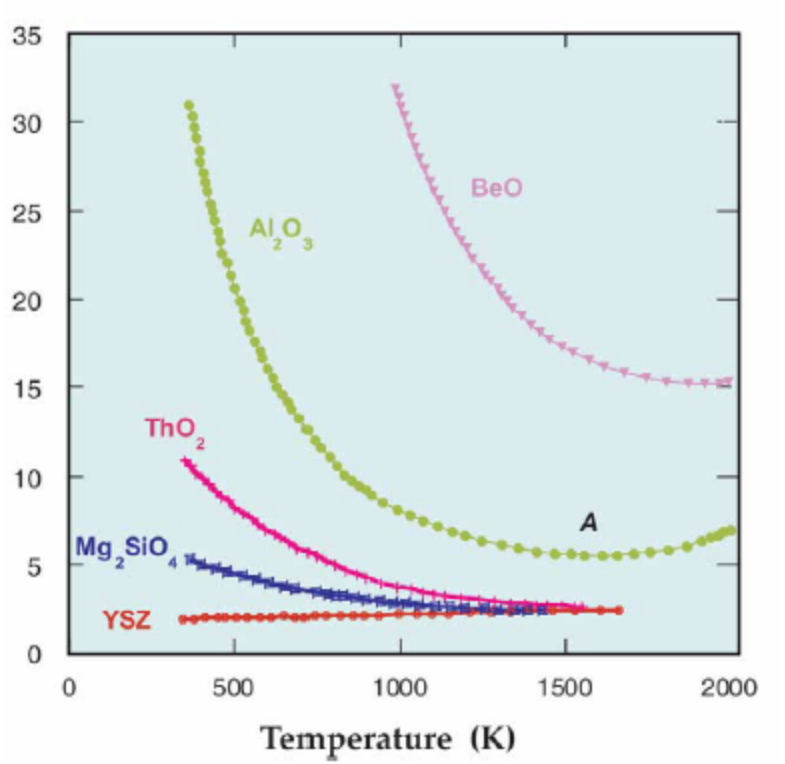


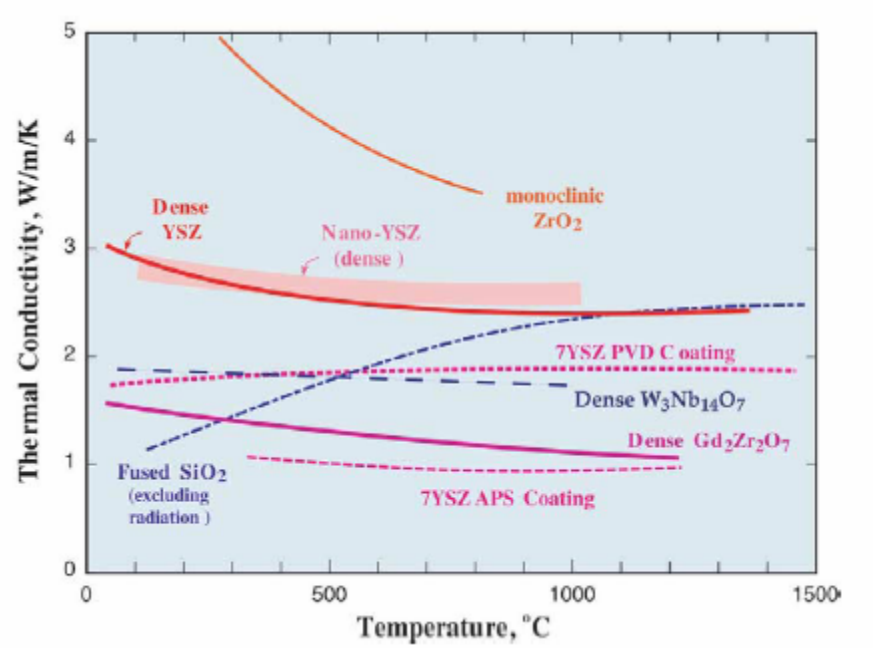
http://www.mse.eng.ohio-state.edu/fac_staff/faculty/padture/padturewebpage/padture/turbine_blade.jpg



D. R. Clarke, UCSB

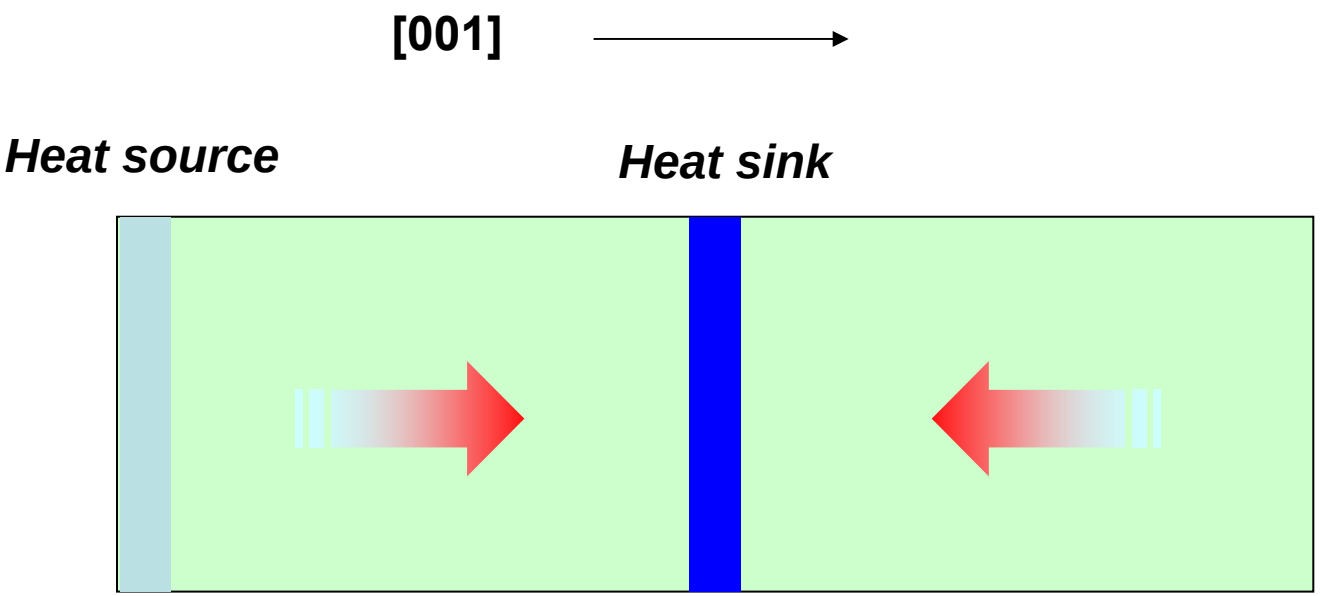
Thermal Conductivity of Oxides





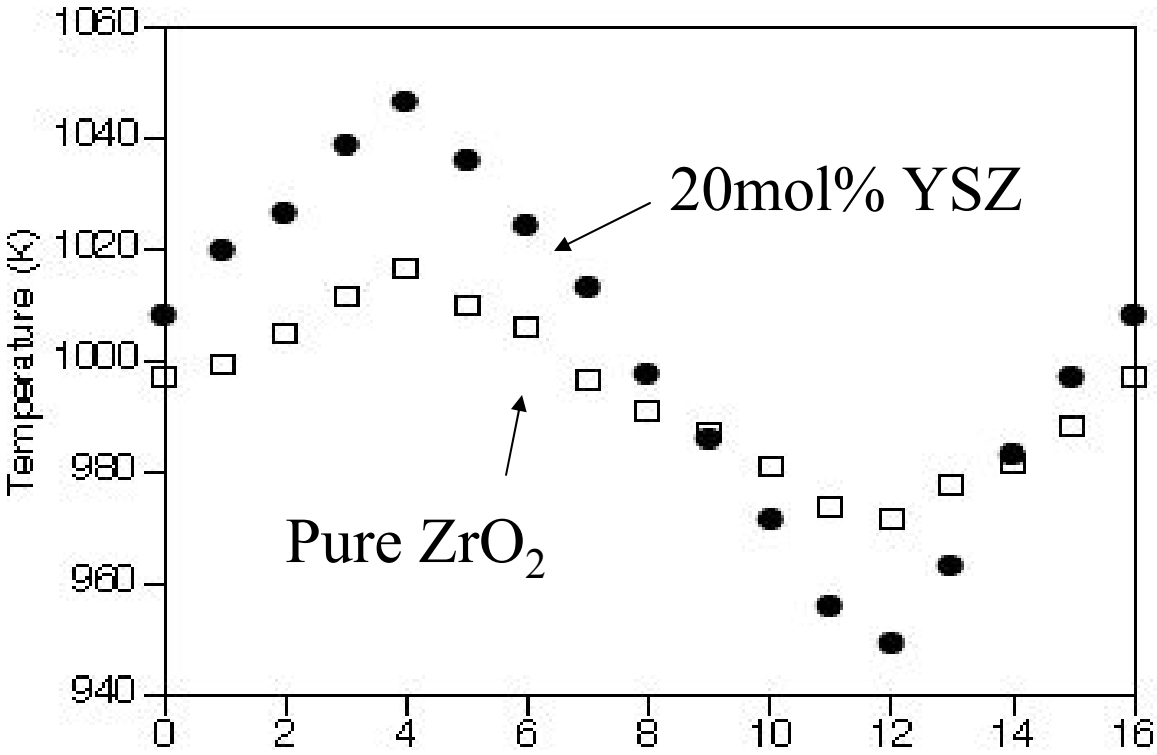
Approach to determination κ

- Non-equilibrium: Add and remove heat



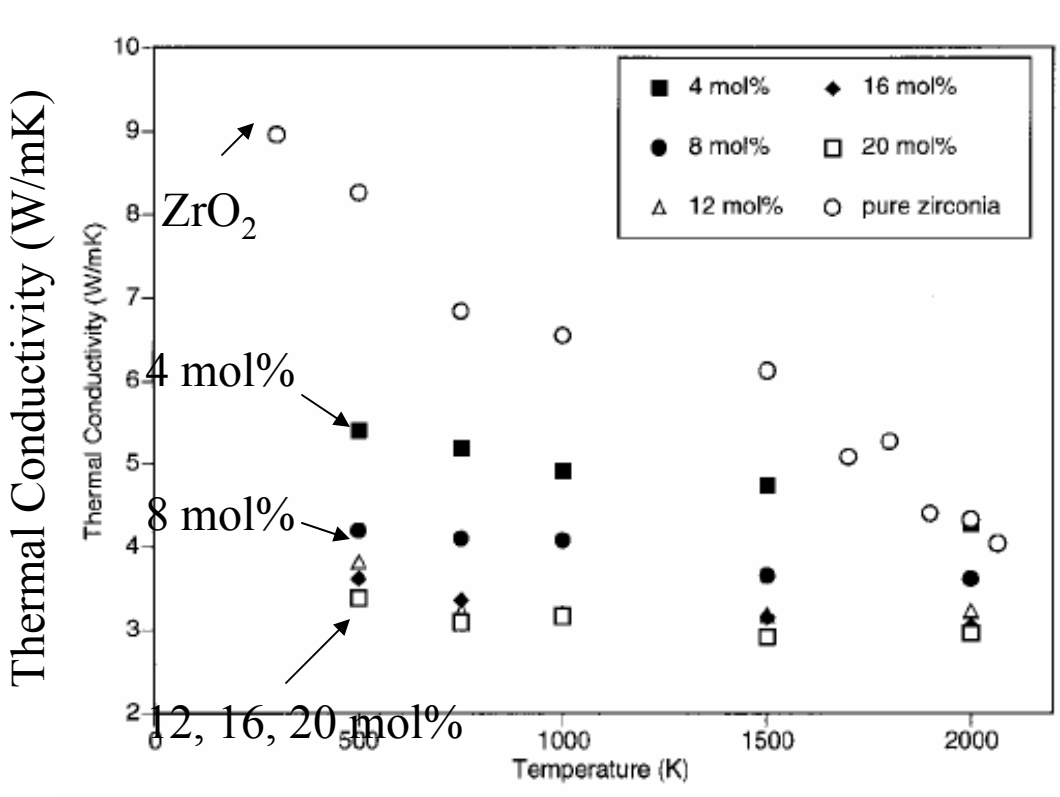
$J=-\kappa\,(dT/dz)$

Steady-State Temperature Profile



$$J = -\kappa \nabla T$$

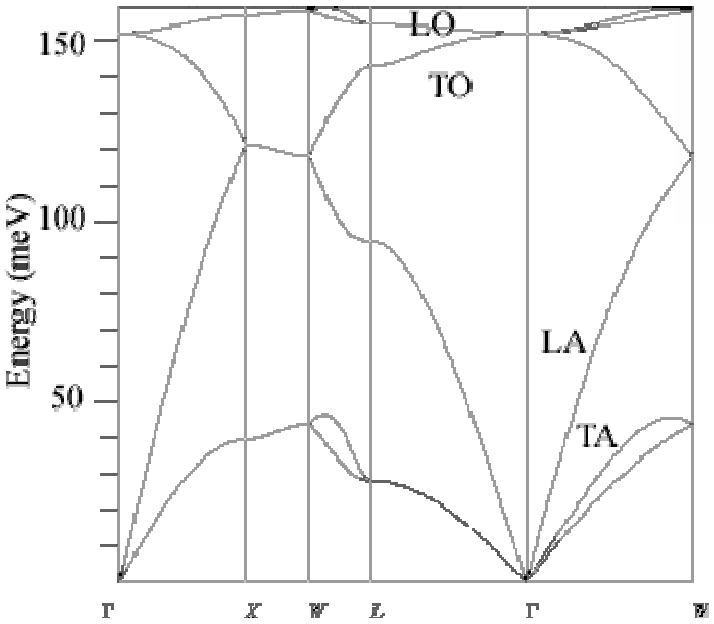
Temperature and Concentration Dependence of κ

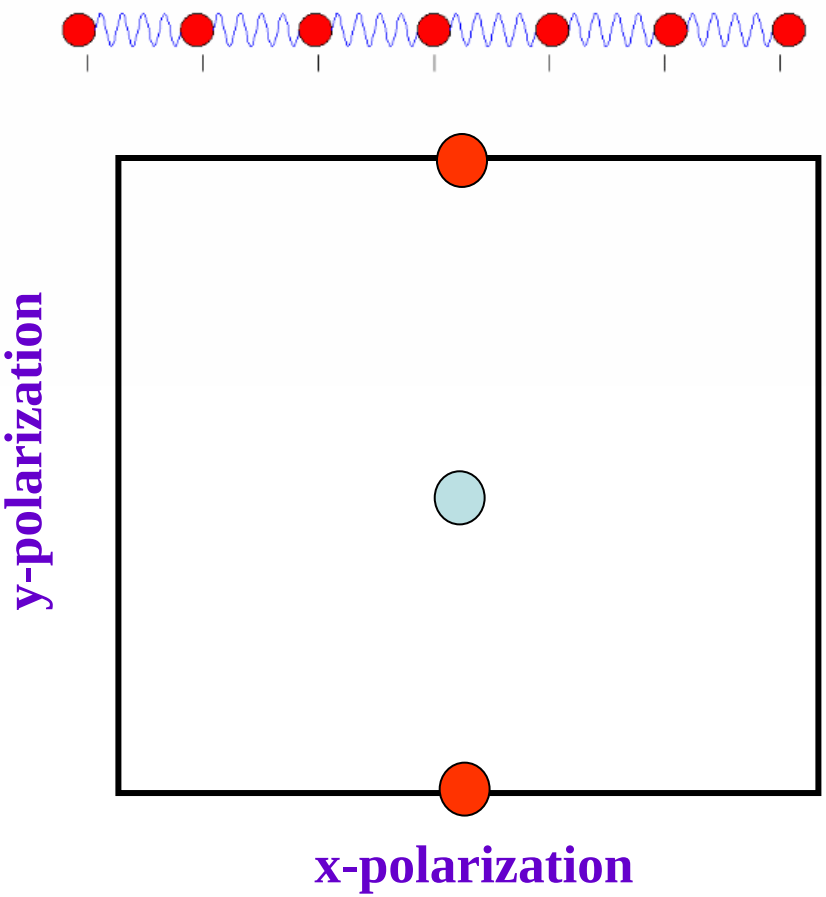


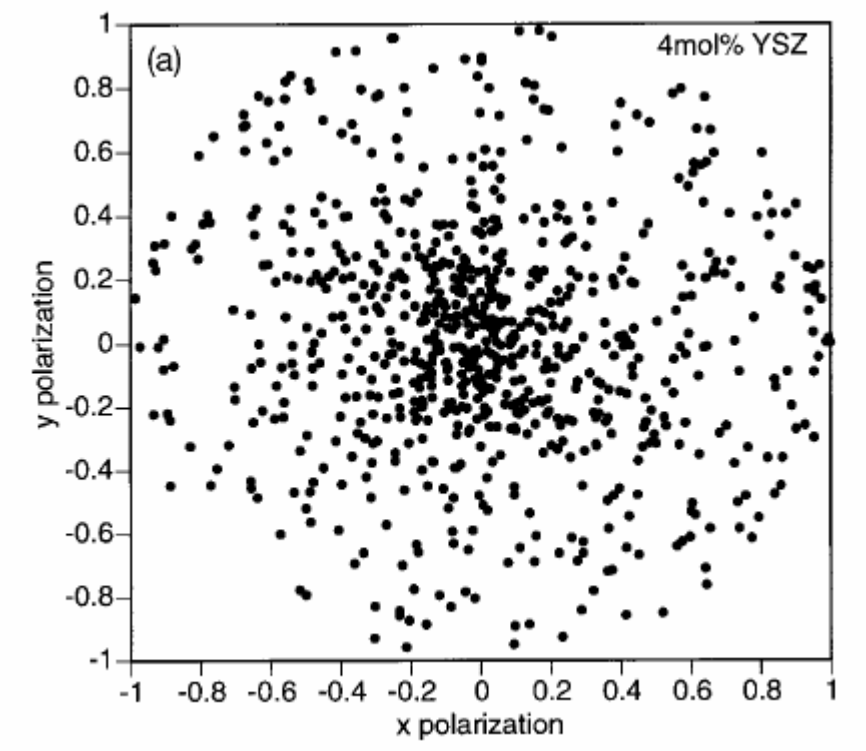
Temperature (K)

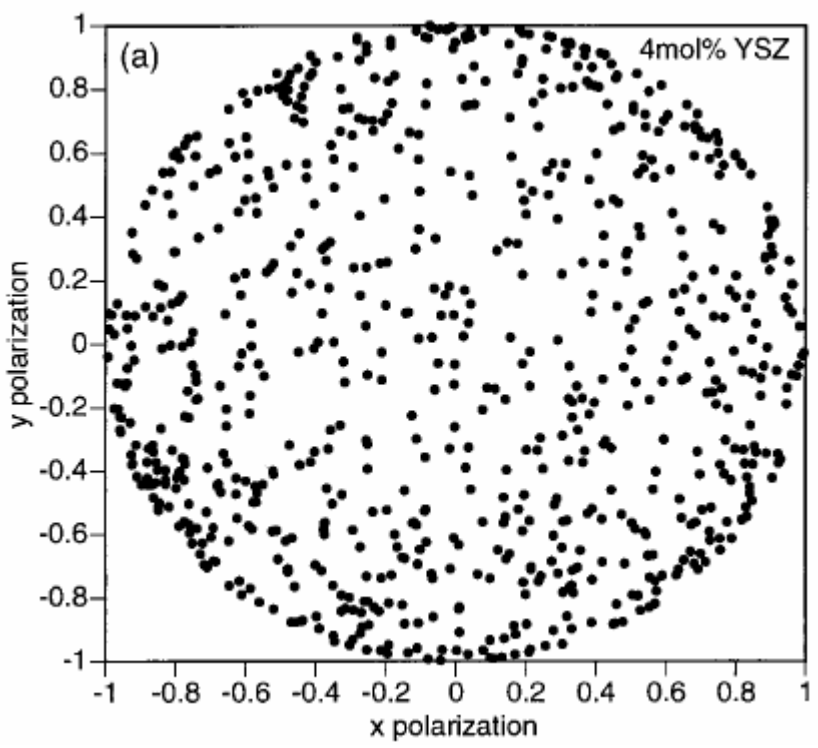
	Sim. (W/mK)	Expt. (W/mK)
ZrO_2 (300K)	κ=8.92	κ=8.22
YSZ (>500K)	κ= 3.0	κ= 2.3

Phonon Polarization









f=1.6THz

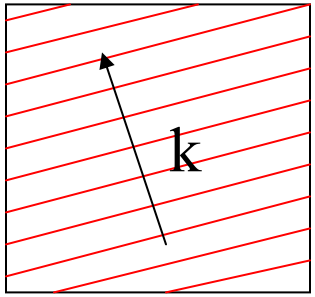
Highly polarized - propagon

f= 3THz

Random polarization - diffusion

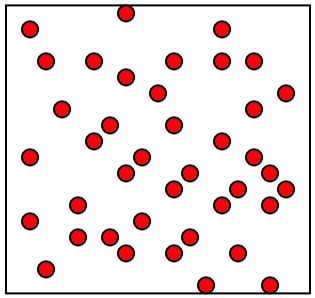
Normal Modes in Amorphous Materials

- Propagons transport heat efficiently



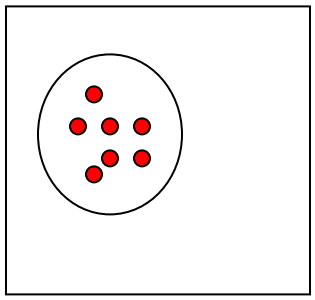
Propagon

- Diffusons less efficient, no directionality



Diffuson

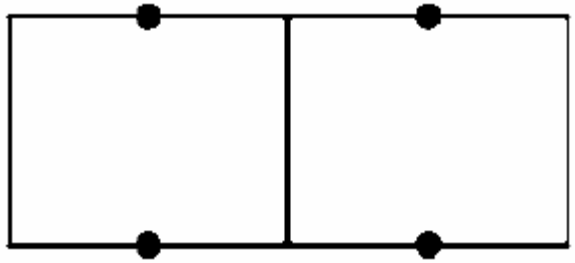
- Energy in locon mode remains localized unless scattered. True insulating state.



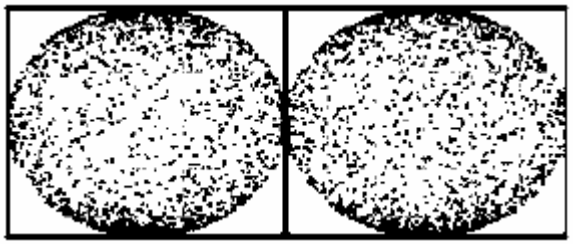
Locon

Feldman and Allen (PRB48, 1993)

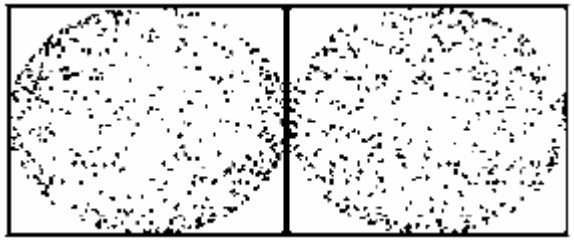
Chemical vs. Structural Disorder



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)

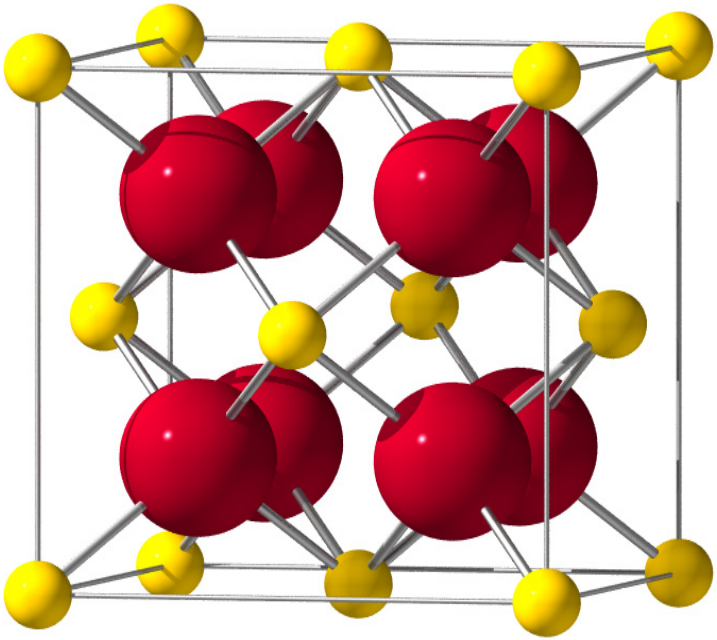
Performance criteria

Low thermal conductivity
high thermal expansion coefficient (match alloy substrate)
Elastically soft / mechanically compliant (match alloy)
Chemical compatibility
Mechanical integrity

Fluorite vs. Pyrochlore

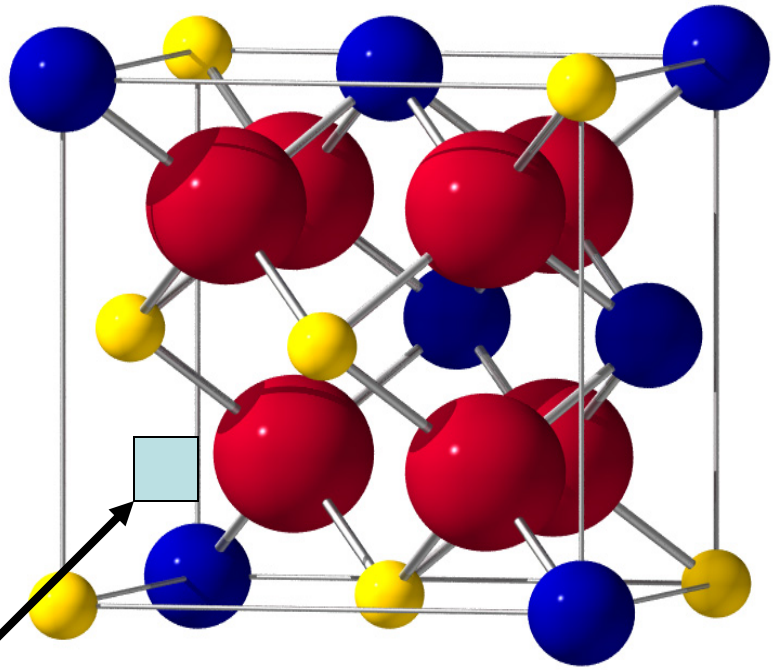
Fluorite

Complete unit cell



Pyrochlore

1/8 unit cell



M 4+
O 2-

MO_2

ZrO_2

Unoccupied 8a site

$A_2B_2O_7$

A_2O_3-$(BO_2)_2$

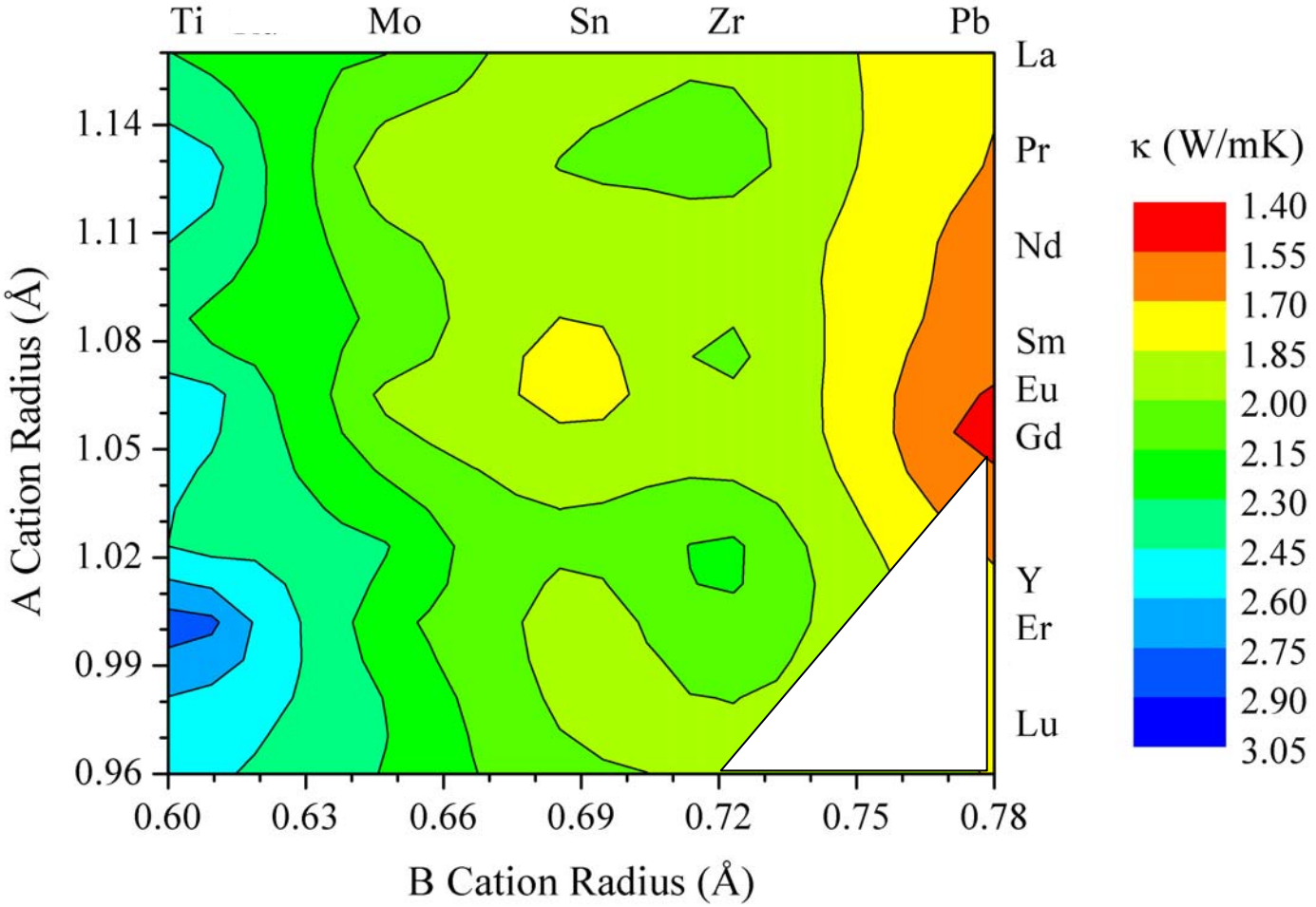
$Gd_2Zr_2O_7$

B 4+
A 3+
O 2-

Comparison with Experiment - Thermal Conductivity

	κ_{expt} (W/mK)	κ_{simul} (W/mK)	$\kappa_{simul}/\kappa_{exptl}$
$La_2Zr_2O_7$	1.56 1.5 1.5	1.98	1.27-1.32
$Nd_2Zr_2O_7$	1.6 1.33	1.83	1.14-1.38
$Sm_2Zr_2O_7$	1.5 1.5	2.09	1.39
$Eu_2Zr_2O_7$	1.6	1.99	1.24
$Gd_2Zr_2O_7$	1.6 1.0 1.1-1.4	1.91	1.19-1.91

Thermal Conductivity @ 1500K



- varies by factor of 2.2

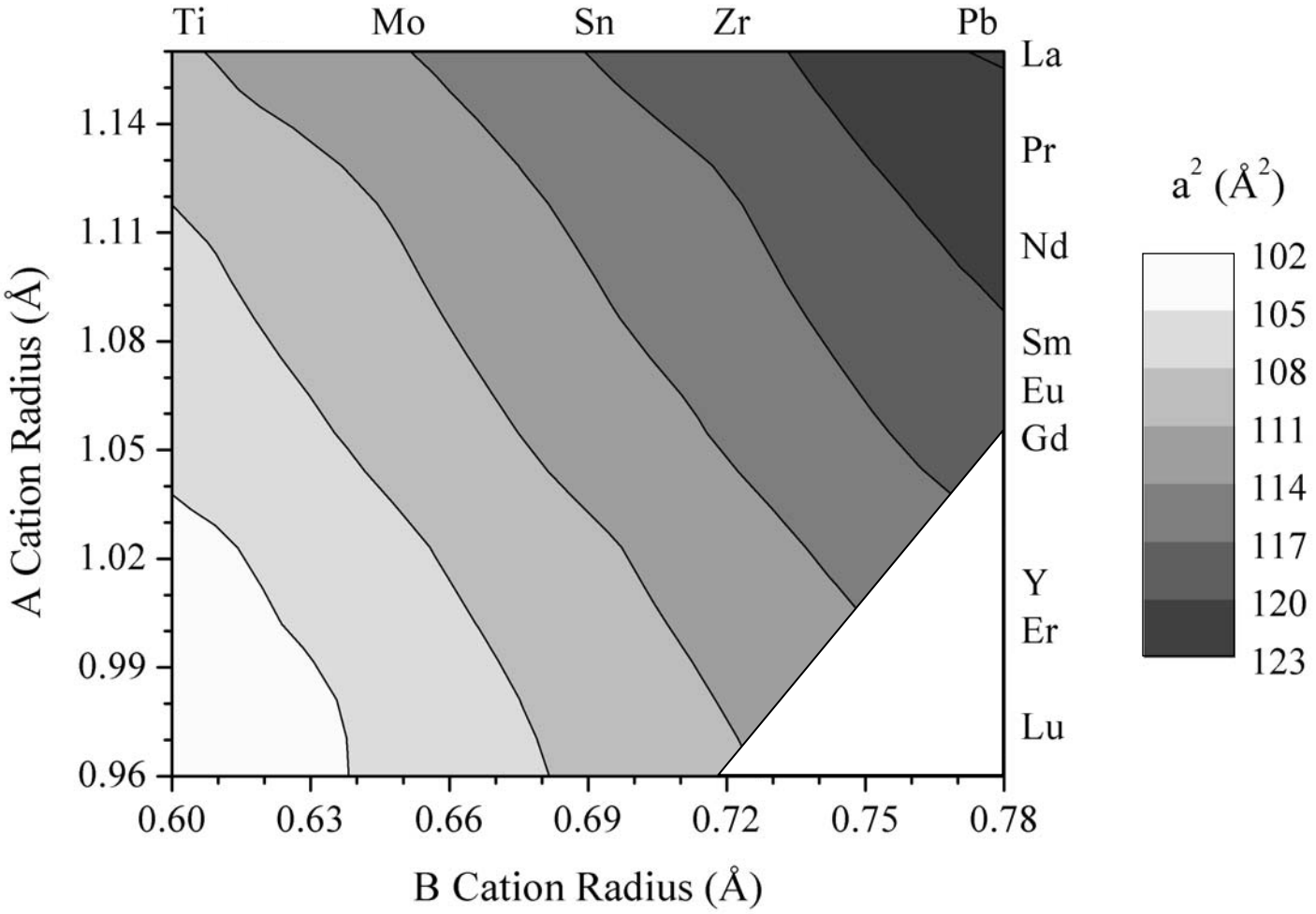
Analysis

$$\kappa = 1/3\ C_v\ v\ \lambda$$

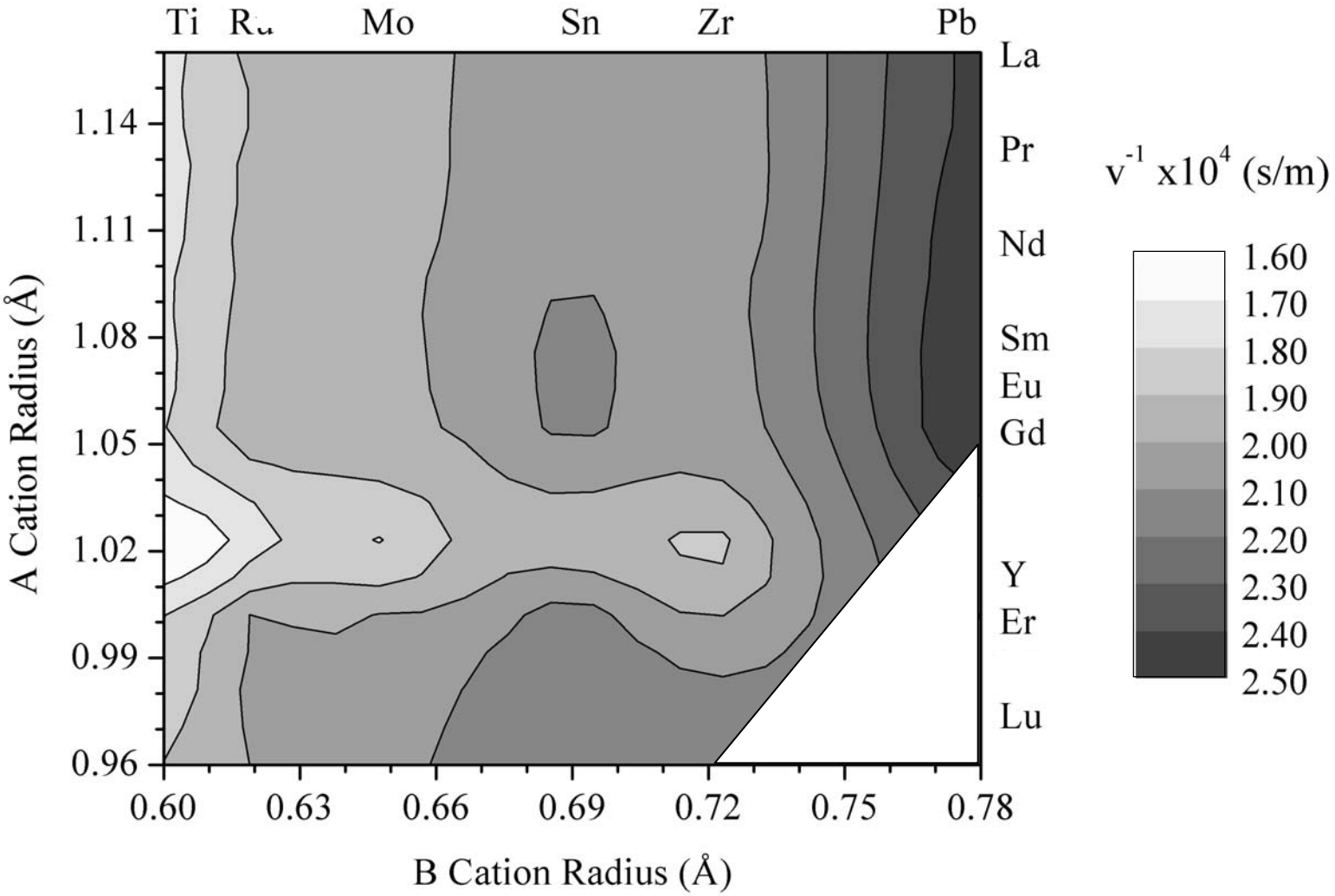
κ- thermal conductivity
C_v - specific heat = $3k_B/a^3$
v - speed of sound
λ - mean free path

$$\lambda/a = \kappa a^2/88k_B v$$

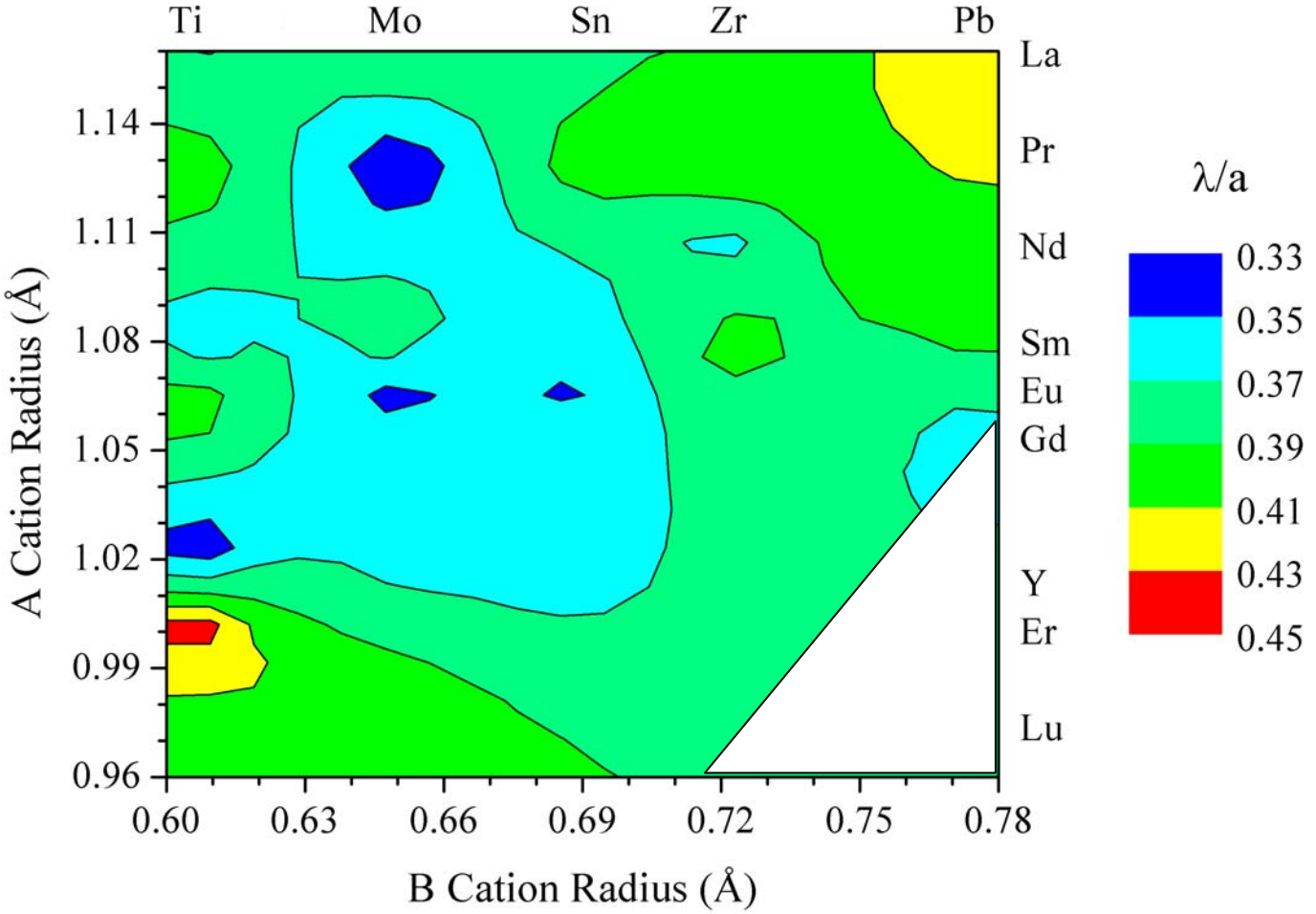
a^2


Ti
Mo
Sn
Zr
Pb
La
Pr
Nd
Sm
Eu
Gd
Y
Er
Lu
1.14
1.11
1.08
1.05
1.02
0.99
0.96
A Cation Radius (Å)
0.60
0.63
0.66
0.69
0.72
0.75
0.78
B Cation Radius (Å)
a² (Å²)
102
105
108
111
114
117
120
123

Inverse Speed of Sound



Mean Free Path



- varies by ~30%

Effect of Cation and Oxygen Disorder

Pyrochlore No disorder	YSZ Anion and cation disorder
$Y_2Zr_2O_7$	$(ZrO_2)_2$ - Y_2O_3
κ = 2.27 W/m-K	κ =1.96 W/m-K

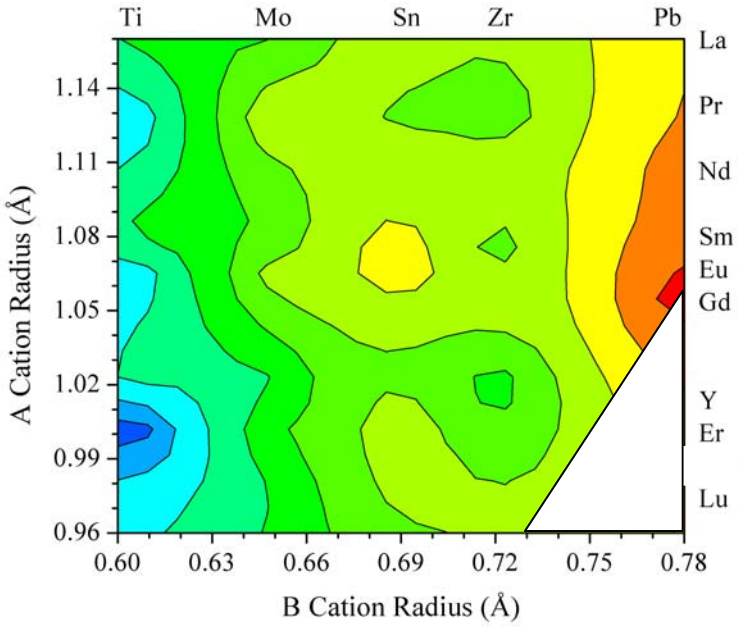
Disorder decreases thermal conductivity by ~10%

Engineering Better Thermal Barriers?

- B ion radius largely determine κ
  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

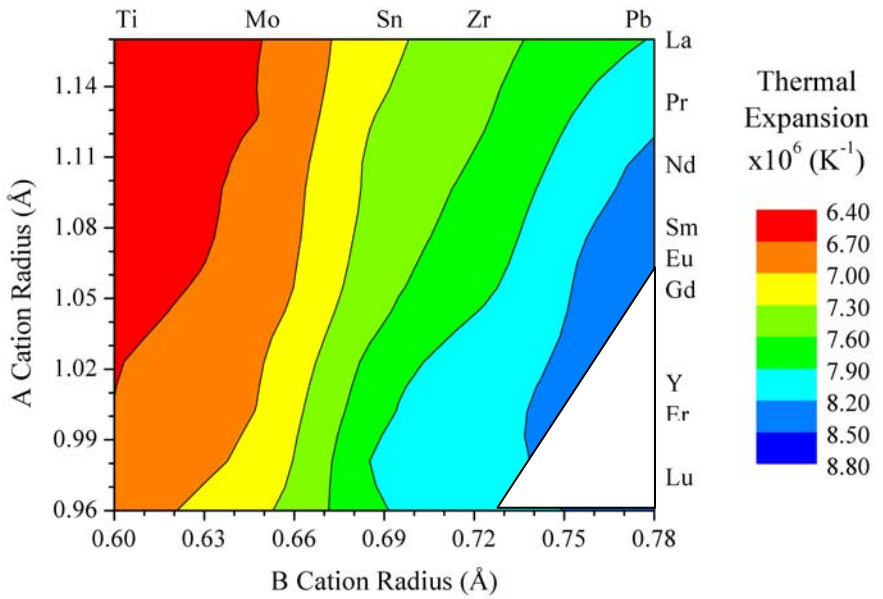


Engineering Better Thermal Barriers?

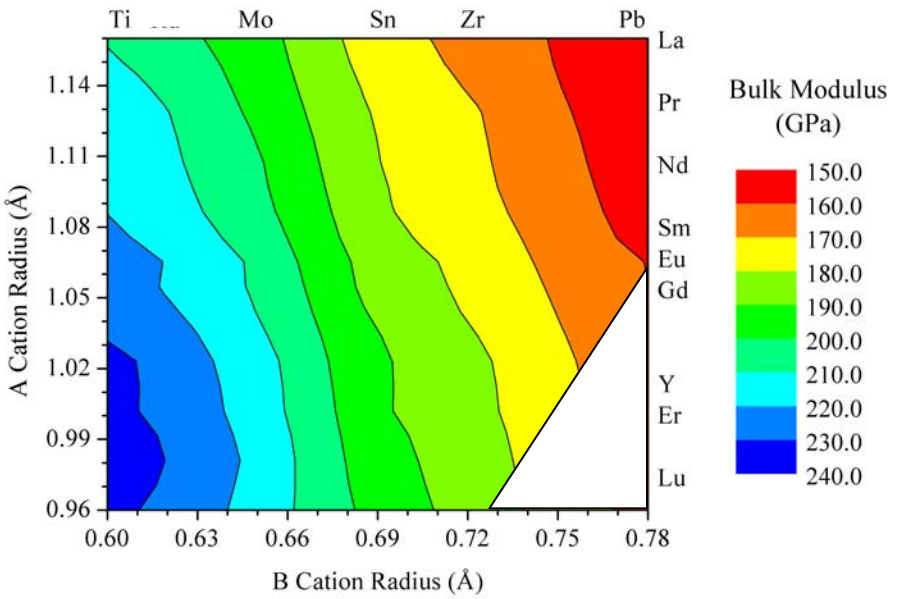
Large B is good for
- lower thermal conductivity
- lower bulk modulus
- higher thermal expansion

Large B is bad for
- phase stability

Thermal expansion coefficient

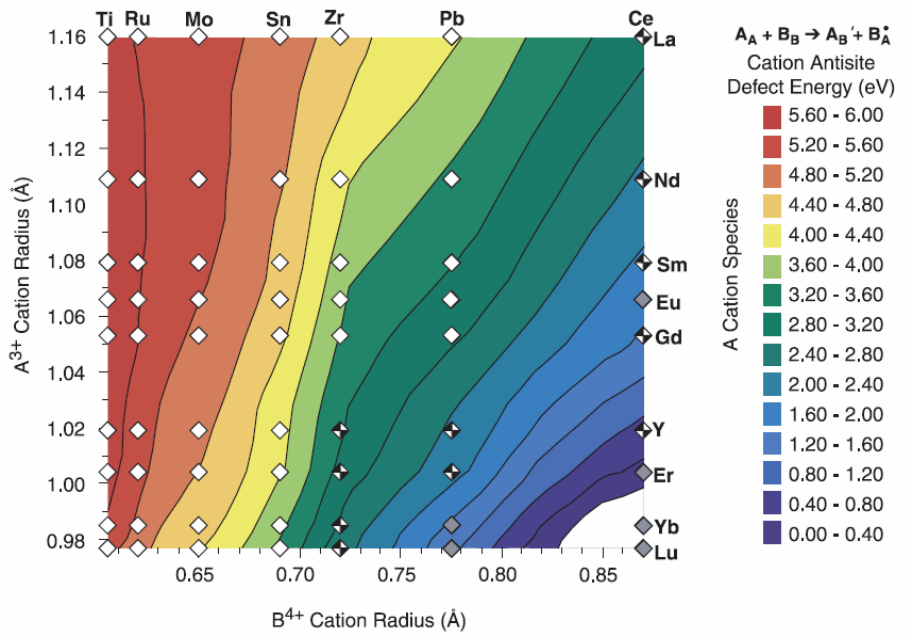


Bulk modulus

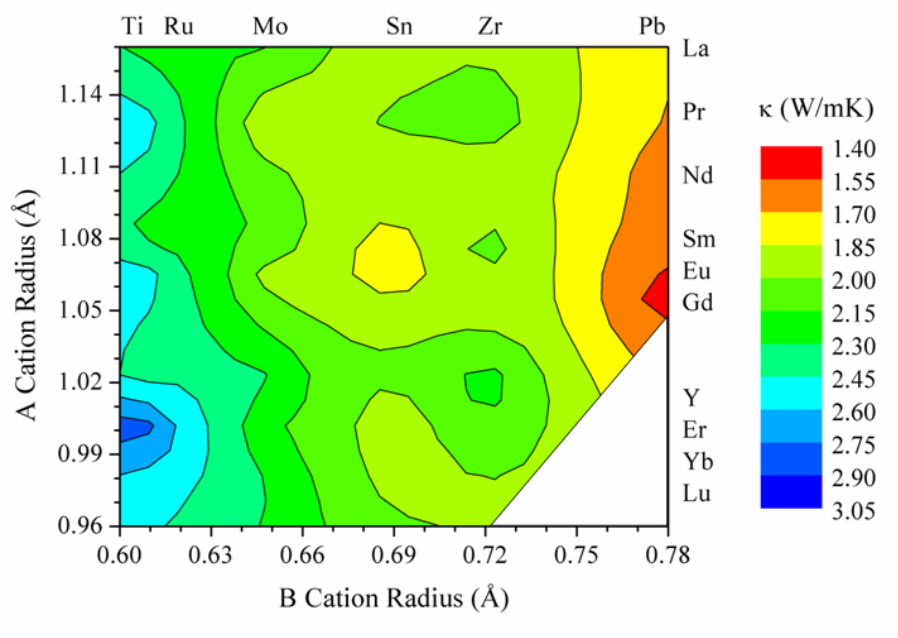


Pyrochlores for Inert Matrix Fuel

Zirconates have low antisite energies → good radiation tolerance



Sickafus, Minervini, Grimes et al. *Science* 2000



Schelling, Phillpot and Grimes, *Phil Mag. Lett* , 2004

However, zirconates have low thermal conductivity

→ composite with higher k material

Can Pyrochlores Be Made Even Better Thermal Barriers?

- **How low can thermal conductivity go?**

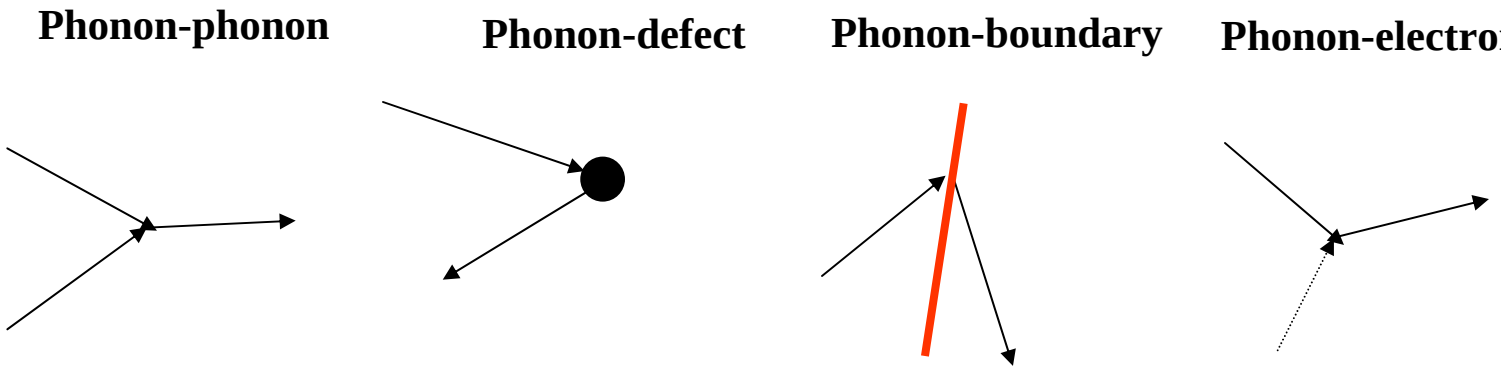
  - $\kappa = 1/3\ C\ v\ \lambda$
  - $\lambda \sim 0.31 - 0.45\ a$
  - nearest neighbor distance ~0.22a
  - further reduction of κ by 1/3 - 1/2 possible

- **How can this be accomplished?**

  - alloying to increase cation and oxygen disorder
  - graded compositions, composites
  - microstructural control (interfacial resistance)

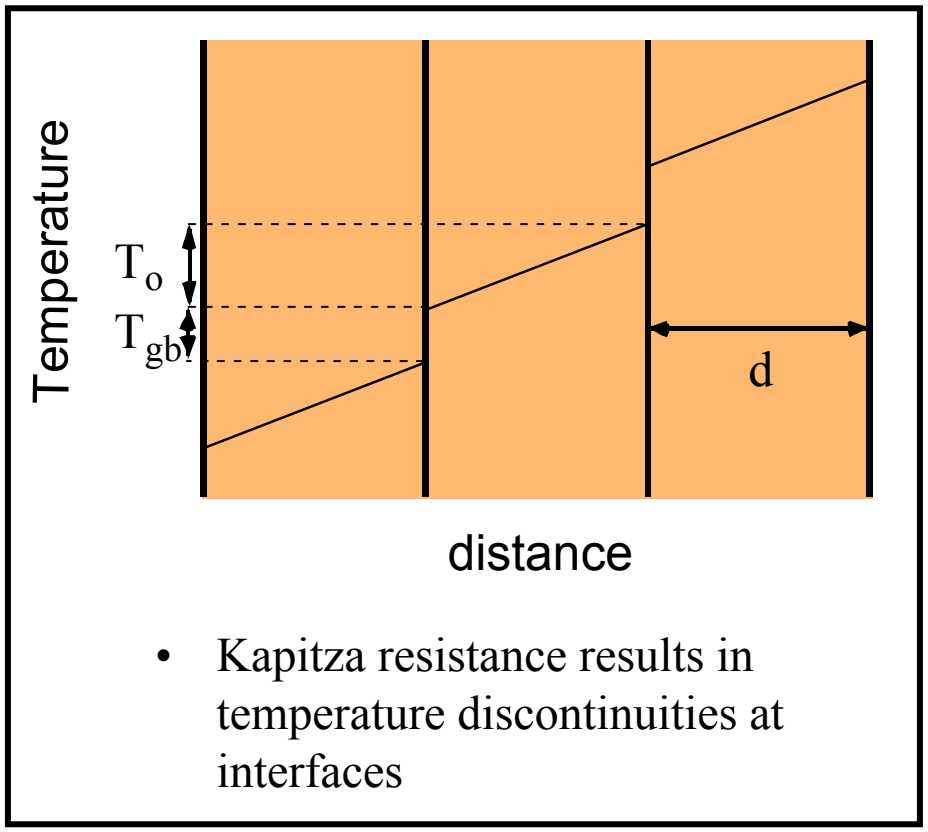
Case Study #2: Interfacial Thermal Conductivity

Phonon Scattering Mechanisms



Macroscale	*****	***	*
Nanoscale	*	***	*****

Interfacial (Kapitza) Thermal Resistance



- Kapitza resistance results in temperature discontinuities at interfaces

$$J = G_K \Delta T$$

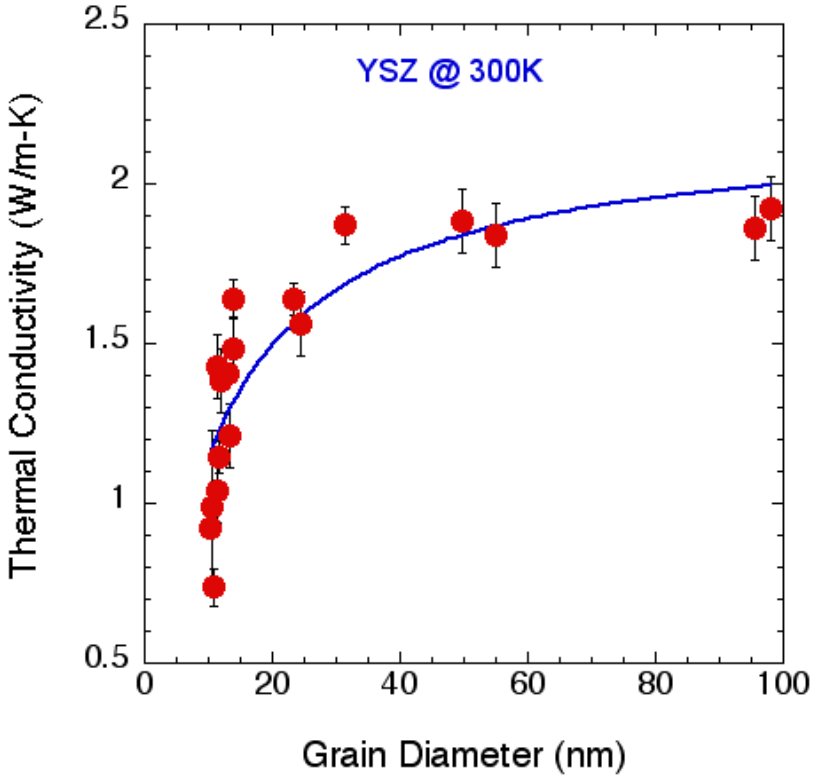
Three grain boundaries:

- **(001) θ=43.6° Σ29**
  - **– high angle, high energy**

(001) θ=11.4° Σ101
  - **– high angle, high energy**

(111) θ=42.1° Σ31
  - **– high angle, high energy**

Kapitza Conductance in YSZ



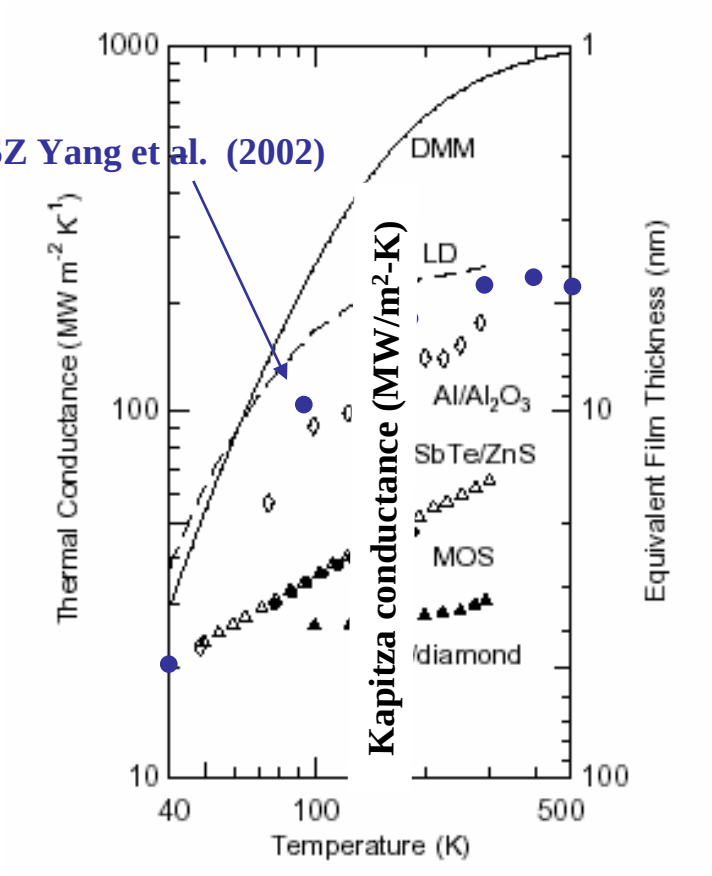
H.-S. Yang *et al.*, *Acta Mater.* (2002)

$$k = \frac{k_o}{1 + \frac{k_o R_k}{d}}$$

- R_k and k_o are obtained by a 2-parameter fit to $k(d)$
- $G_k = 1/R_k$ ← **Kapitza Resistance**

Kapitza Conductance

Kapitza Conductance



Three Si grain boundaries:

- **(001) θ=43.6° Σ29**
  - **high angle, high energy**

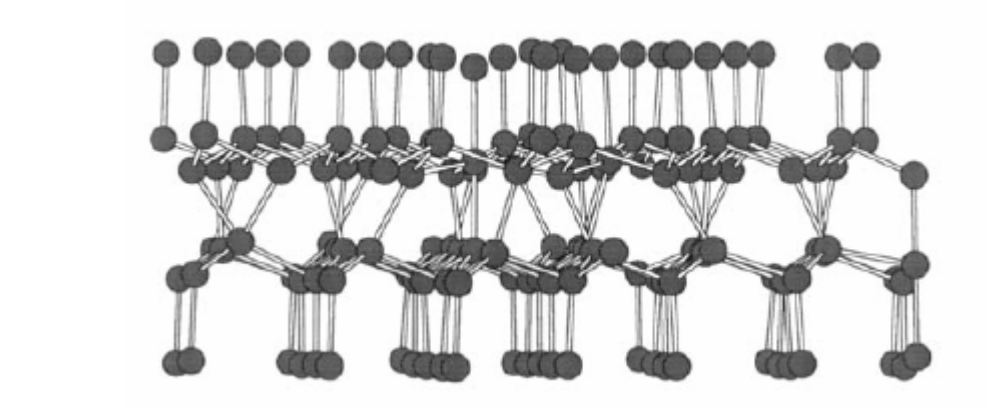
(001) θ=11.4° Σ101
  - **high angle, high energy**

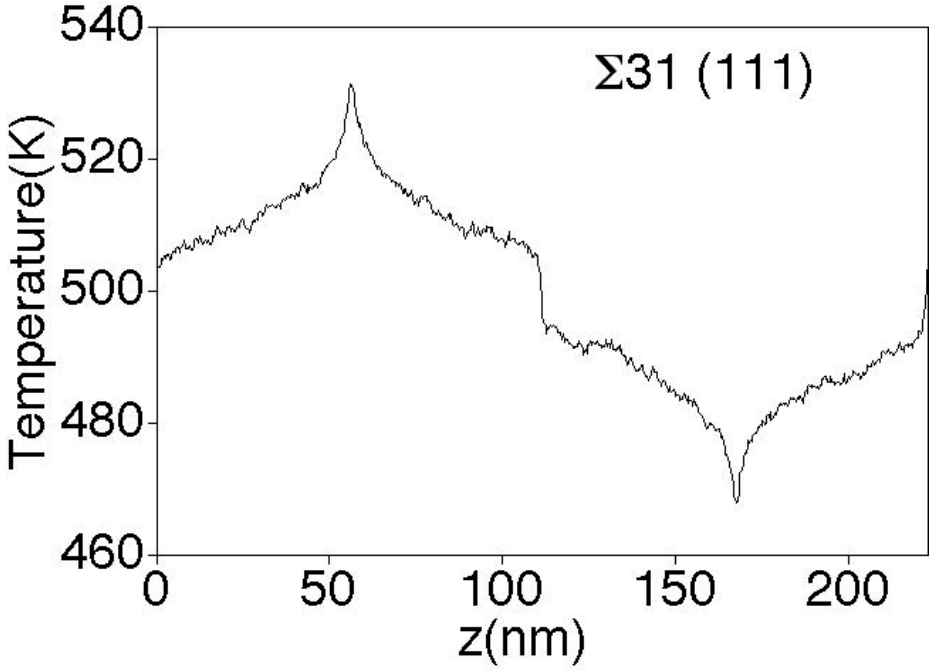
(111) θ=42.1° Σ31
  - **high angle, high energy**

Cahill, Goodson, and Majumdar, *Jn. Heat Transfer*, **124**, 223, (2002)

- data for nanocrystalline YSZ similar to that for several heterophase systems

Low-Energy, High-Angle GB: (111) θ=42.10° Σ31





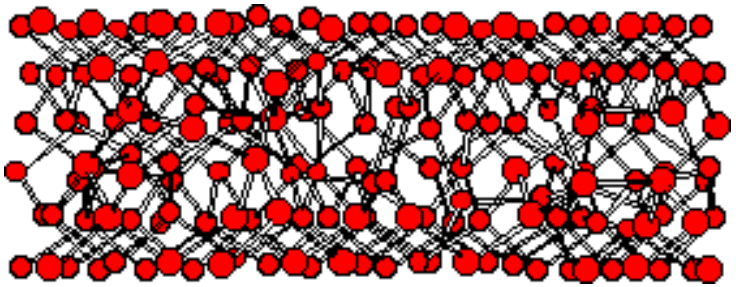
E_{gb} = 0.64 J/m^2

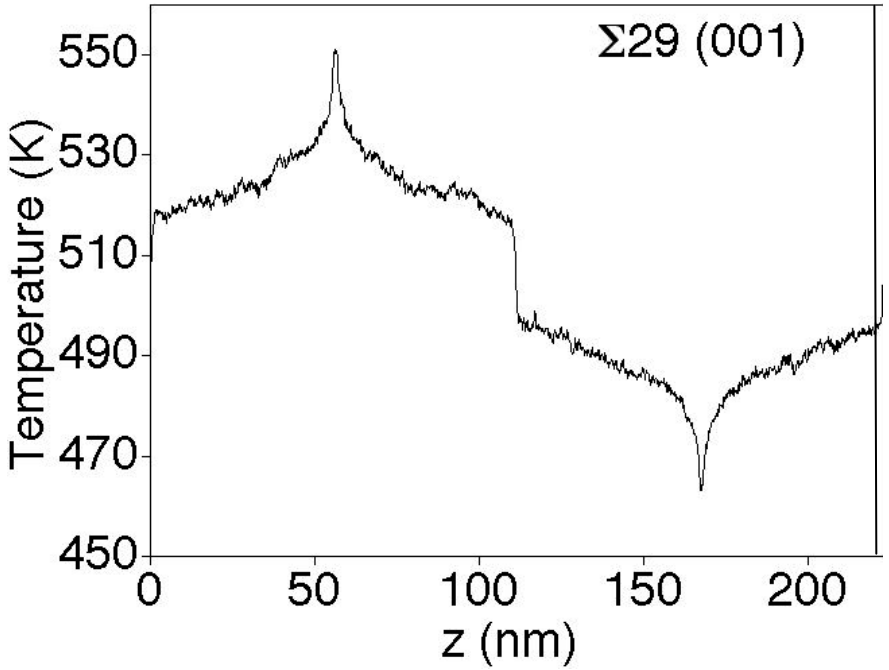
Coordination at GB
C3: 0%
C_4: 94%
C_5: 6%

$$J = G_K \Delta T$$

G_K = 1.53GW/m^{2}K

Typical High-Energy GB: (001) θ=43.60° (Σ29)





E_{gb} = 1.32 J/m^2

Coordination at GB

C_3:8%

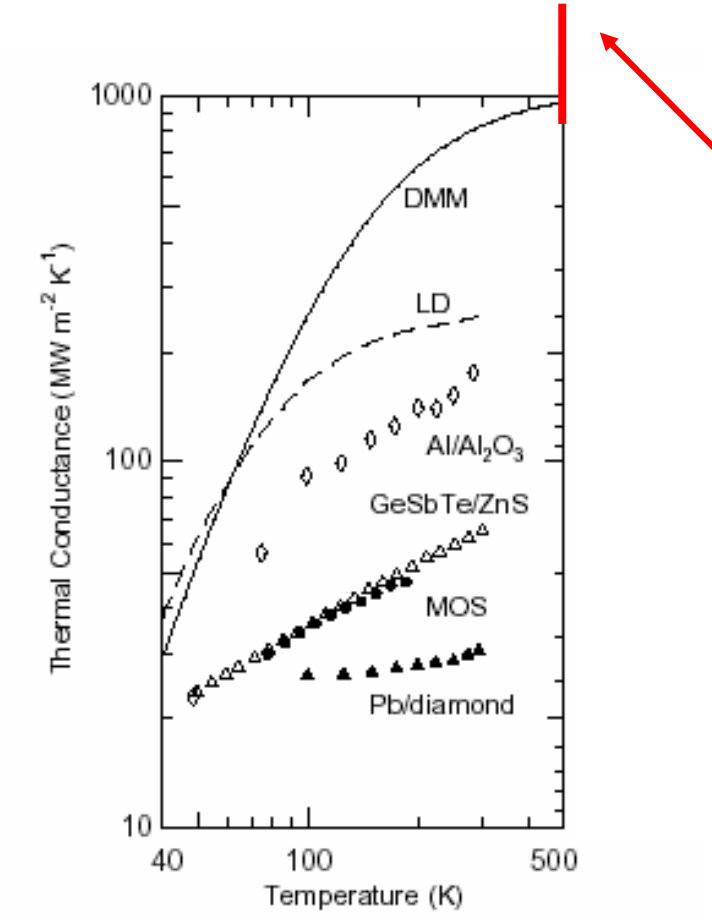
C_4: 82%

C_5: 10%

G_K = 0.85GW/m^{2}K

Interface Conductance

$$J = G_K \Delta T$$



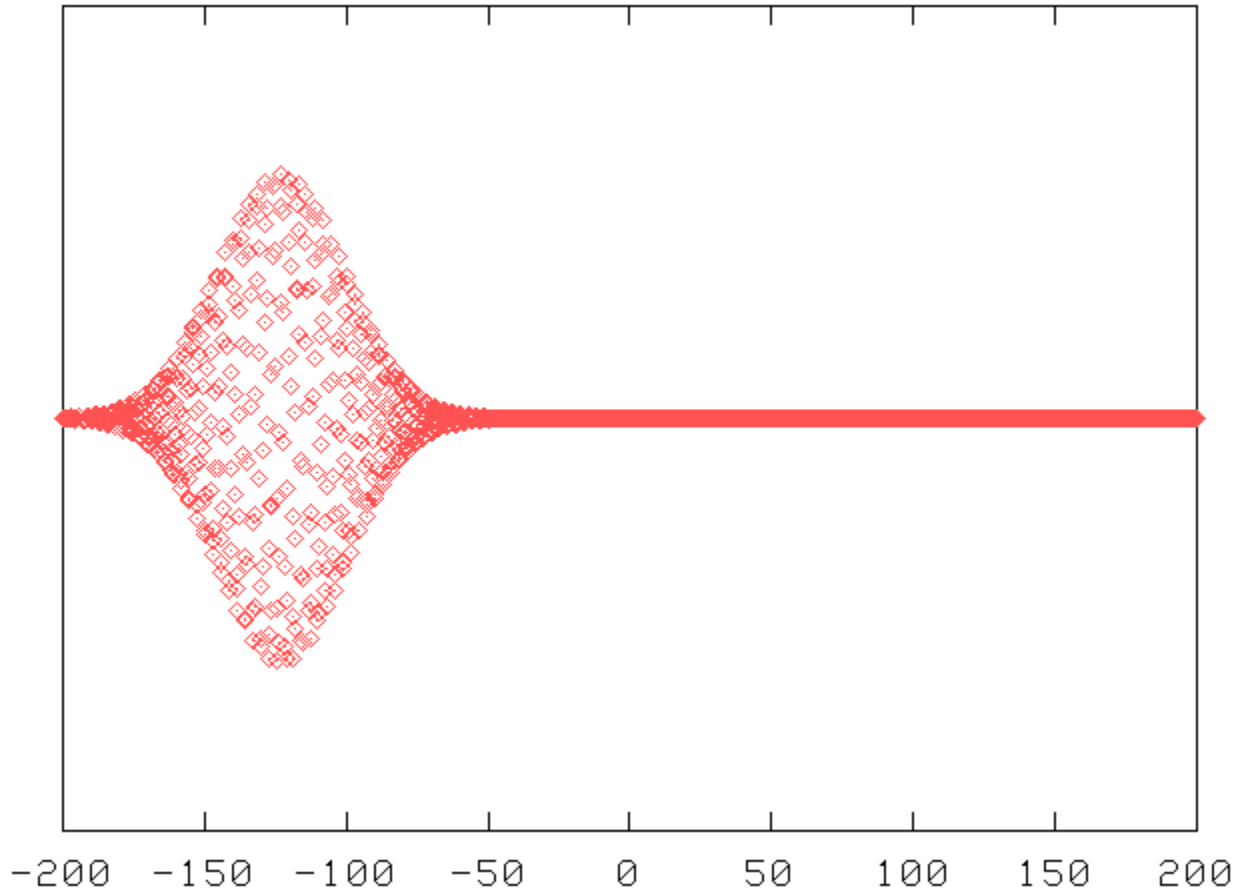
(001) Σ29 θ=43.60°
E_{gb} = 1.32 J/m^2
G_K = 0.85GW/m^{2}K

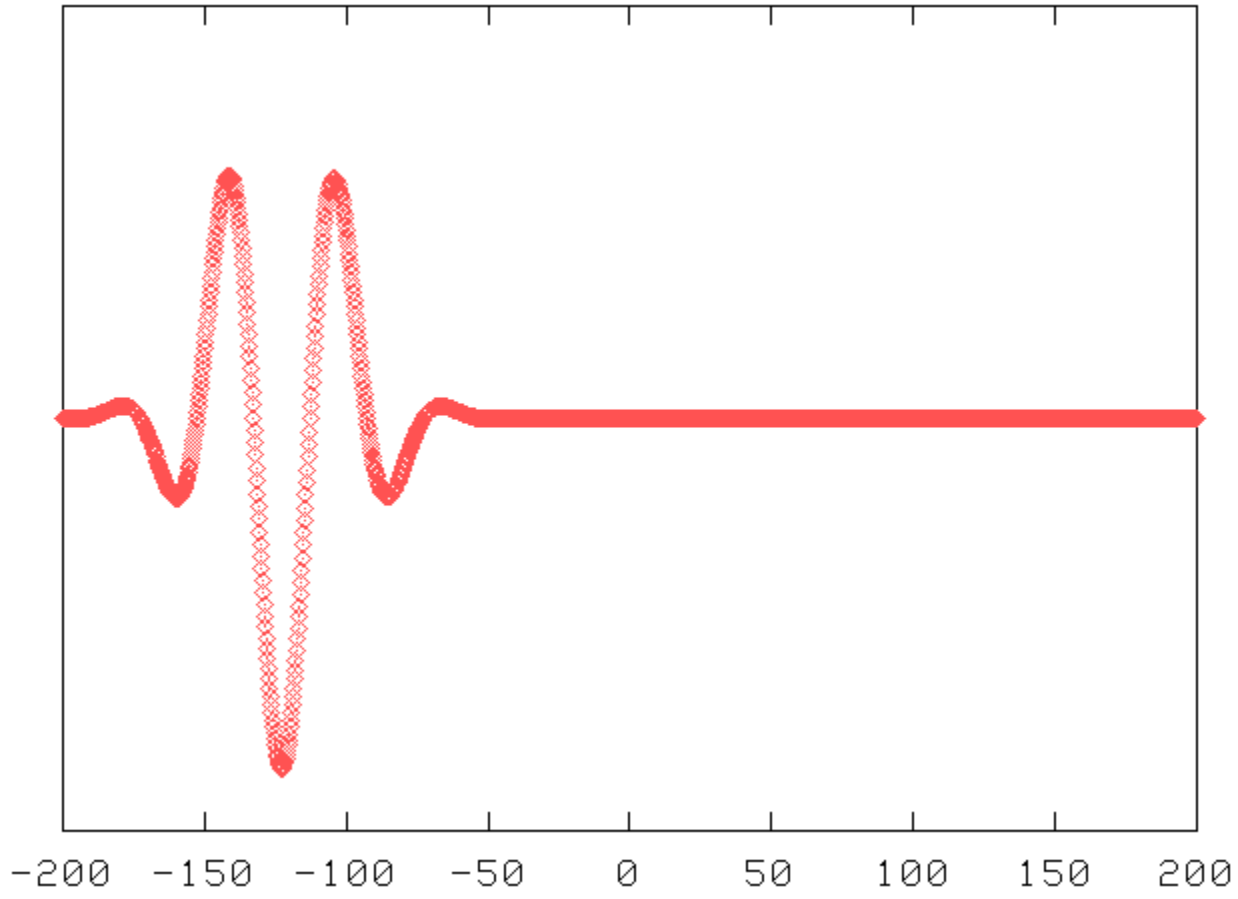
(001) θ=11.42° Σ101
E_{gb} = 0.91 J/m^2
G_K = 1.71GW/m^{2}K

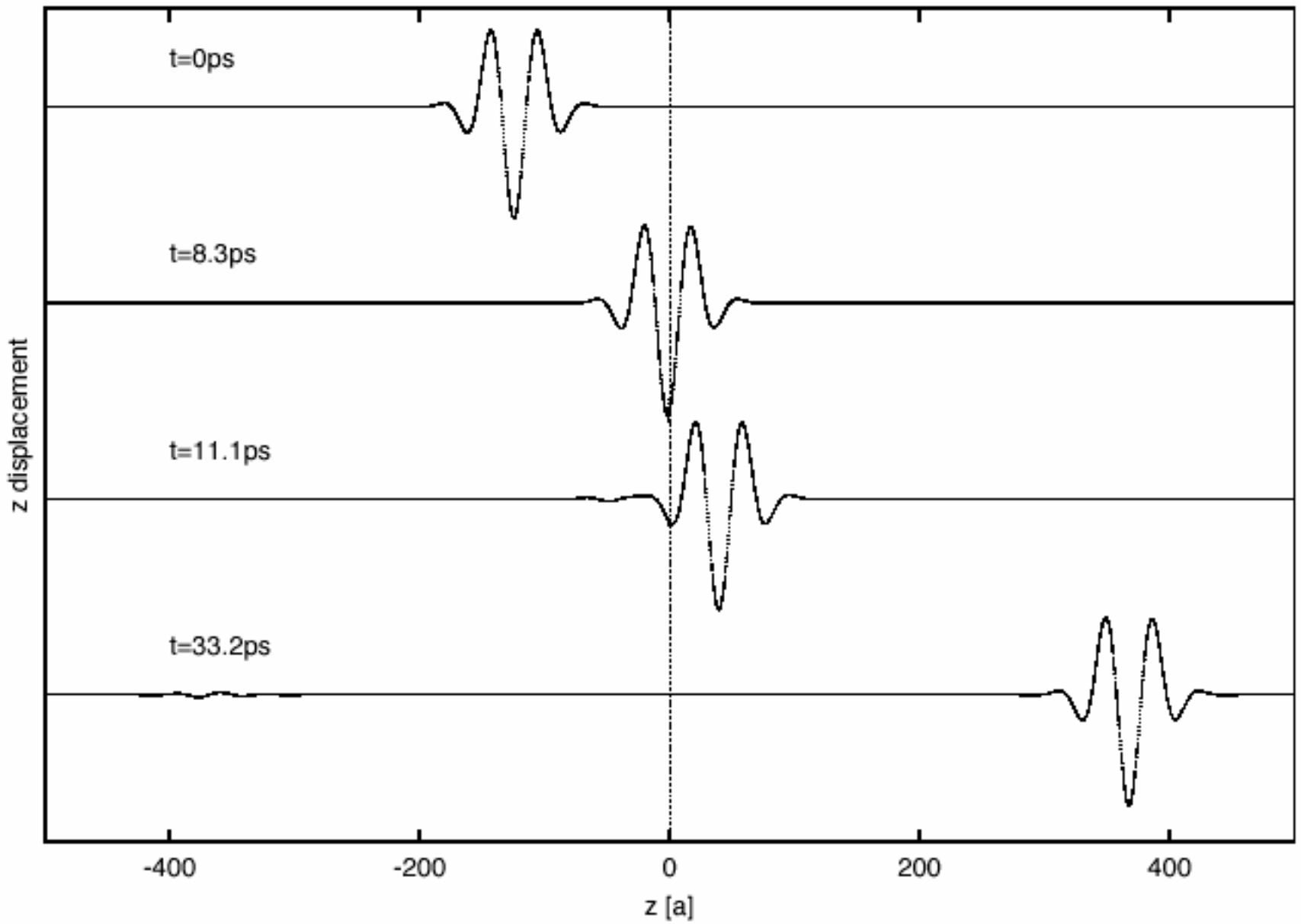
(111) Σ31 θ=42.10°
E_{gb} = 0.64 J/m^2
G_K = 1.53GW/m^{2}K

Maiti et al:
(310) STGB
G_K = 0.9GW/m^{2}K @575K

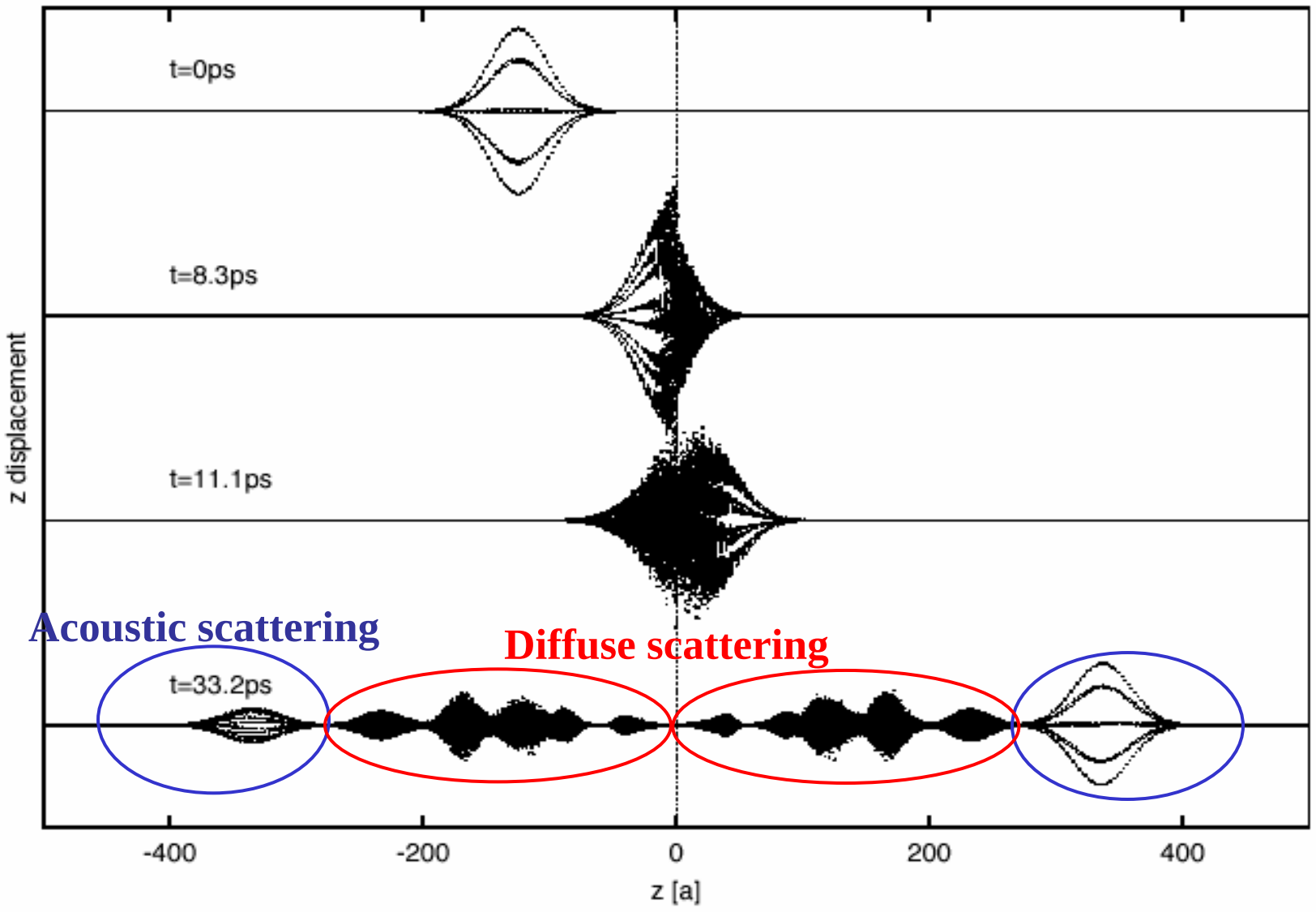
(510) STGB
G_K = 0.8 GW/m^{2}K @ 575K


-200
-150
-100
-50
0
50
100
150
200


-200
-150
-100
-50
0
50
100
150
200

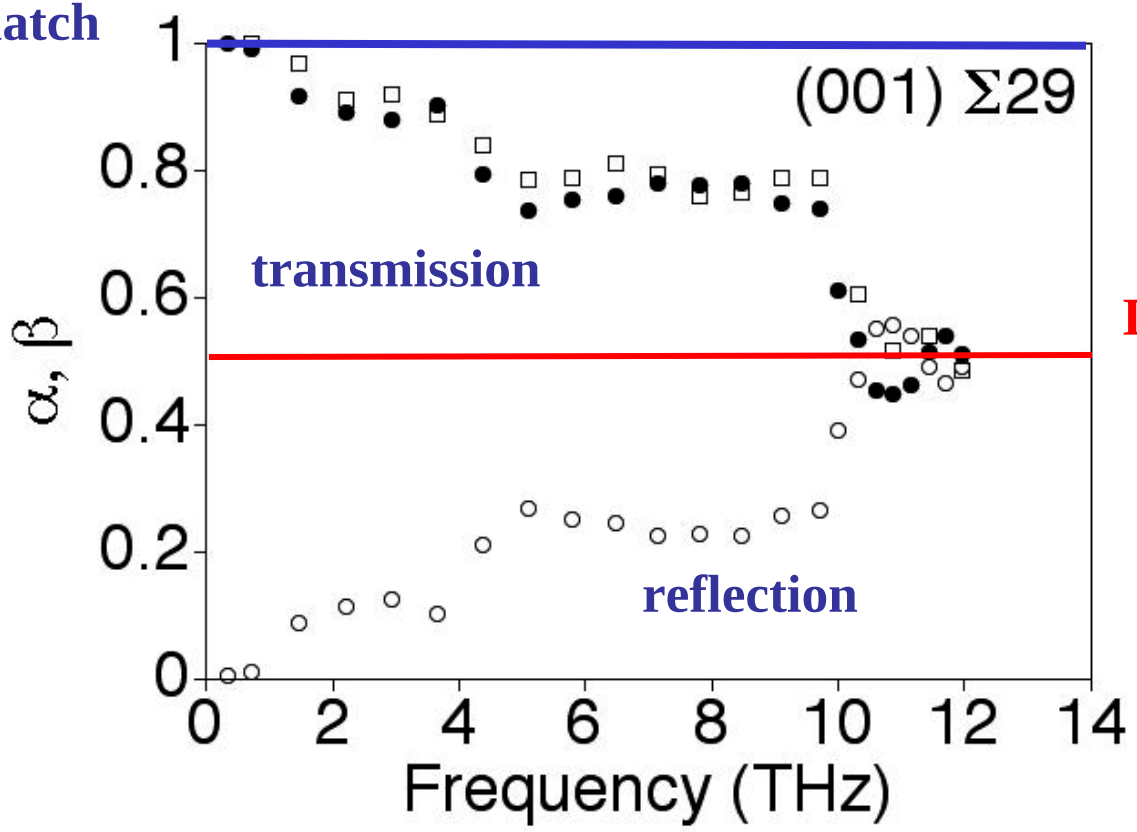

t=0ps
t=8.3ps
t=11.1ps
t=33.2ps
z displacement
-400
-200
0
200
400
z [a]

High-Frequency LA mode



Frequency Dependence of Phonon Scattering

Acoustic Mismatch Model



Diffuse Mismatch Model

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

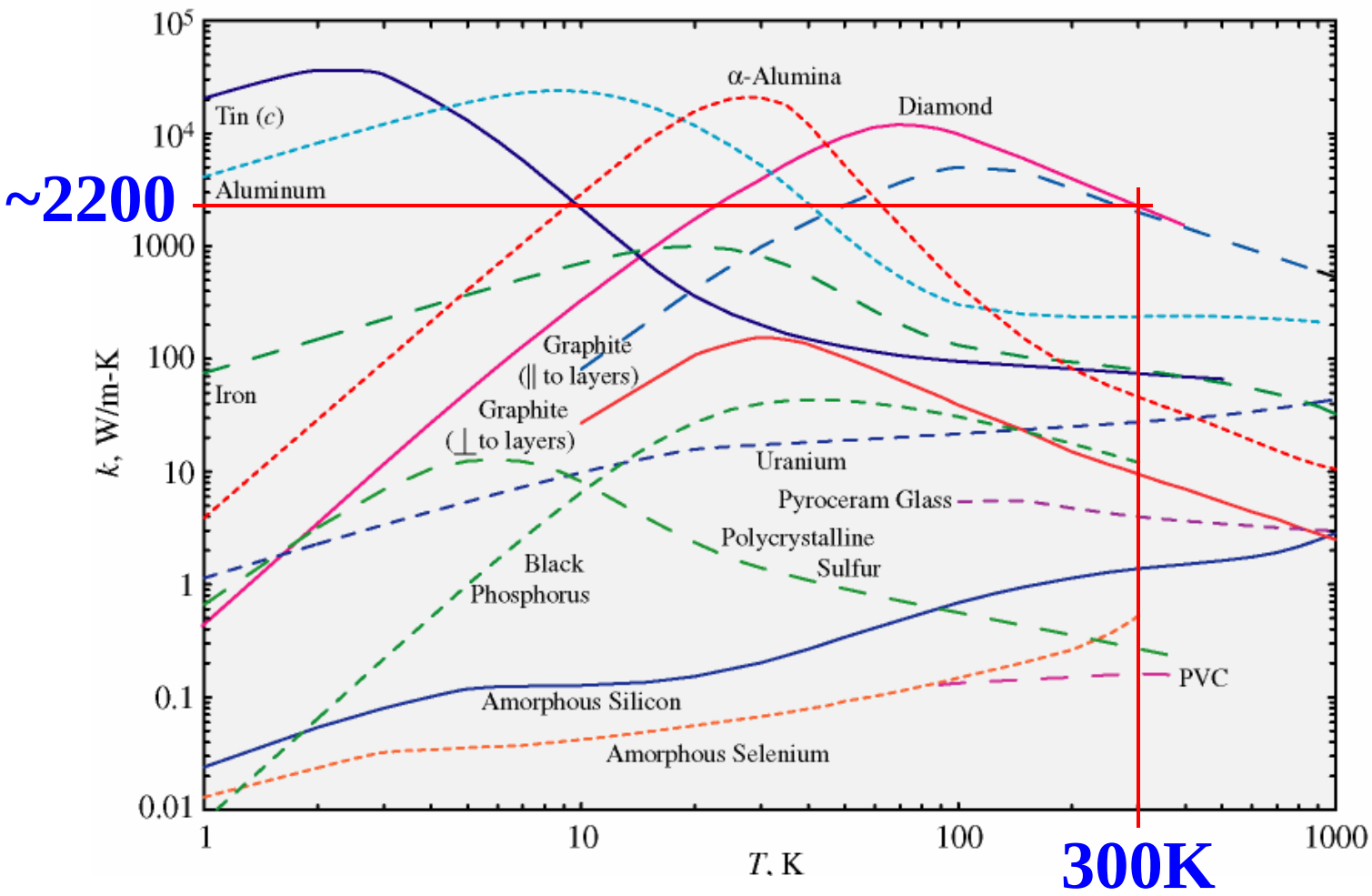
$$\sigma_K(T) = (1/\Omega) \sum \hbar\omega_{\lambda\mathbf{k}}\, \partial n(\omega_{\lambda\mathbf{k}},T)/\partial T\, \partial\omega_{\lambda\mathbf{k}}/\partial k_z\, \alpha_{\lambda\mathbf{k}}$$

	σ_K (MD)	σ_K (computed) GW/m^2K	computed/MD
Σ29	0.855	0.457	0.534
Σ101	1.710	0.904	0.528

1. Computed results only includes LA, TA modes

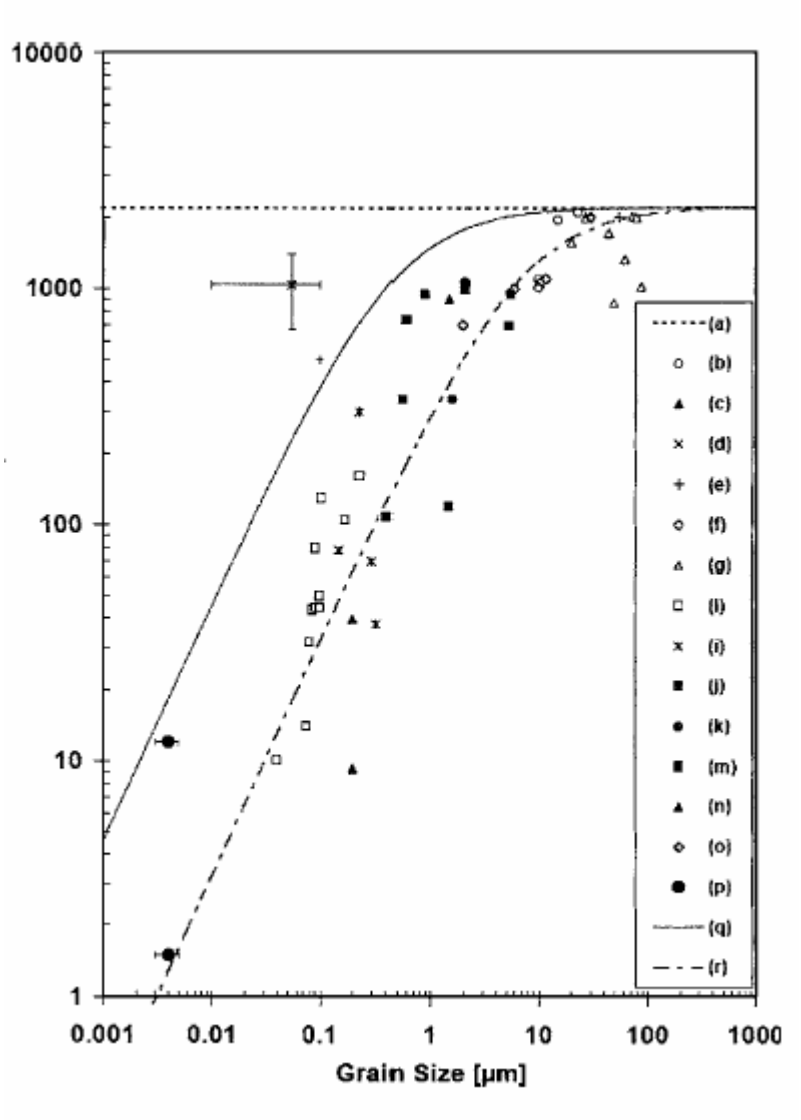
2. The Σ101 computed result assumes $\alpha(\omega)$ same for TA modes as LA

3. Effects of non-normal incidence not included



S.R.Phillpot and A.J.H. McGaughey, Materials Today, June 2005

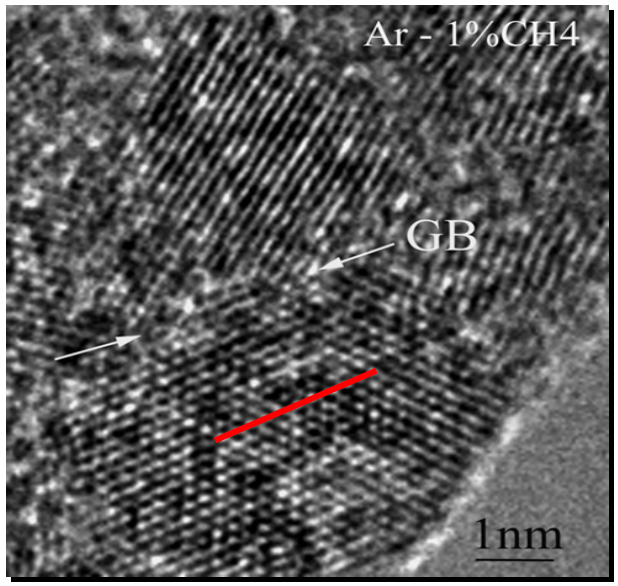
Ultrananocrystalline Diamond (Experiment)



Measured $\kappa = 12$ W/mK

for grain size 3~5 nm at 310K

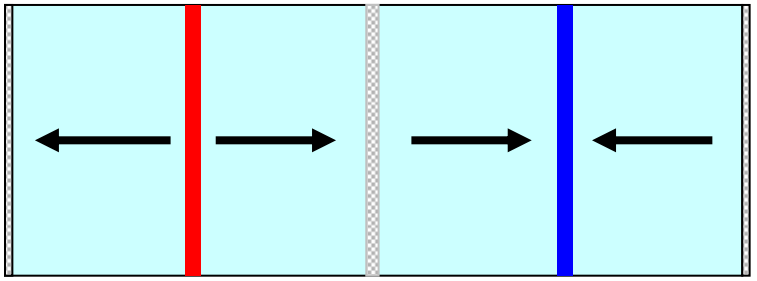
$\rightarrow$ $G_K = 3$ GW/m^{2}K



Angadi et al. JAP 99, 114301 (2006)

A Typical Temperature Profile

Tersoff potential: 3-body interactions and naturally incorporates sp^3, sp^2 hybridization



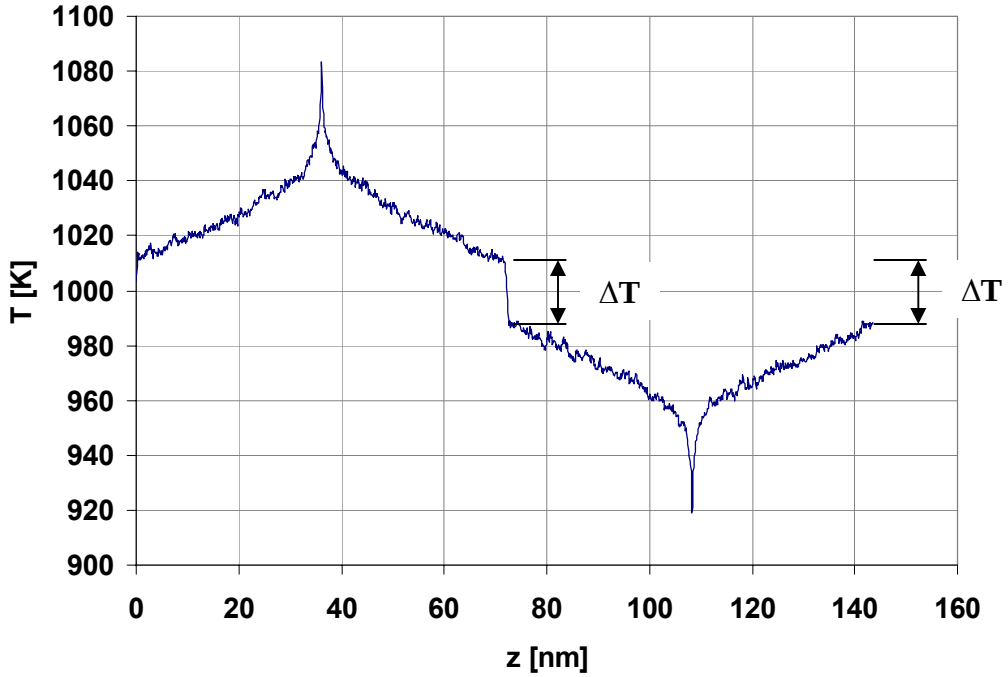
Σ29(001) θ=43.6°

46400 atoms

$<T>$=1000K

ΔT=22.5K

G_K = 9.7 GW/m^{2}K

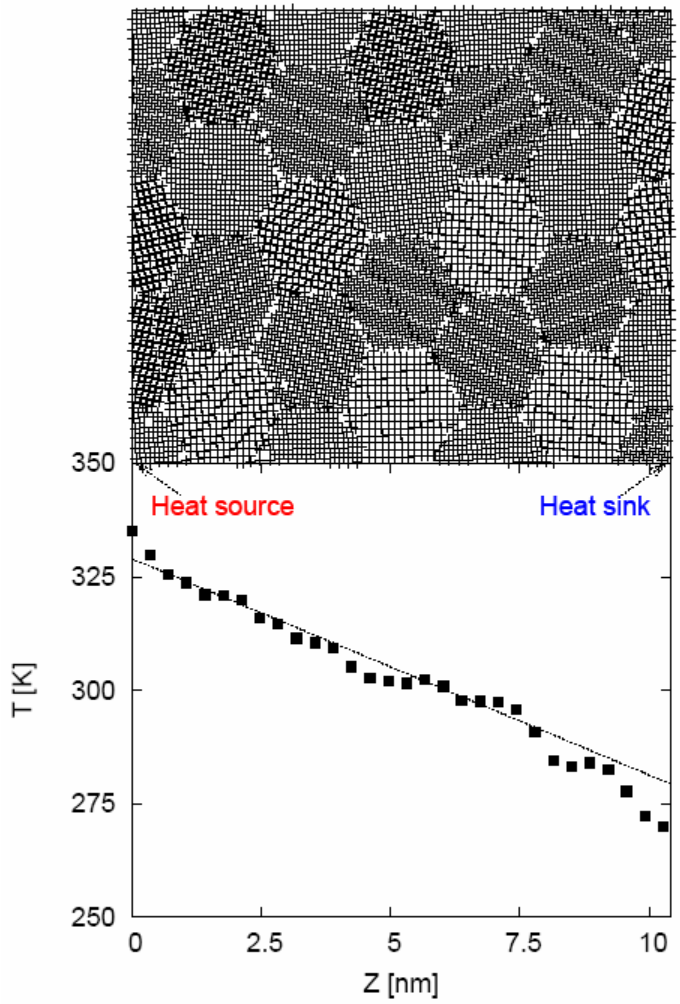


Ultrananocrystalline Diamond (Simulation)

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

Using $d = 3\,nm$,

$\therefore G_K = 4.6\,GW/m^2K$

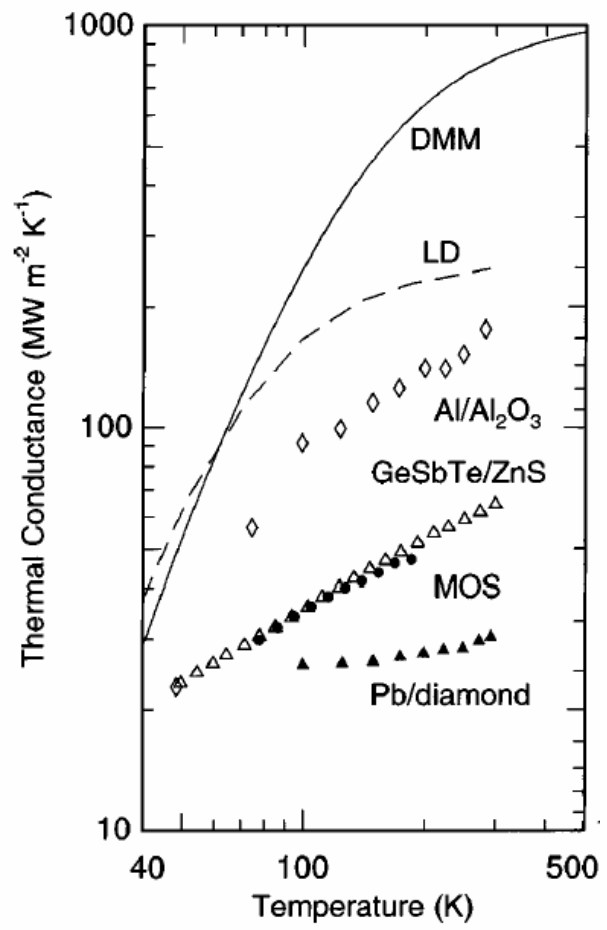


Comparison of Experiment and Simulation

	κ [W/mK]	G_K [GW/m^{2}K]
Experiment	1-12	3
Simulation (Polycrystalline)	14	4.6
Simulation (Grain Boundary)	26	8.5

Note: d = 3 nm, κ_o=2200 W/mK at room temperature

- Experimental and simulation results compare within the factor of 2.
- $\kappa/\kappa_o \sim 1\%$
- G_K of diamond is much higher than that of any other materials.



*Cahill et al. JAP **90** 5 (2003)*

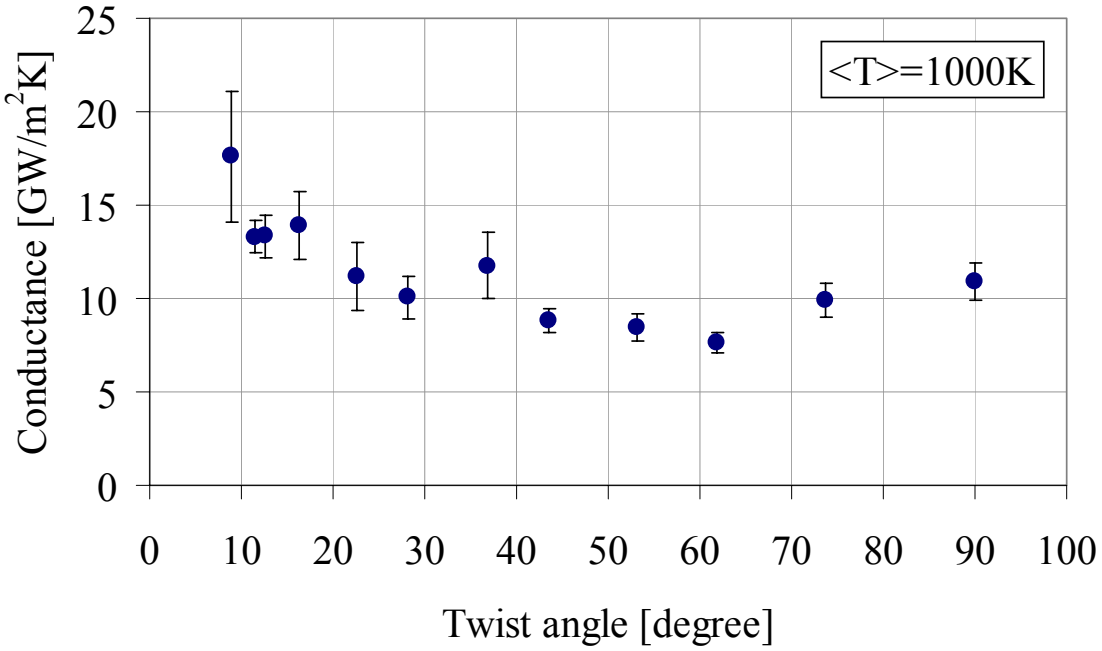
Kapitza Conductance and Twist Angle

• G_K remains fairly constant over a wide range of angle (~20° to 70°)

→ Coordination of atoms in the GBs is very similar

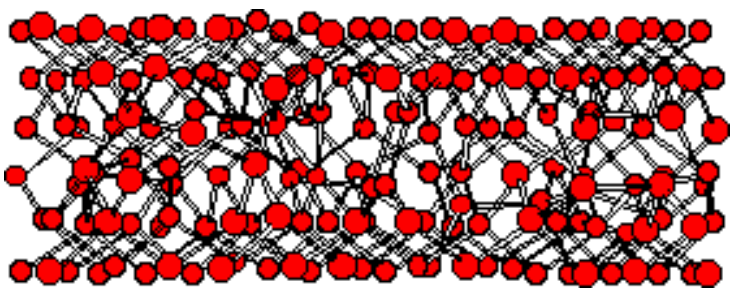
•Higher conductance at low angle (<15°) because of the sparse distribution of dislocation

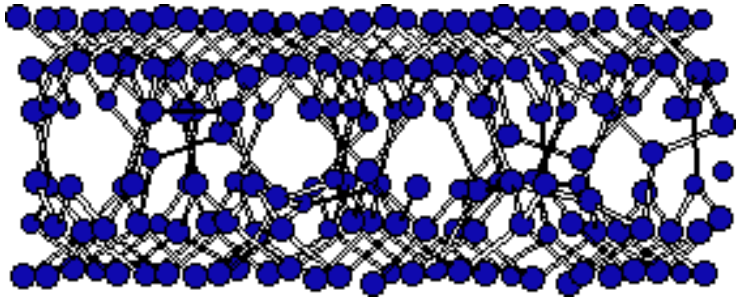
• Slight increase near 90° because of the symmetry of diamond structure



Bonding and Interfacial Conductance: Diamond vs. Si

(001) θ=43.60° (Σ29)





Silicon

Coordination	Si	C
2	0%	2%
3	8%	80%
4	82%	18%
5	10%	0%
<C>	4.02	3.26

Diamond

Better bonding across the silicon GB should lead to better thermal transport

Diamond vs. Silicon

(001) Σ29 Grain Boundary

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

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

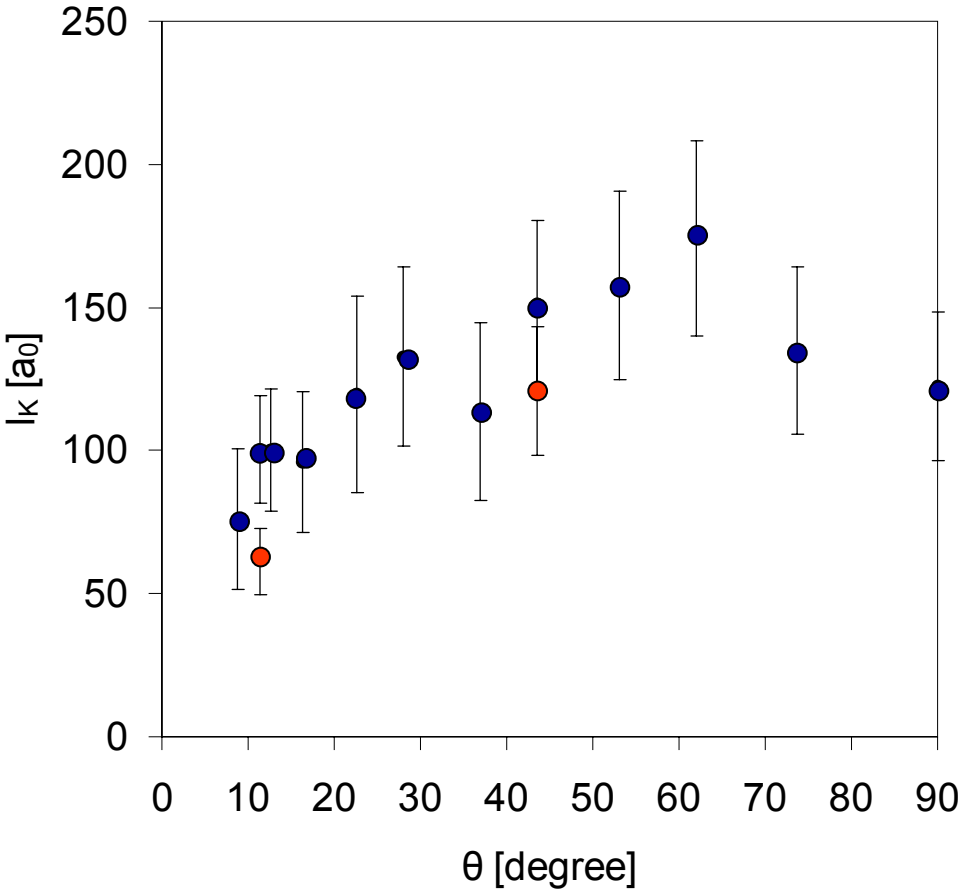
Conclude: Diamond GBs 10X better conductors of heat than Si GBs

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

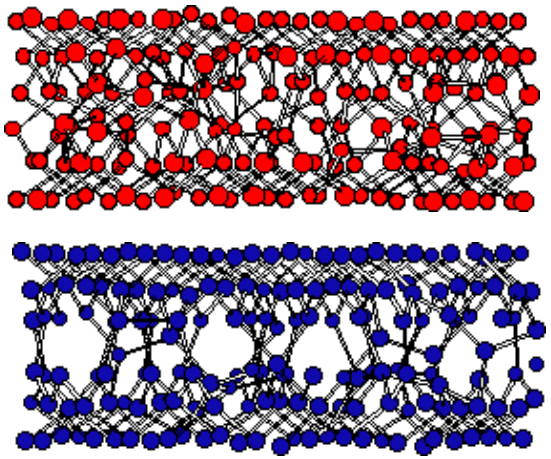
Kapitza length (equivalent thickness of perfect crystal):

$$\lambda_K = k/G_K$$

Normalize Kapitza Length to Lattice Parameter

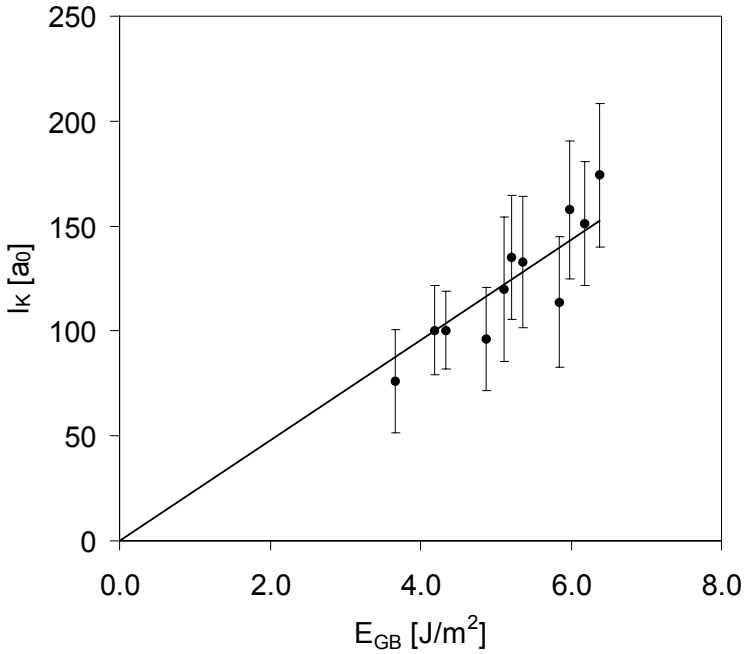


Coordination	Si	C
2	0%	2%
3	8%	80%
4	82%	18%
5	10%	0%
<C>	4.02	3.26



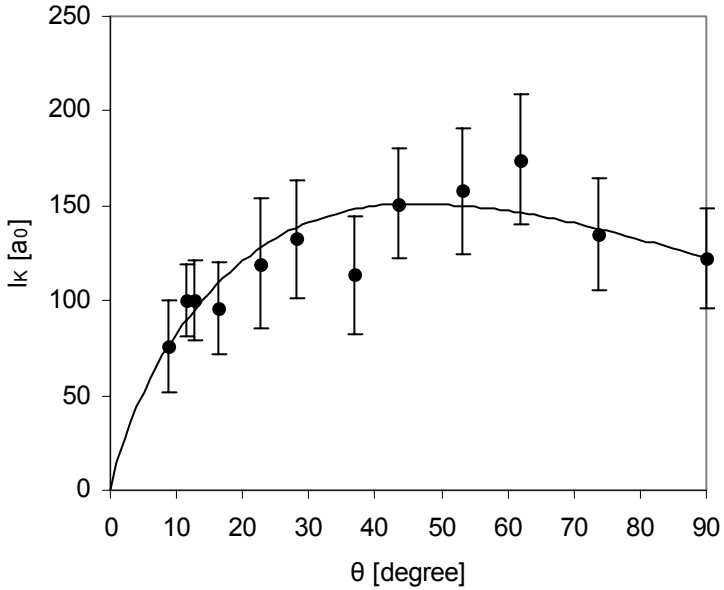
Final conclusion: Silicon GBs are better conductors of heat than diamond GBs!

Kapitza Length



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

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

$1/t \sim c$

$1/t \sim f^4$

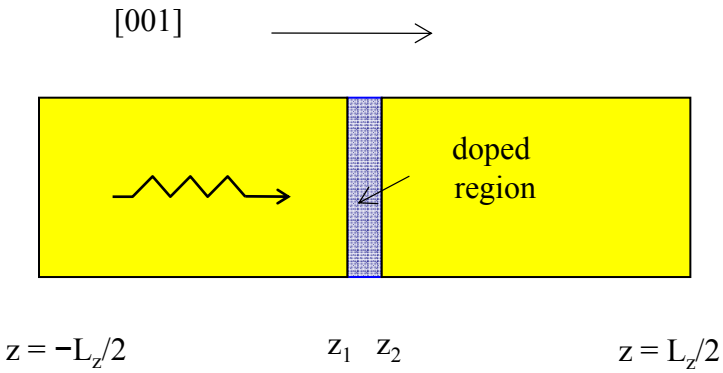
t^{-1} – phonon scattering rate
A – material constant
Δm – mass difference
c - isotope concentration
f – frequency

The formula was derived from weak scattering.

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

P. G. Klemens, Proc. R. Soc. London, Ser. A **68**, 1113 (1955)

Simulation system



Thickness of doped region Δz

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

Dopant concentration c

0.078 - 1.56 atom%

Phonon wave packet frequency f:

1.5 -13THz

- Simulation cell:
  Maximum used:
  2×2×6000 unit cells
  L_z=6000 unit cells
  (3.268μm)
- Simulation time step size:
  dt = 0.55 fsec
- Diamond-structured Si
- Stillinger-Weber potential

Simulation system

- Dopants randomly distributed in doped region
- Differ from Si in mass

  $M_{dop} = 4M_{Si} = 112$ amu (atomic mass unit)

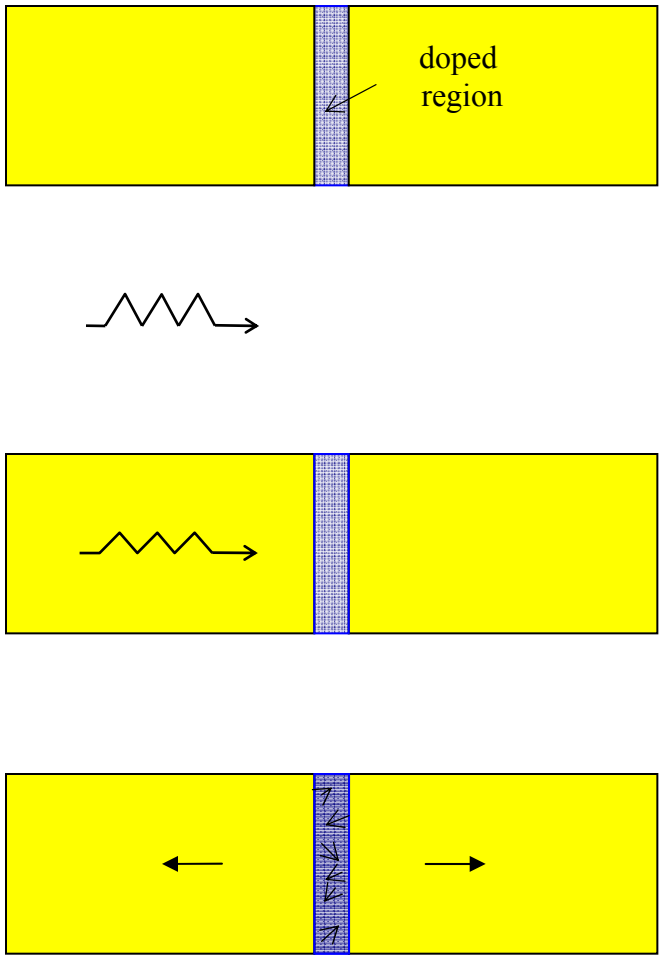
  larger than M_{Ge} (72.59amu)

  – To understand the effects of mass defect
  – To compare with previous simulations of superlattices

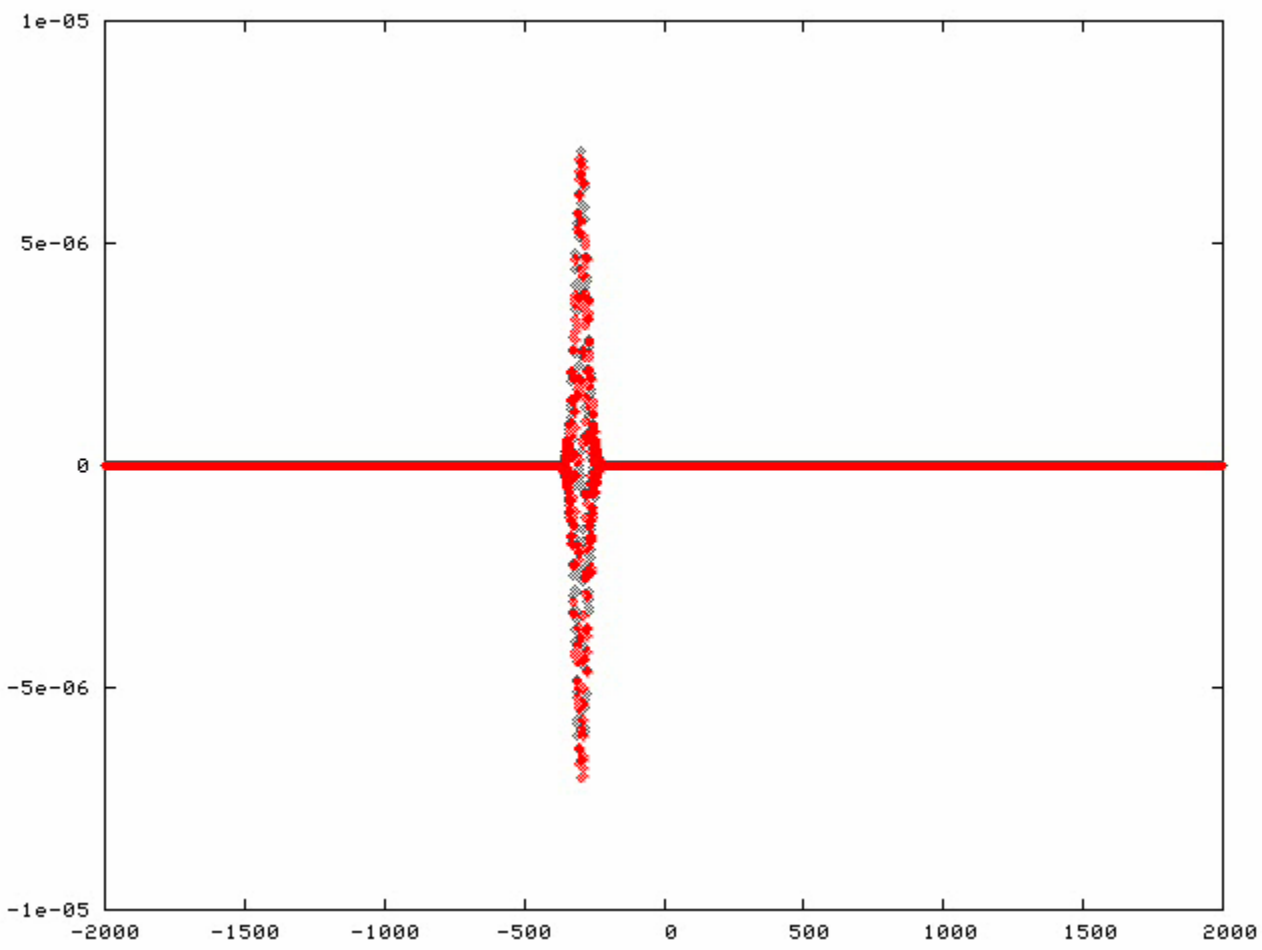
Calculation procedure

Four steps:

- structure creation
- initial phonon wave packet generation
  - well-defined longitudinal acoustic phonon
- MD simulation
- energy analysis



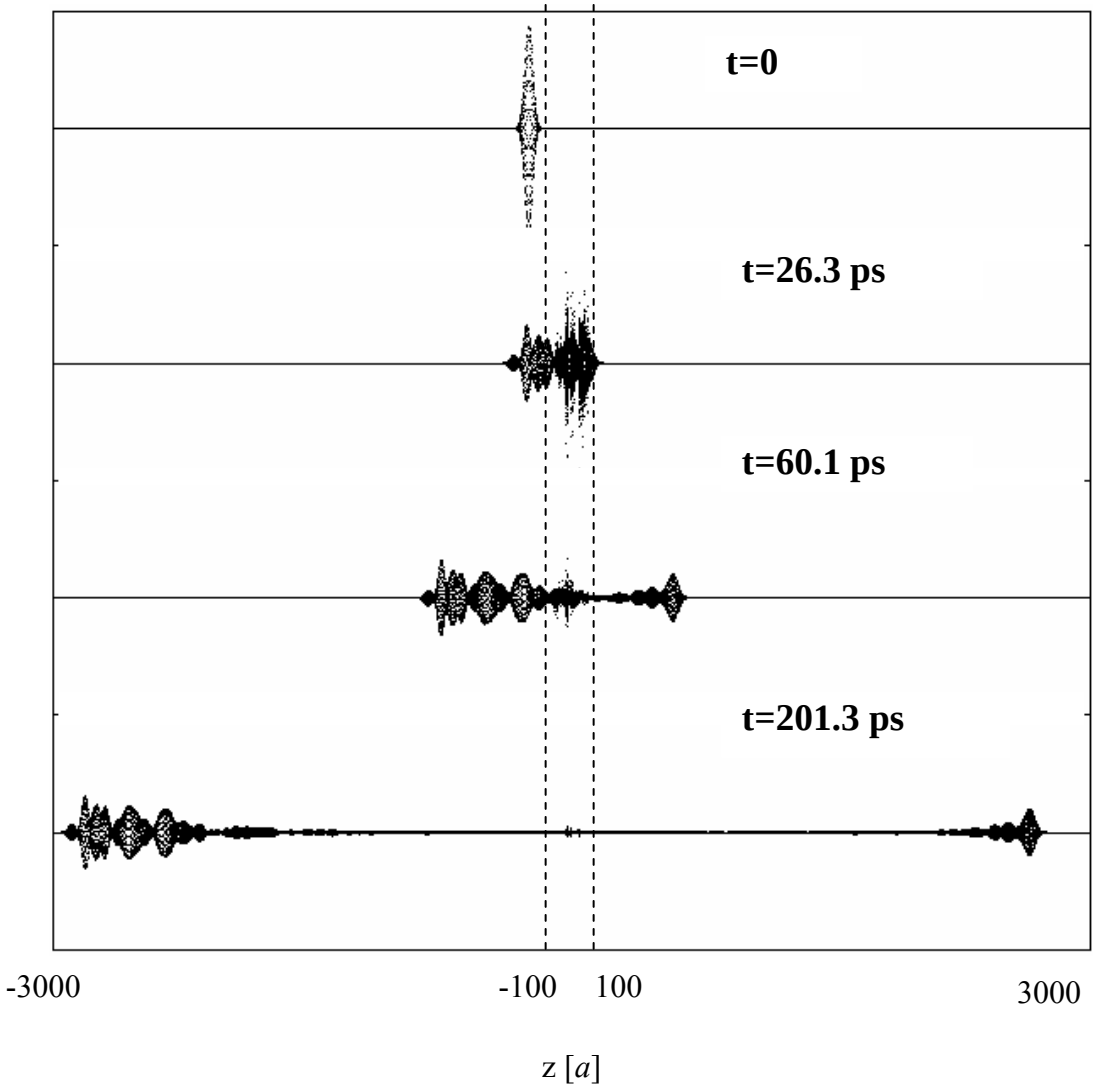
Phonon propagation and scattering description at atomic scale



- Incident phonon frequency: 2.96THz
- 1.56% dopants in doped region
- Δz = 200 unit cell

Snapshots

Energy trapped in the defect region becomes negligible by ~200 ps



Energy analysis

coefficient of reflected energy

$$R = E_{reflect}/E_{total}$$

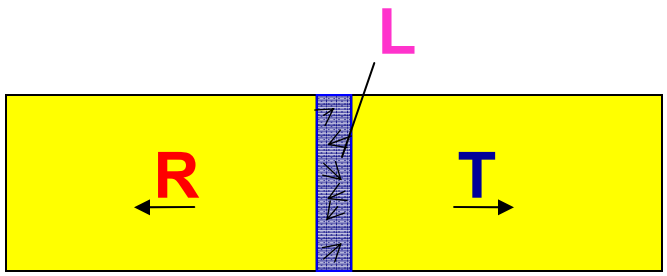
coefficient of trapped energy

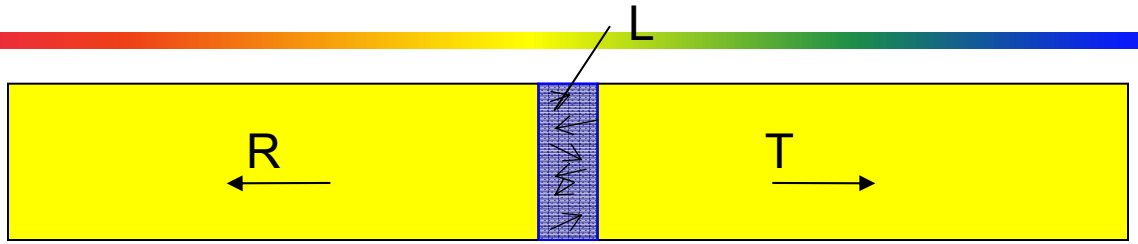
$$L = (E_{total} - E_{reflect} - E_{tran}) / E_{total}$$

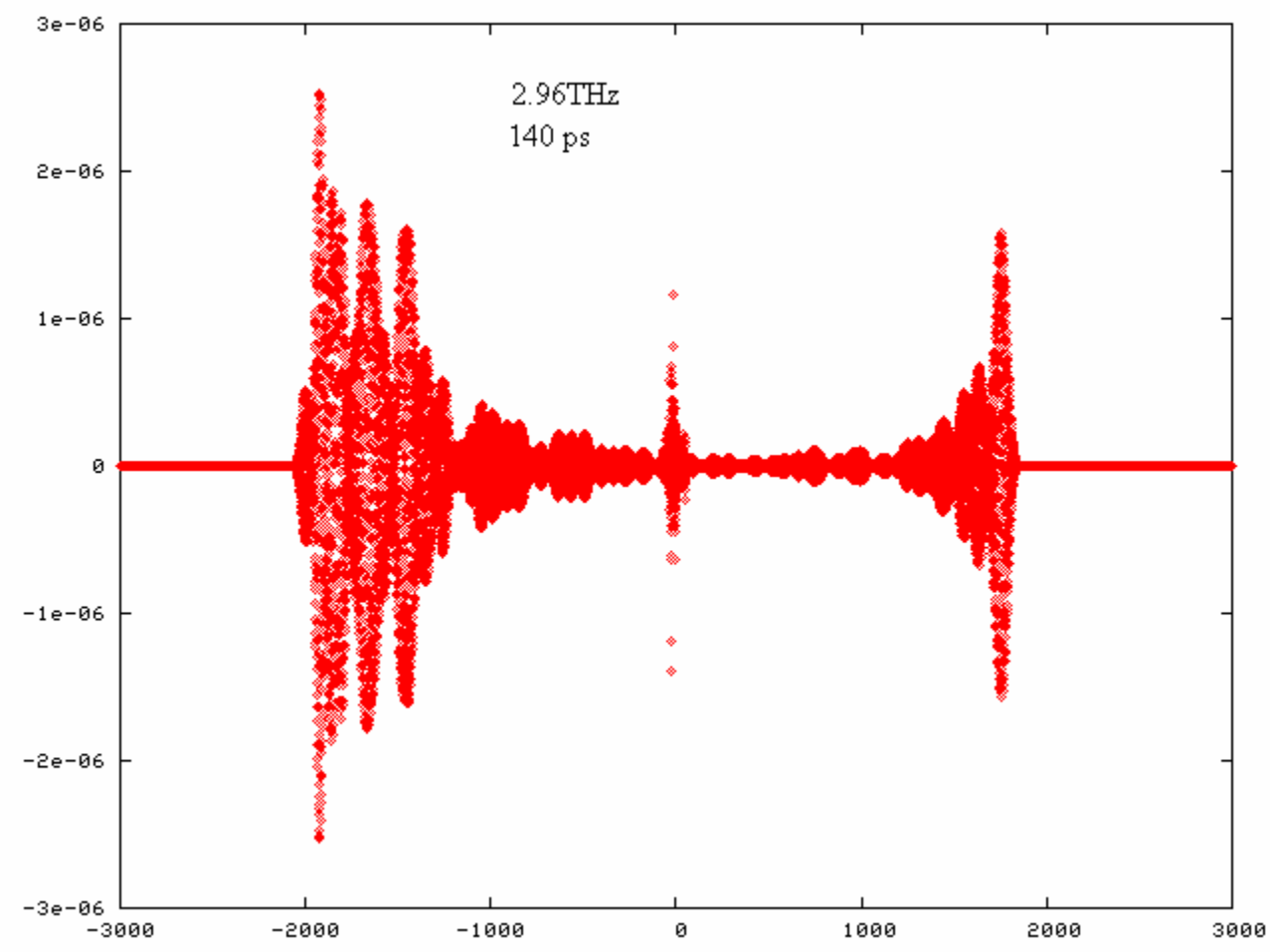
coefficient of transmitted energy

$$T = E_{tran}/E_{total}$$

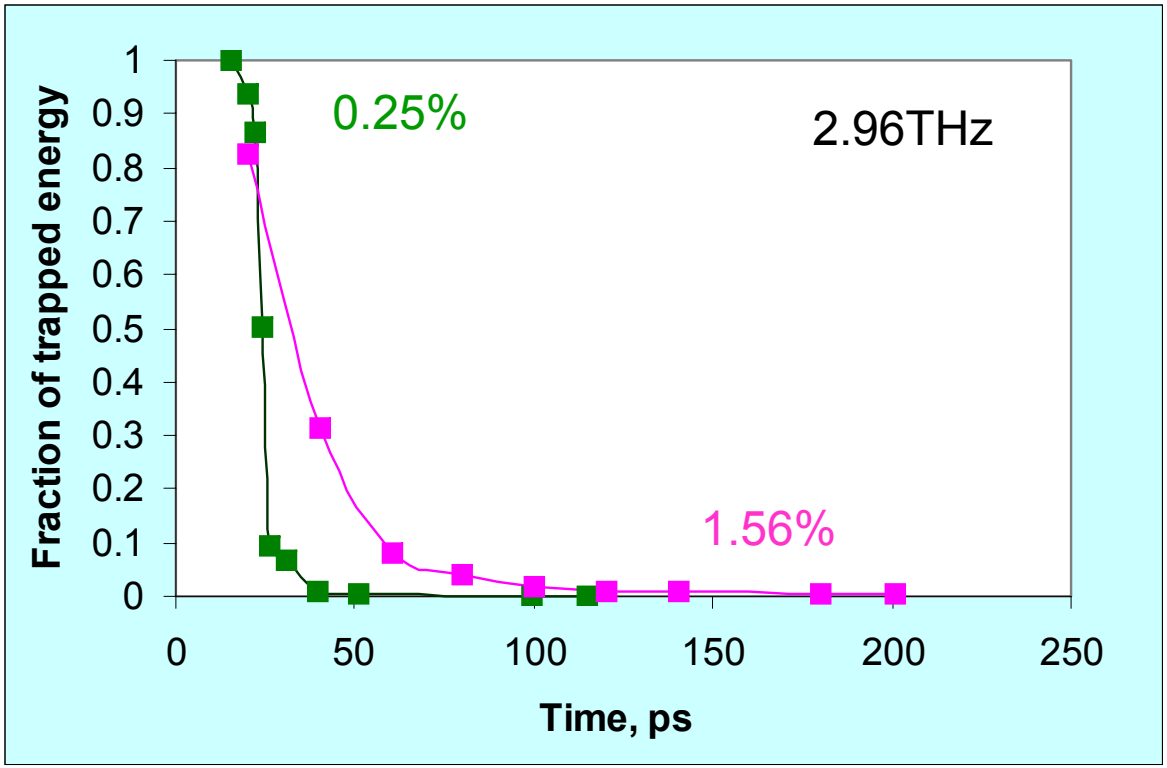
$$R + L + T = 1$$




L
R
T


2.96THz
140 ps
3e-06
2e-06
1e-06
0
-1e-06
-2e-06
-3e-06
-3000
-2000
-1000
0
1000
2000
3000

Time evolution of trapped energy



The higher concentration, the longer time to scatter out.

Physically reasonable results

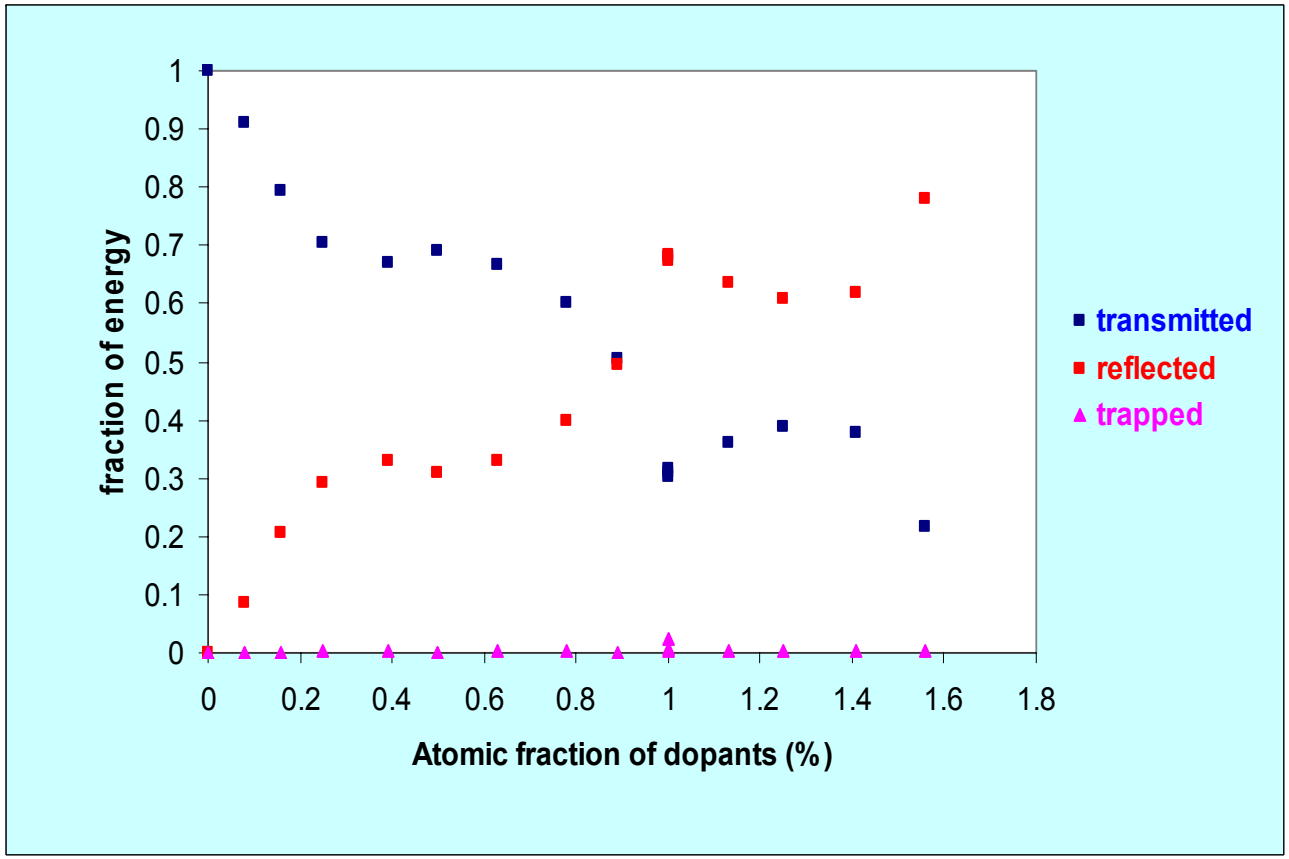
Concentration effect

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

well linear when the concentration is less than 0.3%.

1/t ~ c

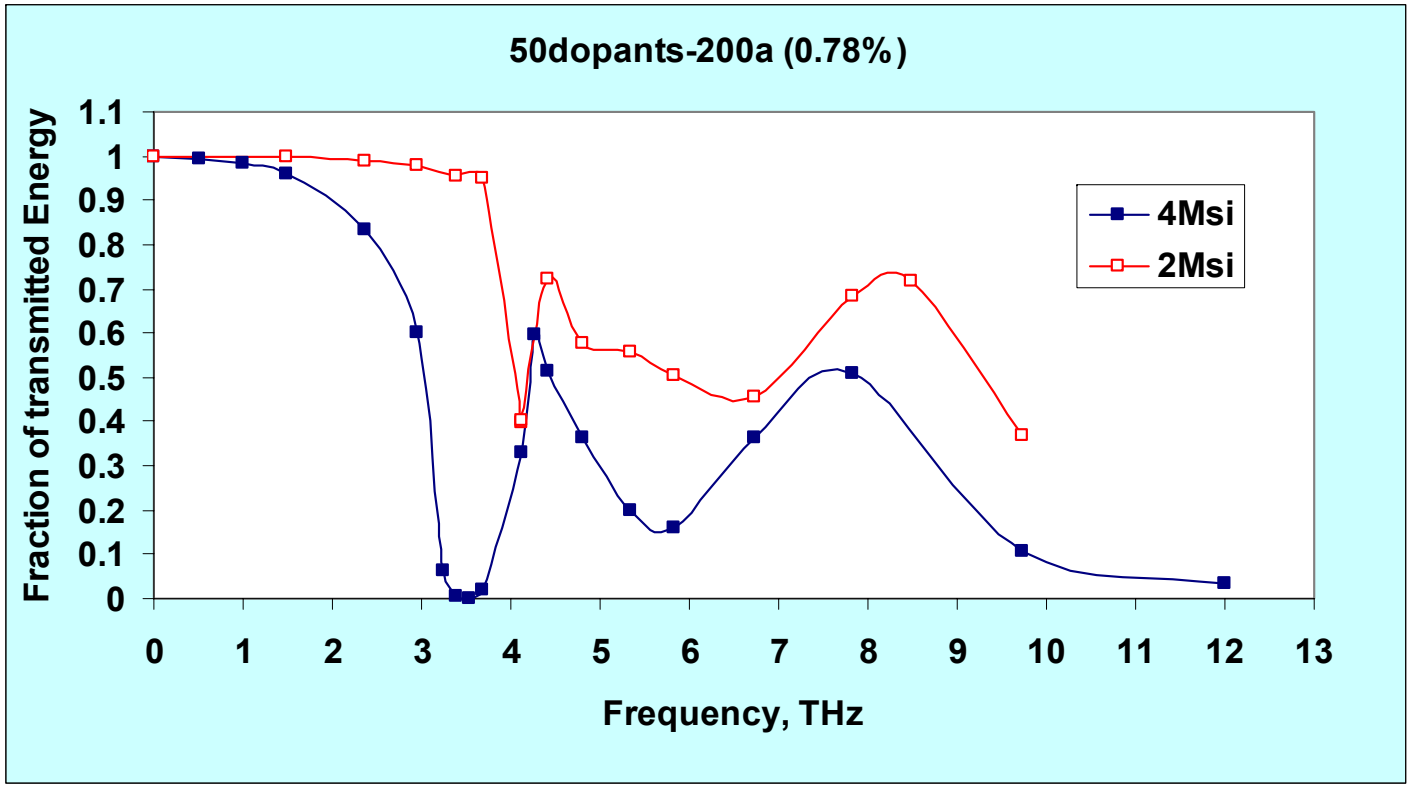
$$[t(f)]^{-1} = A \cdot (\frac{\Delta m}{m})^2 \cdot c \cdot f^4$$



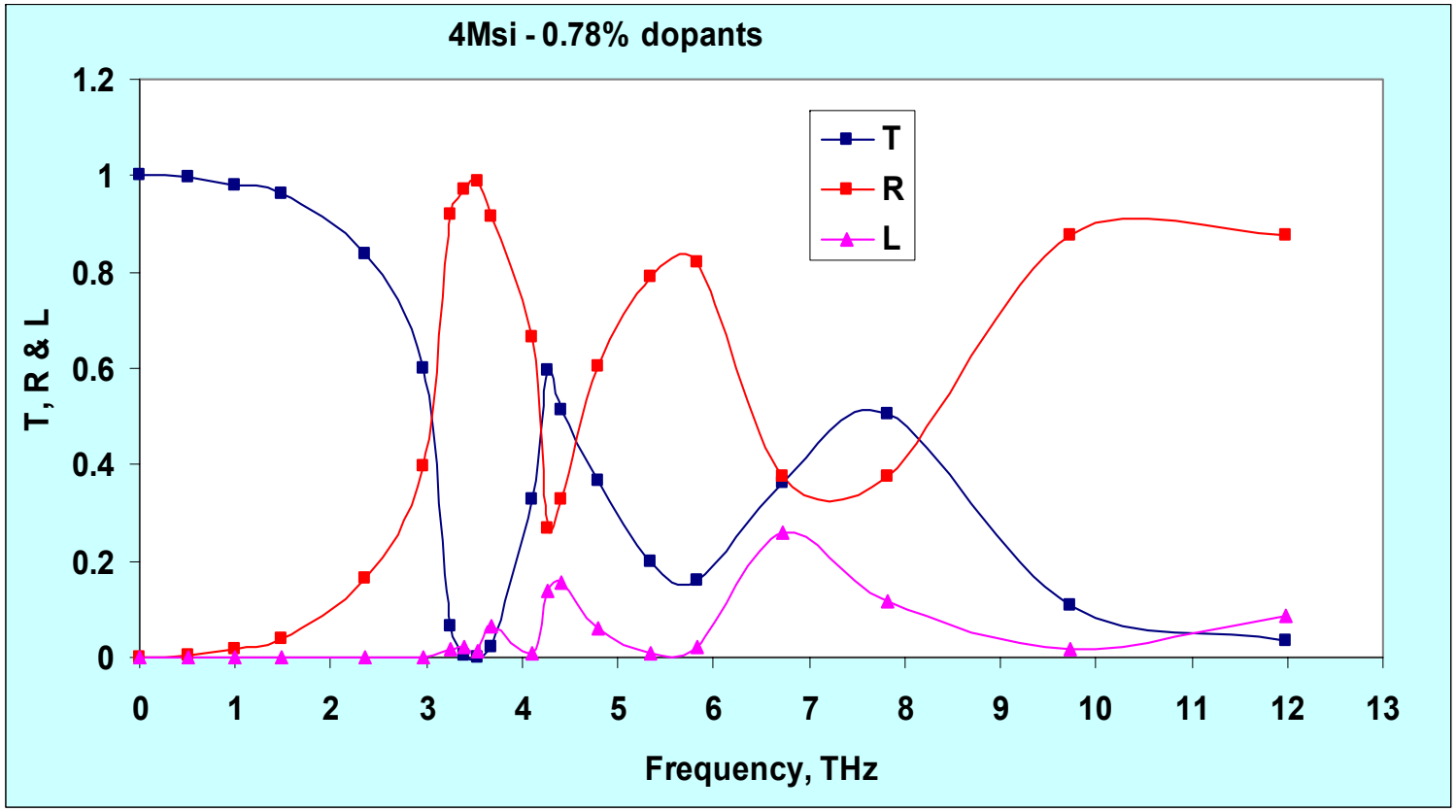
2.96THz
Δz = 200 unit cell

Mass effect

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



Frequency effect

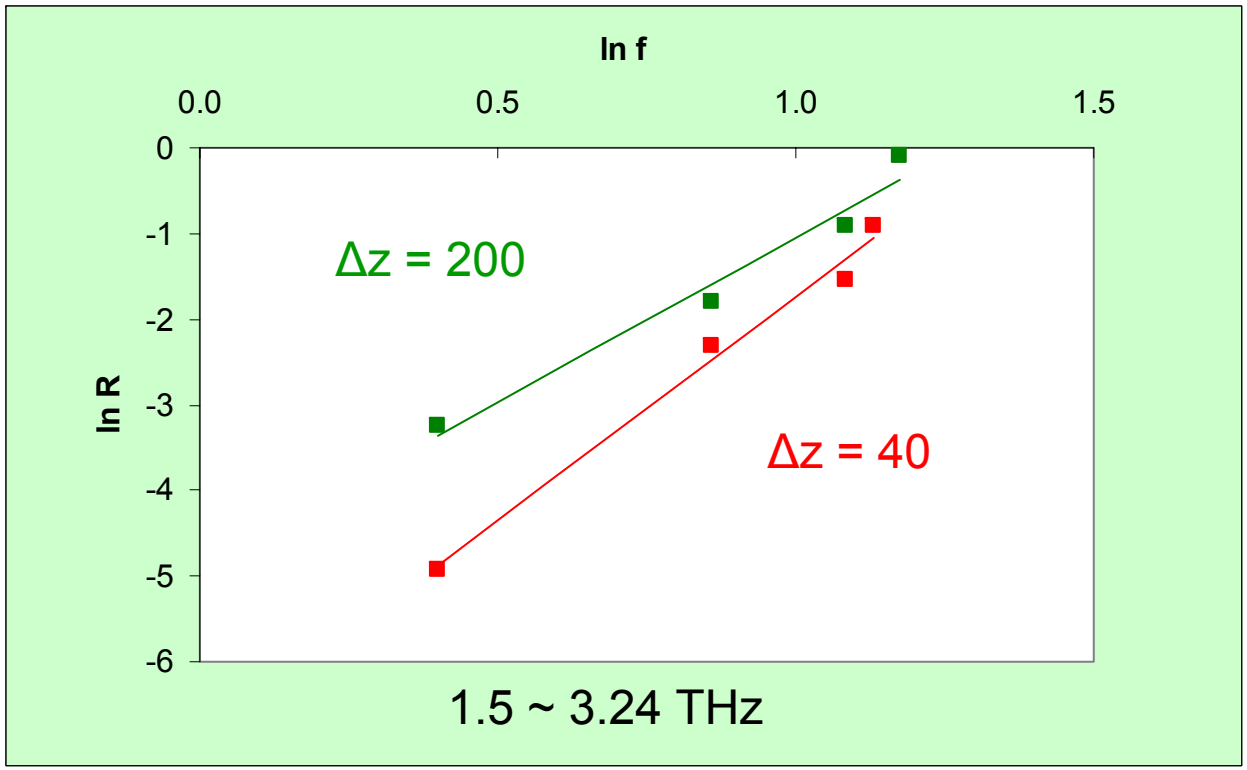


T drops quickly with f decreasing. (f < 3.5 THZ)

T reaches minimum around 3.5 THz

Frequency effect

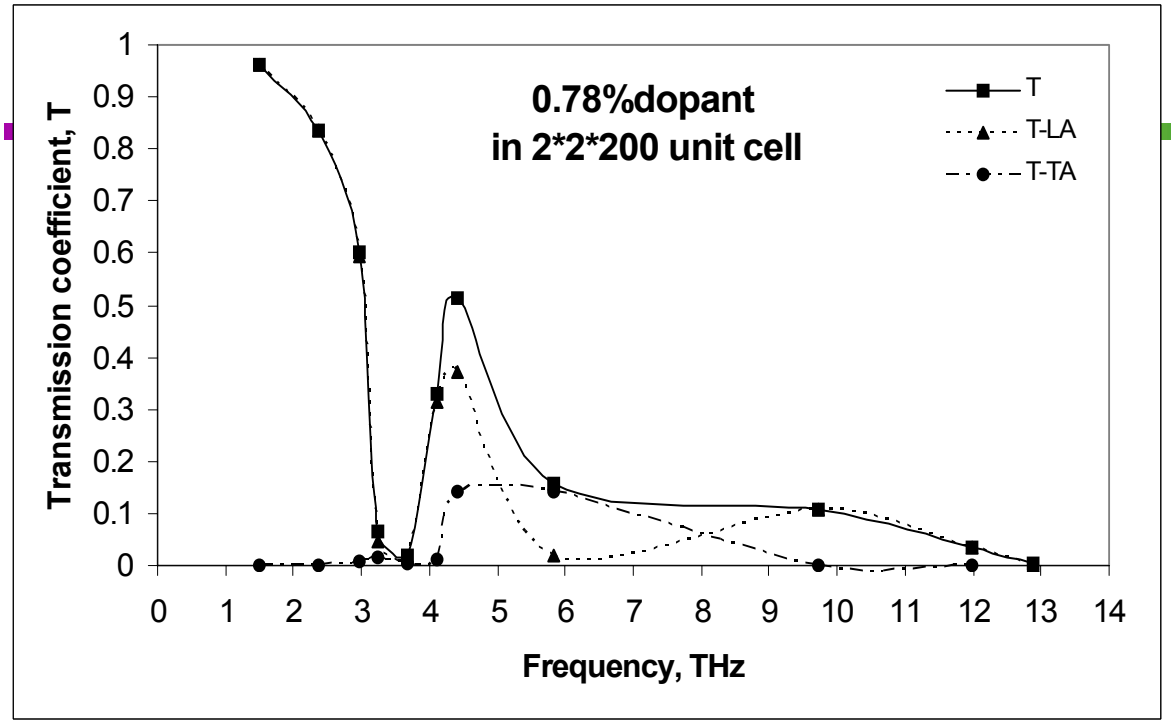
$1/t \sim f^{\alpha}$ $\qquad [t(f)]^{-1} = A \cdot (\frac{\Delta m}{m})^2 \cdot C \cdot f^4$



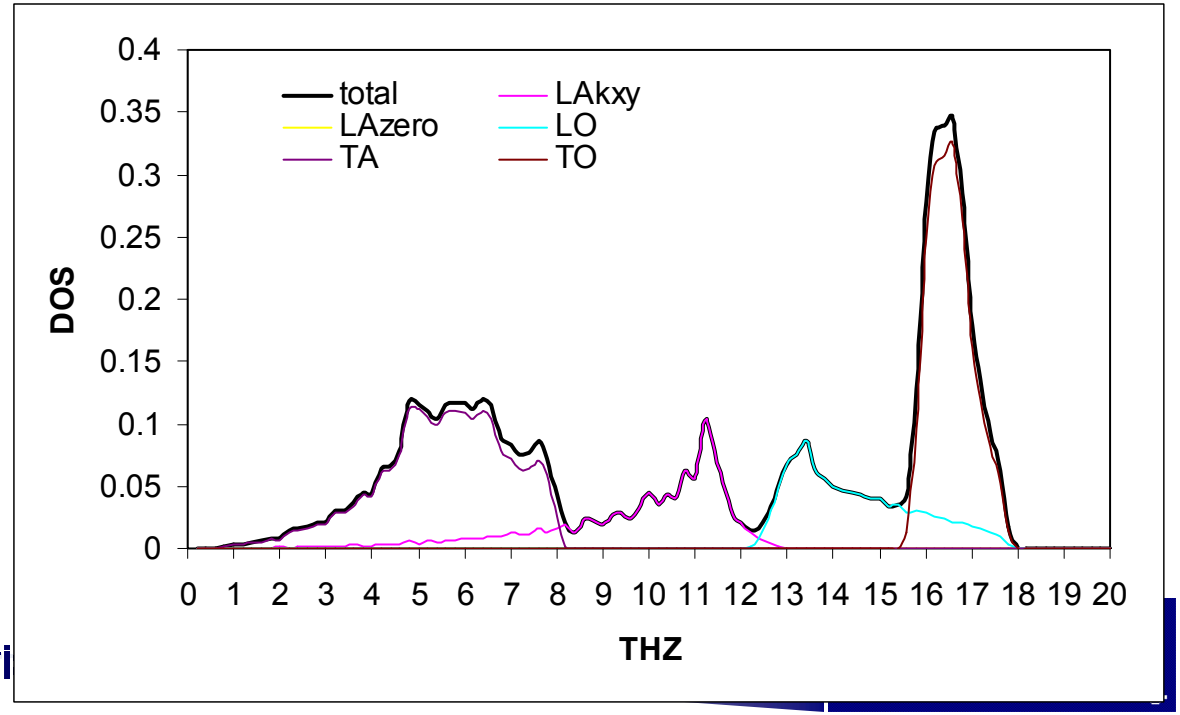
$\alpha = 3.82$
for Δz=200

$\alpha = 5.23$
for Δz=40

compared with classic result
$\alpha = 4$
(assumes Debye DOS)



Phonon density of state for pure Si



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.

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

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