Simulation of Nanoscale Thermal Effects in Semiconductor Devices

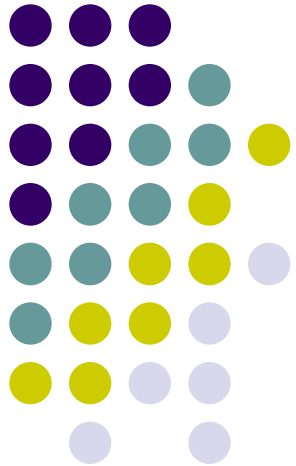
Zlatan Aksamija

Advisor: Umberto Ravaioli

Beckman Institute for Advanced Science and Technology

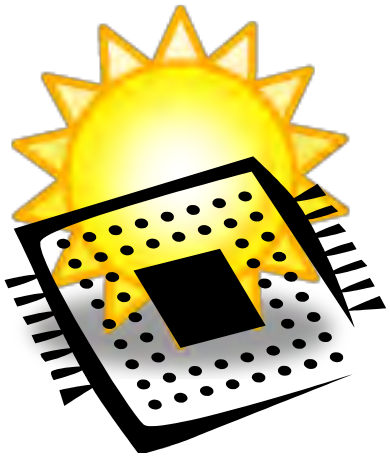
University of Illinois at Urbana/Champaign

aksamija@illinois.edu



Introduction

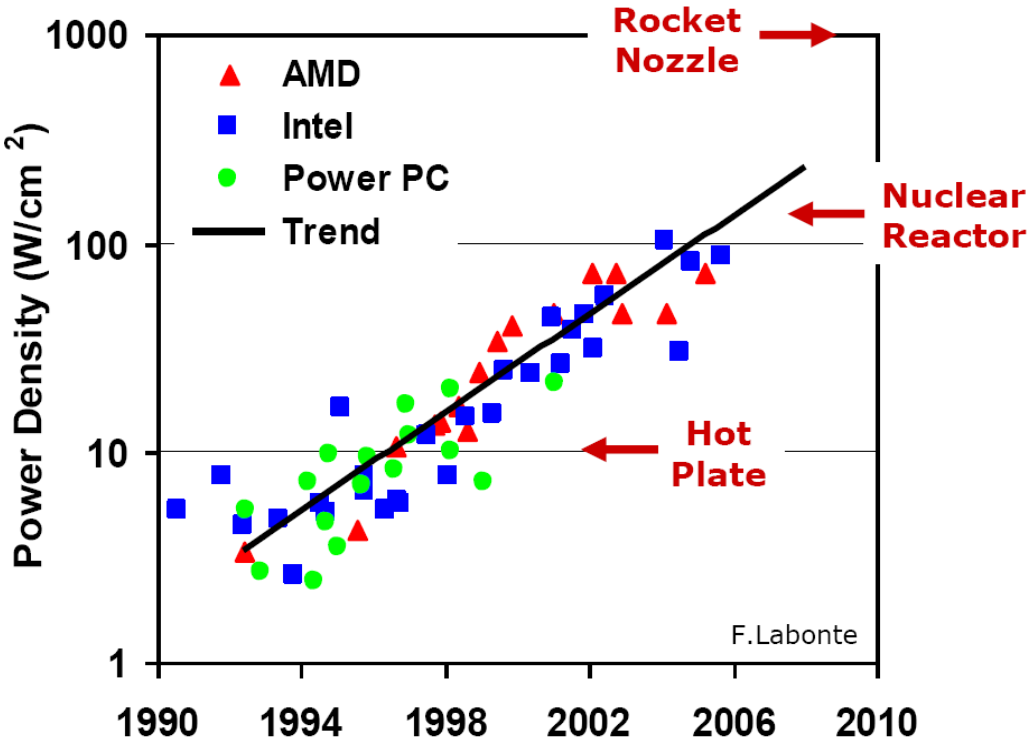
- We want our CPUs to do more than just cook eggs for breakfast!



(http://www.phys.ncku.edu.tw/~htsu/humor/fry_egg.html)

Thermal Power Density

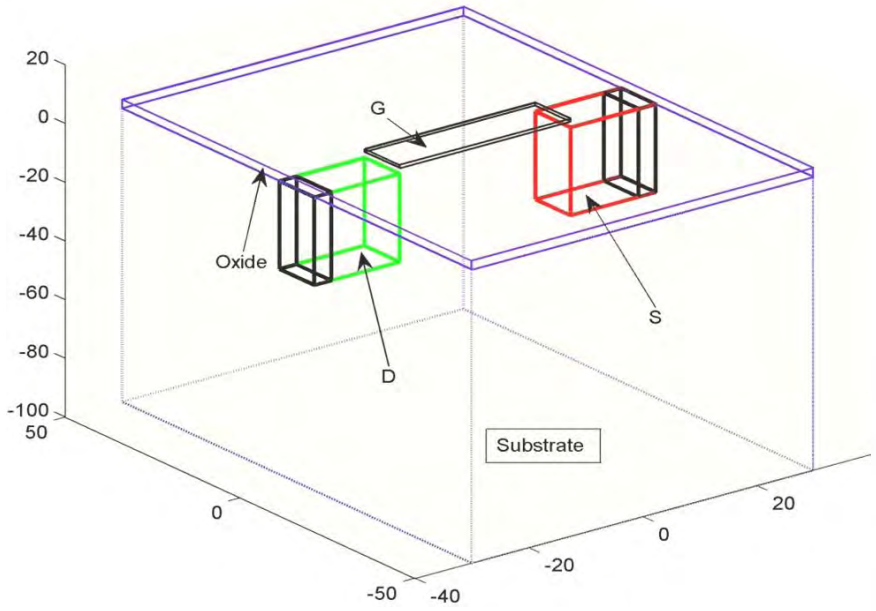
- Aggressive scaling has increased thermal power density exponentially
- Doubles every 3 years
- Increases
  - Cost
  - Noise
  - Power consumption
  - Space
- Environmental impact

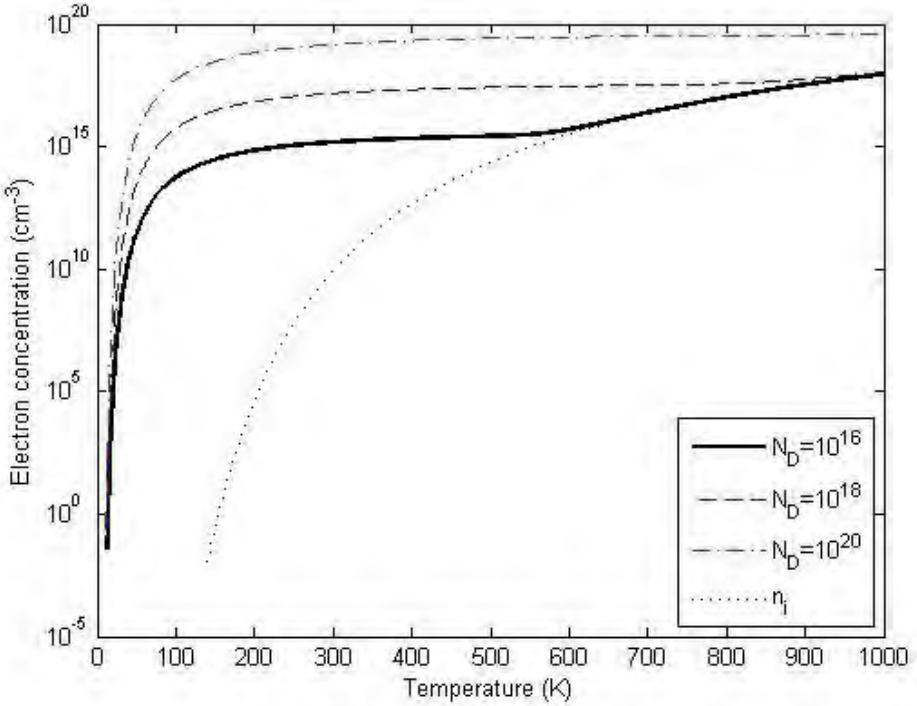


(from E. Pop Proc. IEEE 2006)

Electron Concentration vs. T

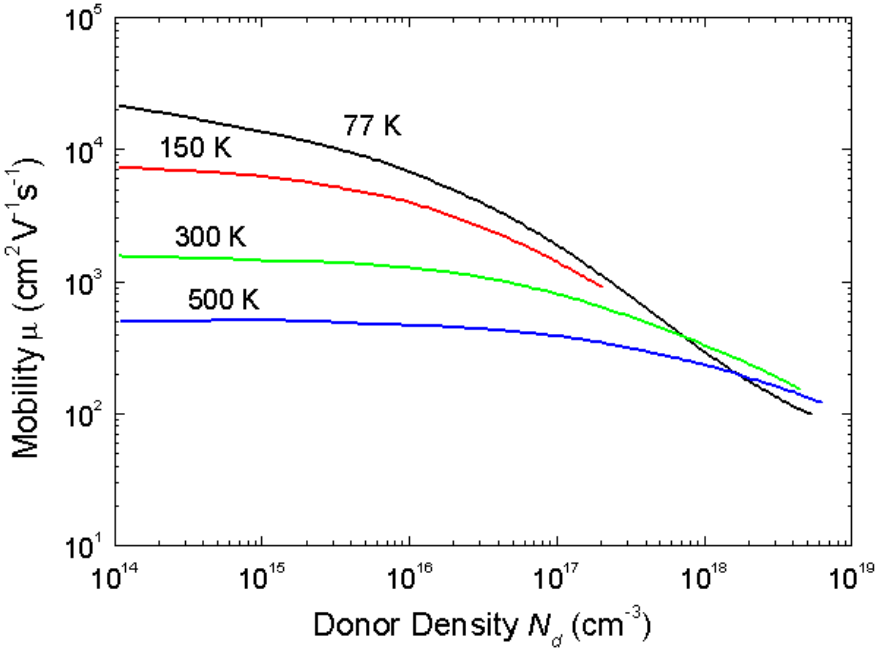
- Semiconductors cease to function in a controllable way long before they melt! (at 1685K)
  - A semiconducting material's function is determined by doping
  - A lightly doped channel ($N_D=10^{16}$) becomes intrinsic above T>600K due to temperature dependence of intrinsic concentration n_i



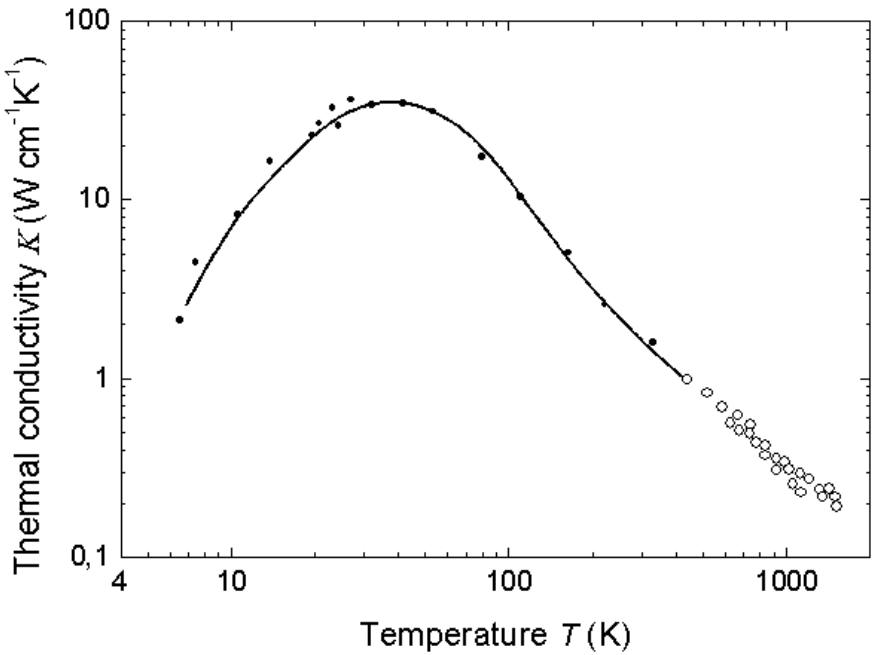


Performance vs. Temperature

- Electrical and thermal performance degrade with temperature
  - Electron mobility and thermal conductivity both decrease due to higher electron-phonon and phonon-phonon scattering

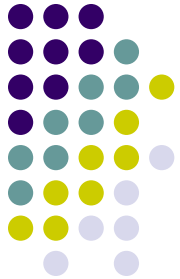


Li, S. S. and W. R. Thurber, *Solid State Electron.* (20) 609



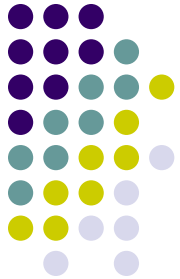
Glassbrenner, C. J. and G. A. Slack, *Phys. Rev.* (134) A1058-A1069

Challenges



- Thermal generation in MOSFETs is seen as the ultimate limit to scaling
- Thermal management solutions are not sufficient to deal with heat generation
- Future designs require a multi-physics electro-thermal approach
- Understand both heat generation and transport
- Couple proven device simulation to thermal transport

Nanoscale heat transfer in semiconductors

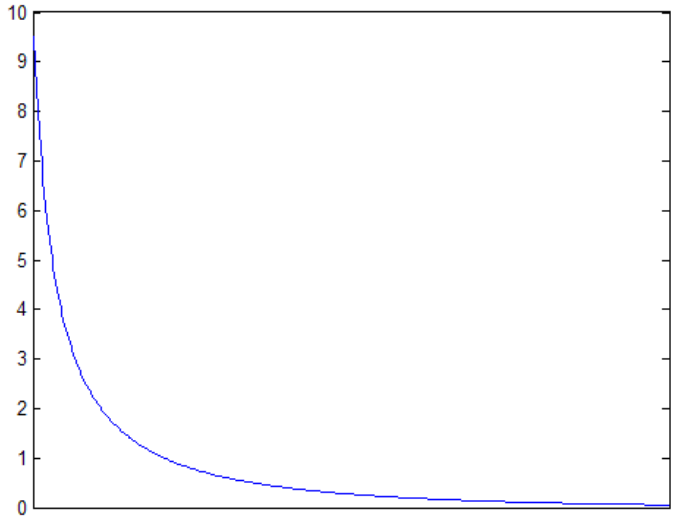


- Heat in semiconductors is carried by lattice vibrations
- A *phonon* is a quantum of physical vibration of the semiconductor lattice
- Phonons represent a physical displacement of the periodic lattice
- Propagate thermal energy through the crystal
- Perturb the atomic potential and scatter electrons, releasing thermal energy
- Scatter with each other due to anharmonic decay
  - Cubic (and higher) terms in the atomic potential cause 3- (or more) phonon coupling
  - This gives rise to finite thermal conductivity

Phonons in semiconductors

- "Phonons are bosons, and electrons fermions" *(say fast 10 times!)*
- Phonons obey Bose-Einstein statistics in equilibrium

$$N(\omega_q) = \frac{1}{e^{\hbar\omega_q / k_B T} - 1}$$



- No exclusion (the more, the merrier!)
- In the low energy limit approximate as

$$N(\omega_q) \approx \frac{k_B T}{\hbar\omega_q} - \frac{1}{2}$$

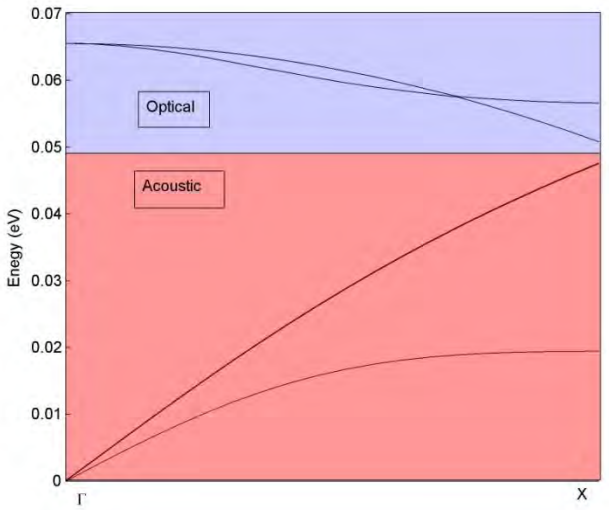
- Called the "equipartition approximation"
- Number of phonons goes down as inverse energy
- In equilibrium low energy phonons are most "popular"
- "Hot" phonons occur when N>>1 even for high-energy phonons

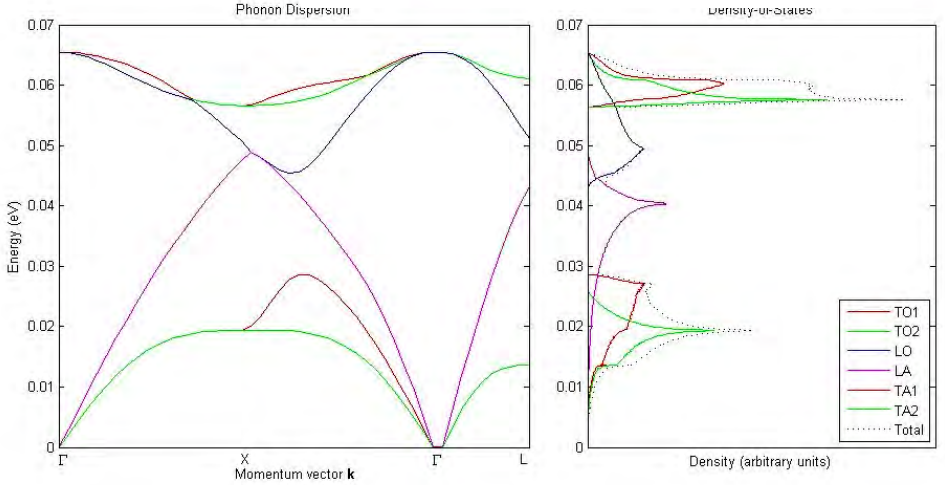
Phonon classification and characteristics

- Phonon dispersion can be determined from various models:
  - valence shell
  - bond-charge
  - *Ab initio*/DFT/Linear Response/Frozen phonon
- Classified by mode and frequency:
  - Longitudinal and two transverse
  - Acoustic and optical modes
- All the necessary properties are computed from the dispersion:
  - Phonon Density-of-States (DOS)
  - Computed by linear analytic method
  - Sum all modes near a given energy

$$g(\omega) = \iiint_{1stBZ} \delta(\omega - \omega(\vec{q}))d\vec{q} = \oiint_{\omega=\omega(\vec{q})} \frac{d\vec{S}}{\left|\nabla_{\vec{q}}\omega(\vec{q})\right|}$$

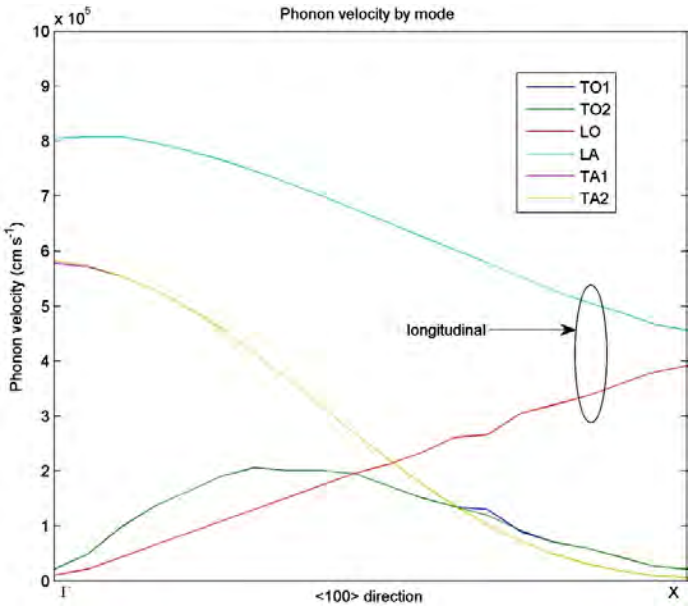
  - Lattice thermal energy
  - Heat capacity

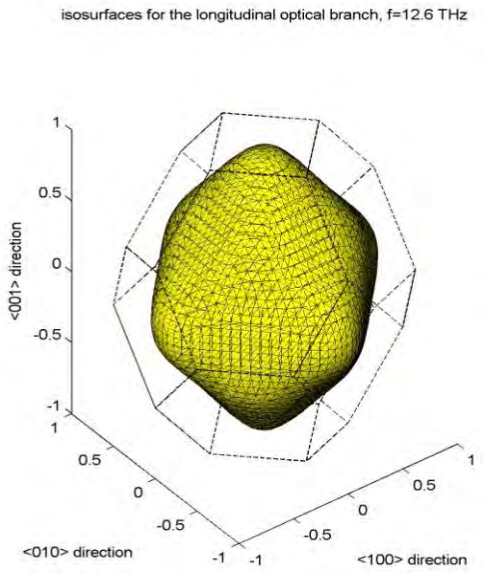


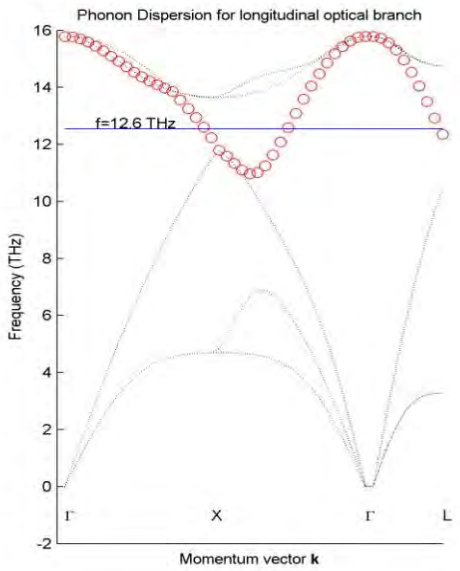


Phonon velocity and direction

- Velocity is the gradient of the dispersion $v(\vec{q}) = \nabla_{\vec{q}}\omega(\vec{q})$
- Velocity is always perpendicular to the equal energy surface
- Optical modes are much slower
- Heat flows in preferred directions normal to the flat faces of the isosurfaces
  - In the LO branch (below), these are perpendicular to the bond directions

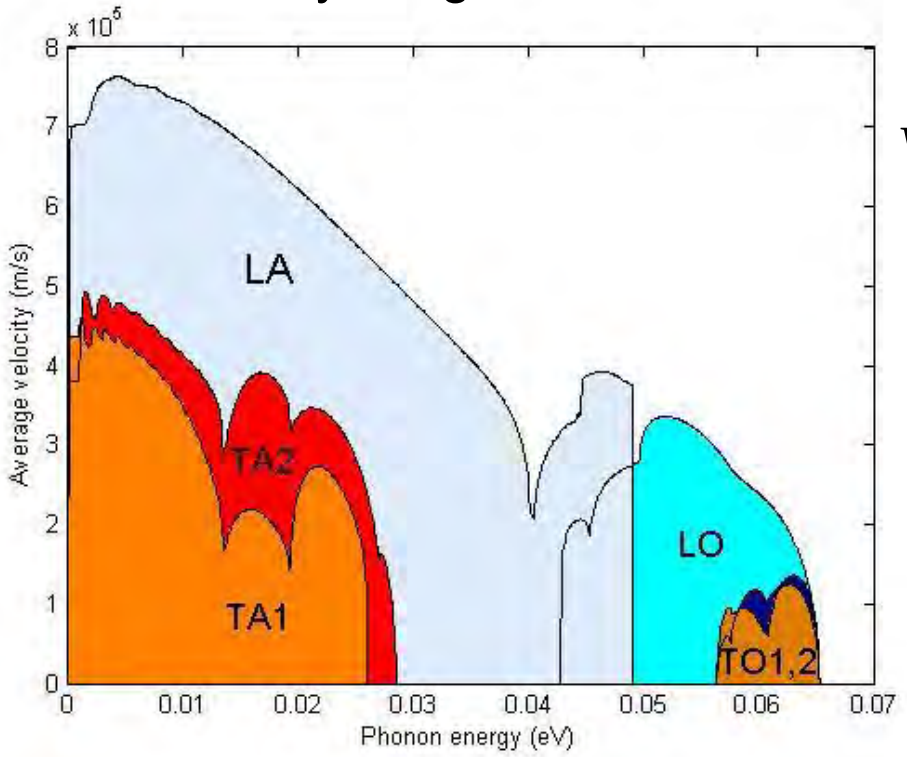






Average phonon velocity

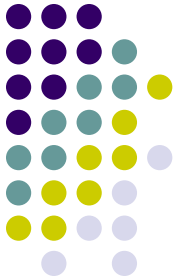
- Velocity depends on direction and magnitude of momentum vector **q**
- Take the average velocity over the energy isosurface $\omega = \omega(\vec{q})$
- Numerically integrate velocities of all modes near a given energy



$$v(\omega) = \frac{1}{g(\omega)} \iiint v(\vec{q}) \delta(\omega - \omega(\vec{q})) d\vec{q}$$

- Velocity decreases with energy
- Faster phonons carry less energy and vice versa
- LO branch has v~2000m/s
- TO branches contribute very little to thermal transport!

Boltzmann Transport Equation (BTE) for electrons

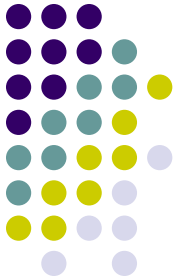


- Conservation of particles: equate time rate of change to change due to scattering
- Assume momentum and position are functions of time only, apply product rule
- Include degeneracy for metallic (small bandgap)

$$\frac{df(\vec{r},\vec{k},t)}{dt} = \frac{\partial f(\vec{r},\vec{k},t)}{\partial t} + \nabla_{\vec{k}} f(\vec{r},\vec{k},t) \bullet \frac{e\vec{F}}{\hbar} + \nabla_{\vec{r}} f(\vec{r},\vec{k},t) \bullet v(\vec{k})$$

$$= \sum_{\forall \vec{k}'} \left[S(k',k) f(\vec{r},\vec{k}',t) - S(k,k') f(\vec{r},\vec{k},t) \right]$$

Phonon BTE



- Phonons are treated in a way similar to electrons
- No spin means no interaction with fields
- Phonon scattering treated in relaxation time
- Additional term due to generation of phonons by the electron-phonon interaction

$$\frac{dN(\vec{r},\vec{q},t)}{dt} = \frac{\partial N(\vec{r},\vec{q},t)}{\partial t} + \nabla_{\vec{r}} N(\vec{r},\vec{q},t) \bullet v(\vec{q})$$

$$= \left.\frac{dN(\vec{r},\vec{q},t)}{dt}\right|_{el-ph} + \frac{N(\vec{r},\vec{q},t) - N_{eq}(\vec{q})}{\tau(\vec{q})}$$

Interpreting the BTE:

The BTE is saying that probability is conserved along the path of the particle:

- Use Taylor expansion in phase space:

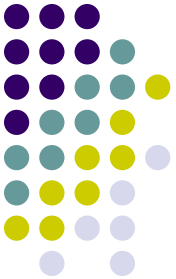
$$f(\vec{r}+d\vec{r},\vec{k}+d\vec{k},t+dt) = f(\vec{r},\vec{k},t) + \frac{\partial f(\vec{r},\vec{k},t)}{\partial t}dt + \nabla_{\vec{k}} f(\vec{r},\vec{k},t)\bullet d\vec{r} + \nabla_{\vec{r}} f(\vec{r},\vec{k},t)\bullet d\vec{k}$$

- Factor out the "dt" term and group together:

$$f(\vec{r}+d\vec{r},\vec{k}+d\vec{k},t+dt) = f(\vec{r},\vec{k},t) + dt\left(\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}dt + \nabla_{\vec{k}} f(\vec{r},\vec{k},t)\bullet\frac{d\vec{r}}{dt} + \nabla_{\vec{r}} f(\vec{r},\vec{k},t)\bullet\frac{d\vec{k}}{dt}\right)$$

$$= f(\vec{r},\vec{k},t) + dt\sum_{\forall\vec{k}'}\left[S(k',k)f(\vec{r},\vec{k}',t) - S(k,k')f(\vec{r},\vec{k},t)\right]$$

Monte Carlo method for the BTE:



- The BTE poses tremendous computational burdens due to “curse of dimensionality”
  - 7-D=3-D space+3-D momentum + 1D time
- Simplify: only consider samples of the f(r,k,t)
- Monte Carlo method for device simulation
  - Particles will move in space according to their velocity,
  - Particles change momentum due to the forces acting on them:

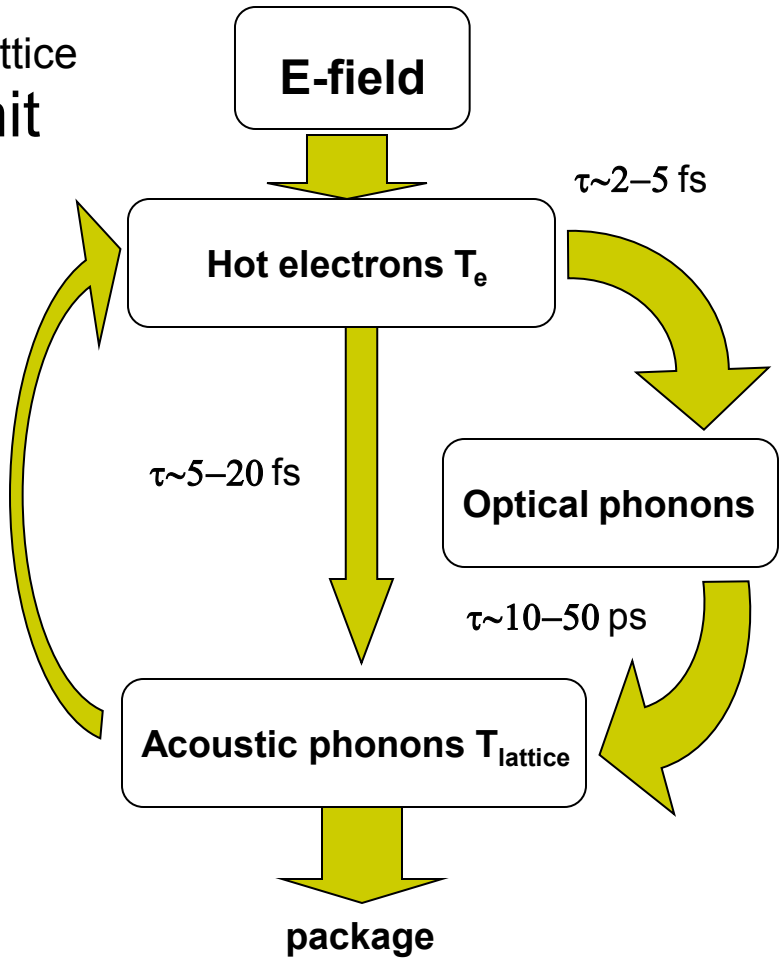
$$d\vec{r} = \frac{d\vec{r}}{dt}dt = v(\vec{k})dt \qquad d\vec{k} = \frac{d\vec{k}}{dt}dt = \frac{e\vec{F}(\vec{r})}{\hbar}dt$$

  - Particles scatter in and out of momentum state **k** due to interactions with electrons, phonons, photons, plasmons, impurities, boundaries, etc.

$$S(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}\left|\left\langle \vec{k}\left|H'\right|\vec{k}'\right\rangle\right|^2 \delta\left(E(\vec{k}) - E(\vec{k}') \pm \hbar\omega(\vec{q})\right)$$

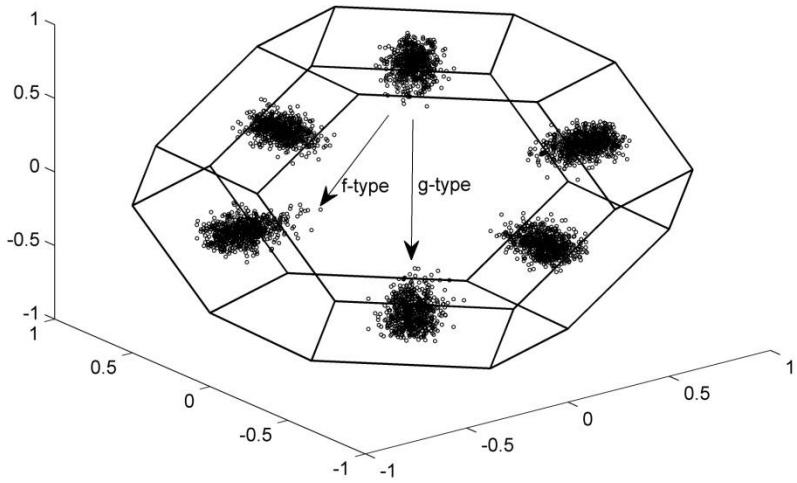
Energy Flow Diagram

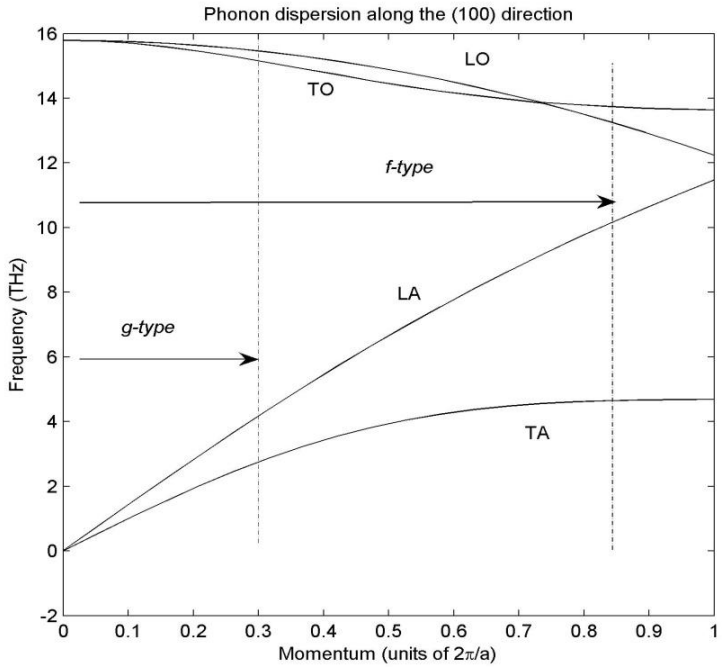
- Energy supplied by the electric field
- E-field heats the electrons $T_e > T_{lattice}$
- Electrons release energy and emit phonons
- Slow optical and high-energy acoustic phonons generated
- Decay due to phonon-phonon coupling (anharmonic decay)
- Fast acoustic phonons carry thermal energy
- Phonon decay slow compared to electron-phonon scattering



Scattering mechanisms and heat

- The dominant optical transitions happen between different X valleys
- Transitions to the opposite valley are called g-type.
- Transitions to any of the four nearest X valleys are called f-type.

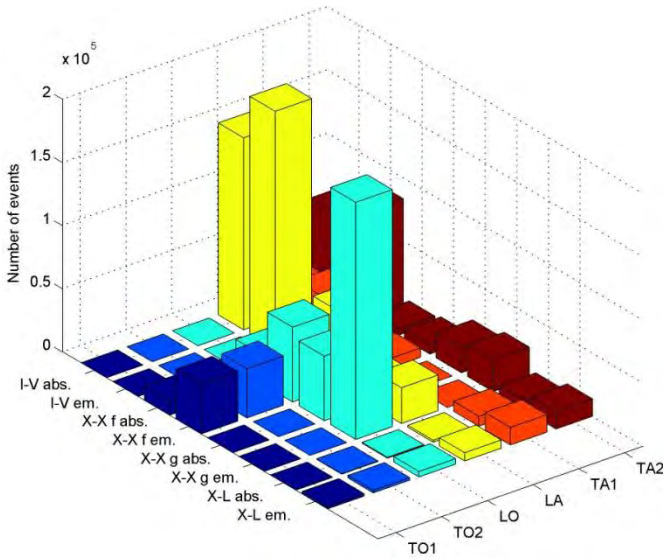


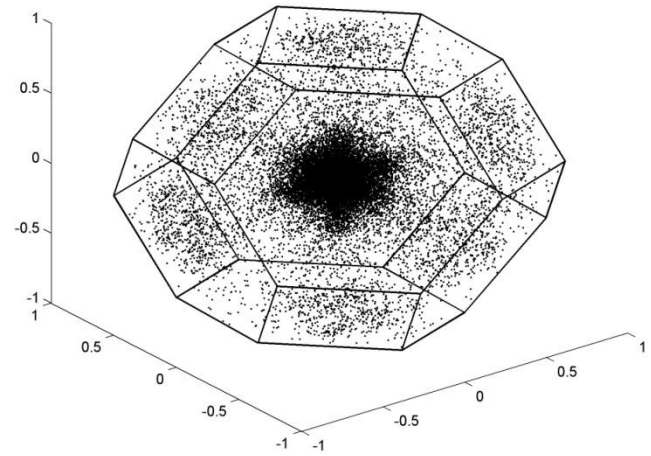


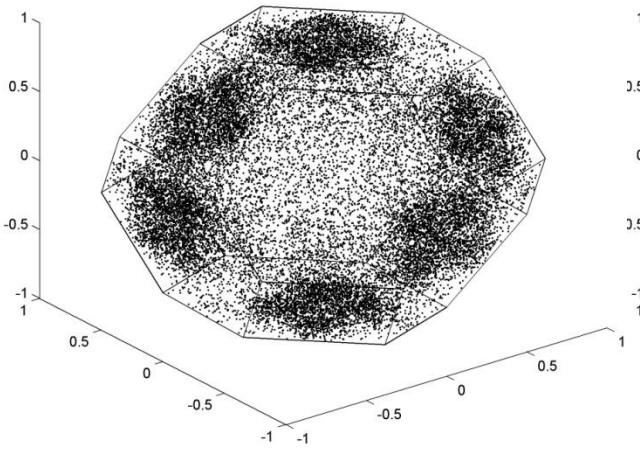
- Acoustic transitions mostly intra-valley (small **q**).
- Higher fields means more electrons at high energies
- Larger phonon **q** transitions possible for acoustic scattering.

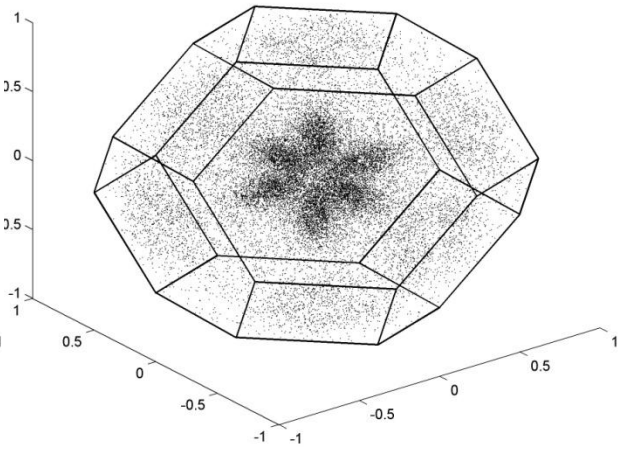
Scattering mechanisms and heat

- Acoustic transitions mostly intra-valley (small **q**).
- Optical phonons are either f- or g-type with **q** near Brillouin zone edge or near 0.3 (inter-valley)
- LO emission dominates
- Both LA emission and absorption strong



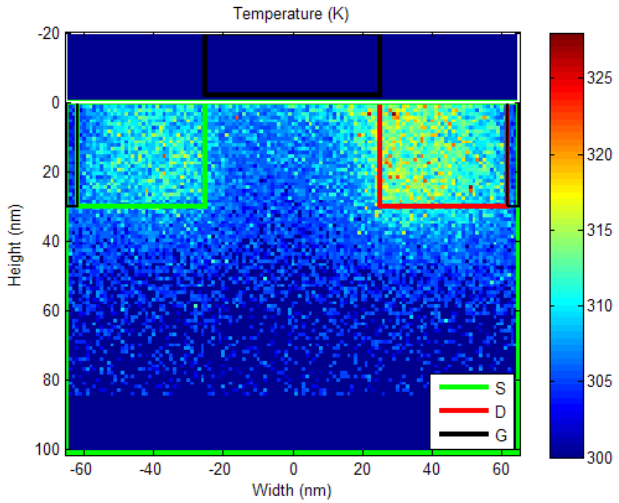


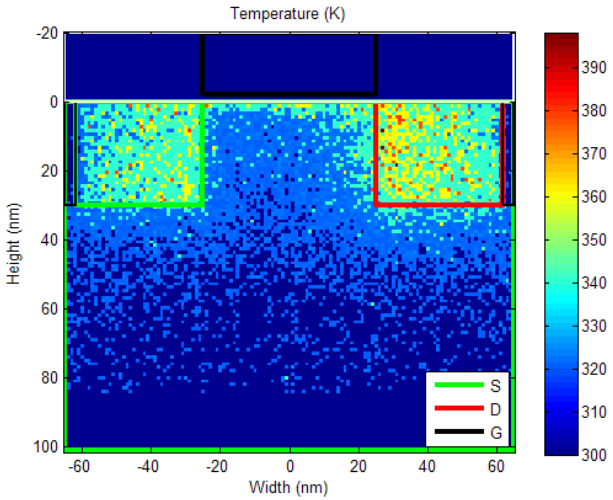


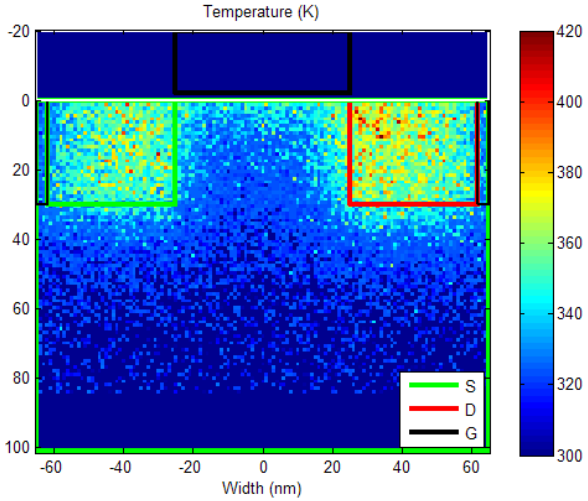


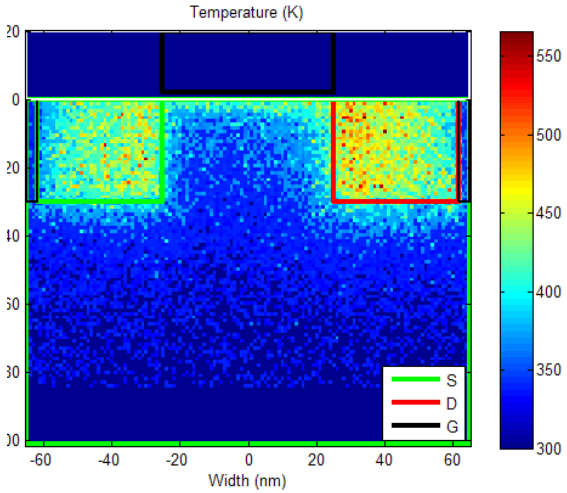
Phonon branch temperatures

- Branch temperature higher for optical phonons (optical modes move slower)
- Modal temperature lower for acoustic phonons, especially TA modes (right image).
- Longitudinal Acoustic modes move faster and have absorption (bottom left)
- Very high temperatures (>500K) for LO mode (bottom right image)



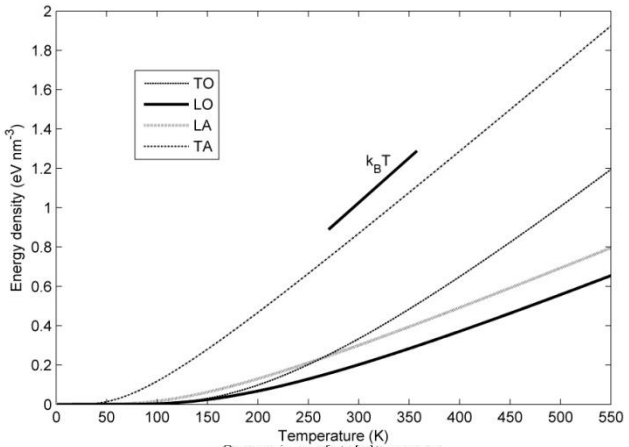


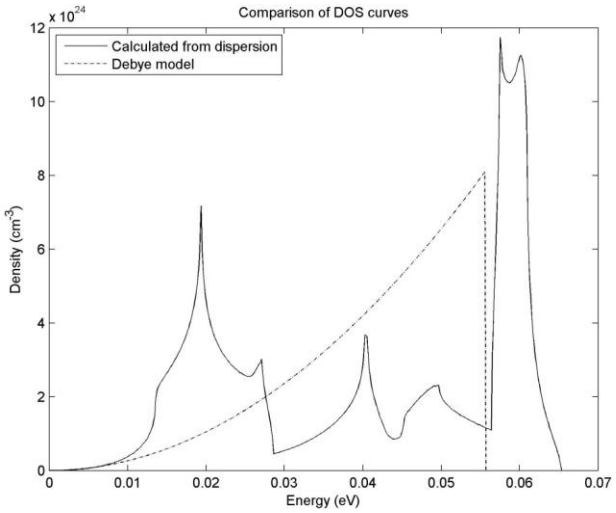


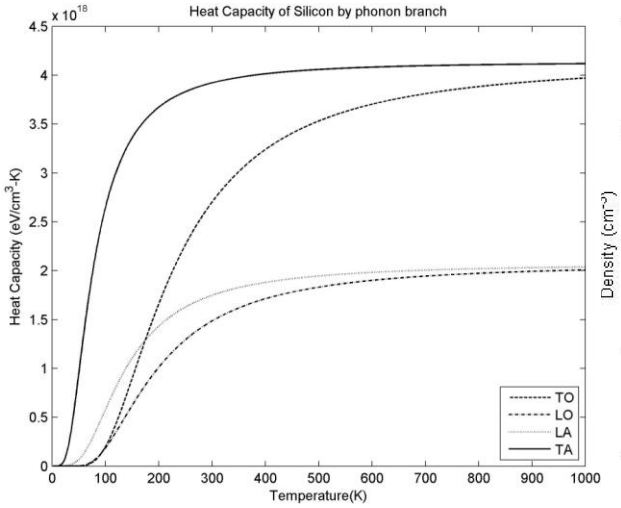


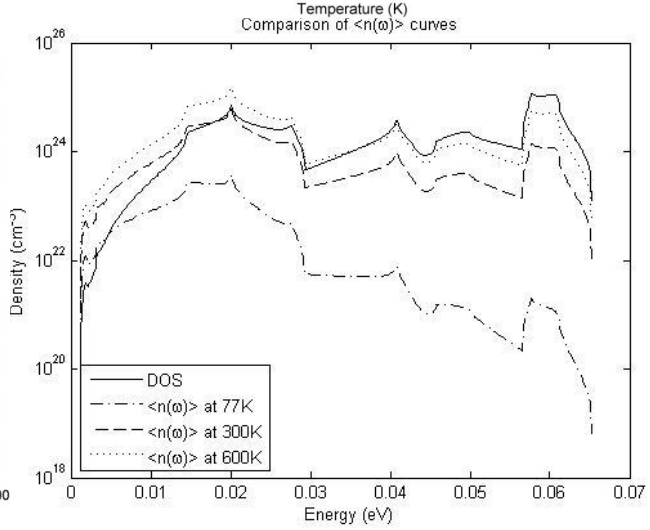
Role of optical phonon modes

- Optical DOS high but equilibrium occupancy low
- Only low energies occupied at low temperatures
- Optical modes fill only near 645K (Debye temperature)
- Thermal energy smaller due to DOS
- Heat capacity of longitudinal modes lower
- Room temperature optical contribution in equilibrium small



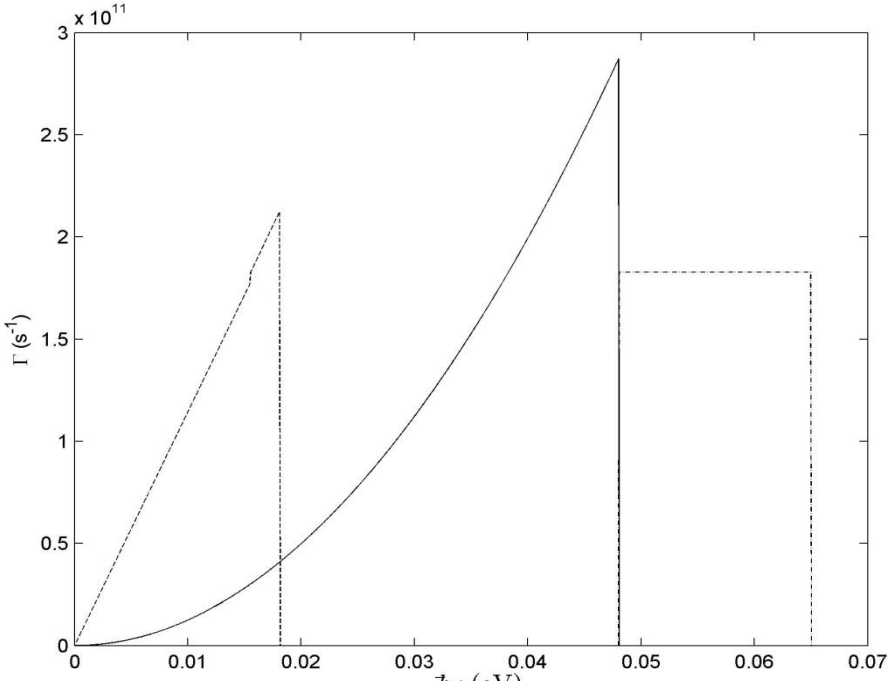


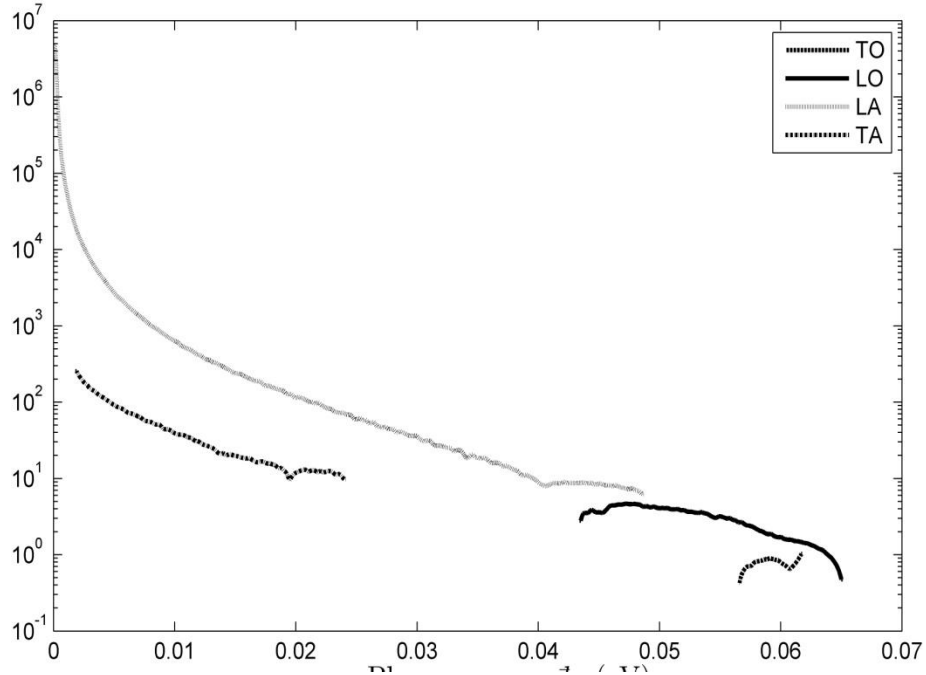




Phonon anharmonic decay rates and mean-free-paths

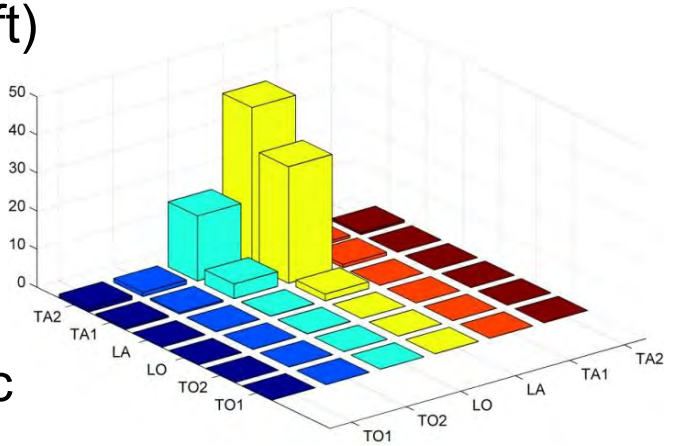
- Optical phonons (LO and TO) have short paths
- LO and TO phonons are slow and decay rapidly
- Phonon mean-free-path decreases with energy
- LA mean-free-path exceeds typical dimension of active region

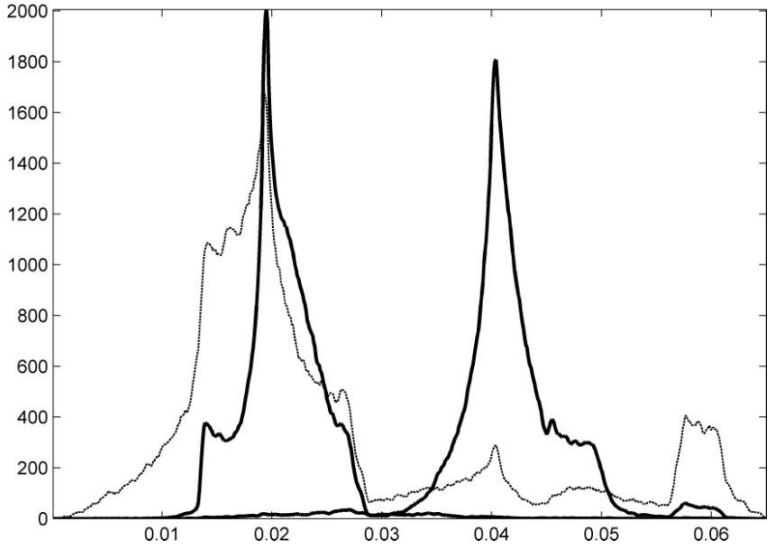


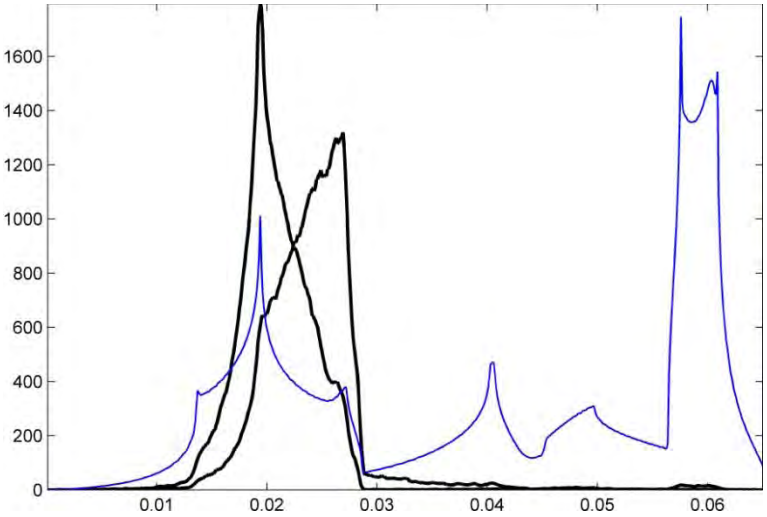


Anharmonic 3-phonon decay

- g-type LO phonons decay mostly into combinations of LA and TA modes (LA+TA left)
- This creates faster LA and TA phonons at intermediate energies
- LA phonons decay into TA+TA pairs
- Overall the decay process produces another bottleneck to heat flow from optical to acoustic

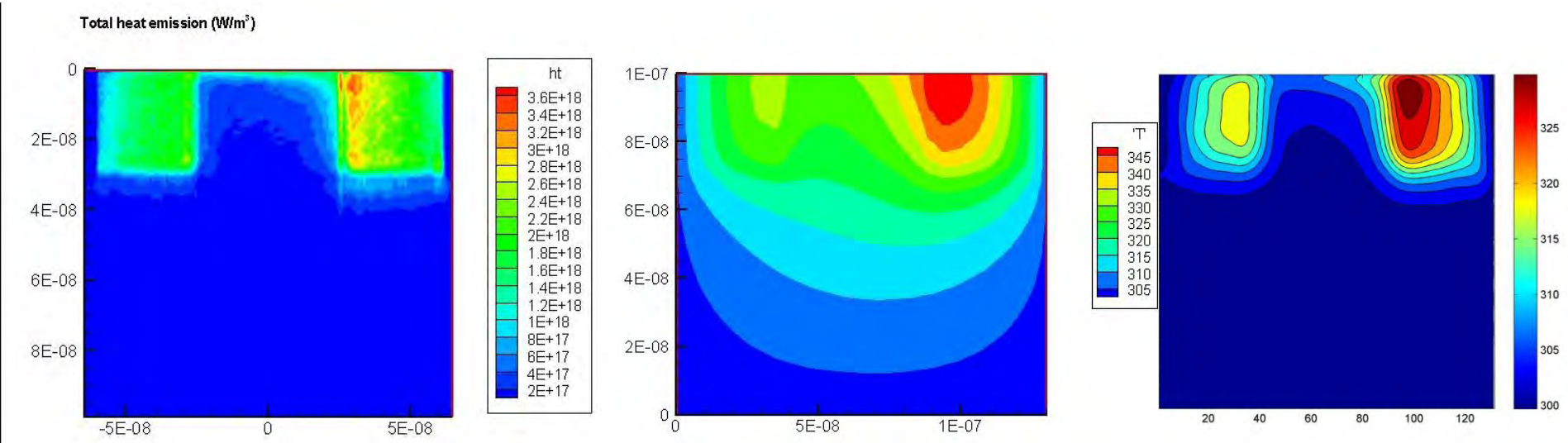




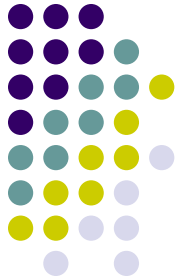


Phonon BTE simulation results

- Heat generation concentrated at drain end
- Most emission in the “hot spot” region
- Phonon BTE shows ~45K temperature rise
- After anharmonic decay of optical and longitudinal phonons, heat transport is well described by classical heat diffusion



Conclusions and comments



- This procedure allows us to probe the heating process in microscopic detail
- Most emission in a small hot-spot in the drain
  - Large temperature peak in the drain region
- High fields increase longitudinal acoustic phonons
  - Explore the effects of hot longitudinal optical phonons
- Backscattering produces g-type optical phonons
  - They have lower velocity and travel in a preferred directions aligned with the diagonals
- Few phonons directed into the substrate
  - Many directed towards the oxide where they are reflected ($Si0_2$ has low thermal conductivity)
- After phonon decay, transport well described by heat equation

Questions?