# 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 – relevant to SRC members

# Nanoscale Heat Transport

- **Heat diffusion equation (D » Λ)**

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

- **Phonon Boltzmann Transport Equation (BTE) (D < Λ)**

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

$e''$ = phonon energy density
$Q'''$ = electron − phonon energy density transfer rate

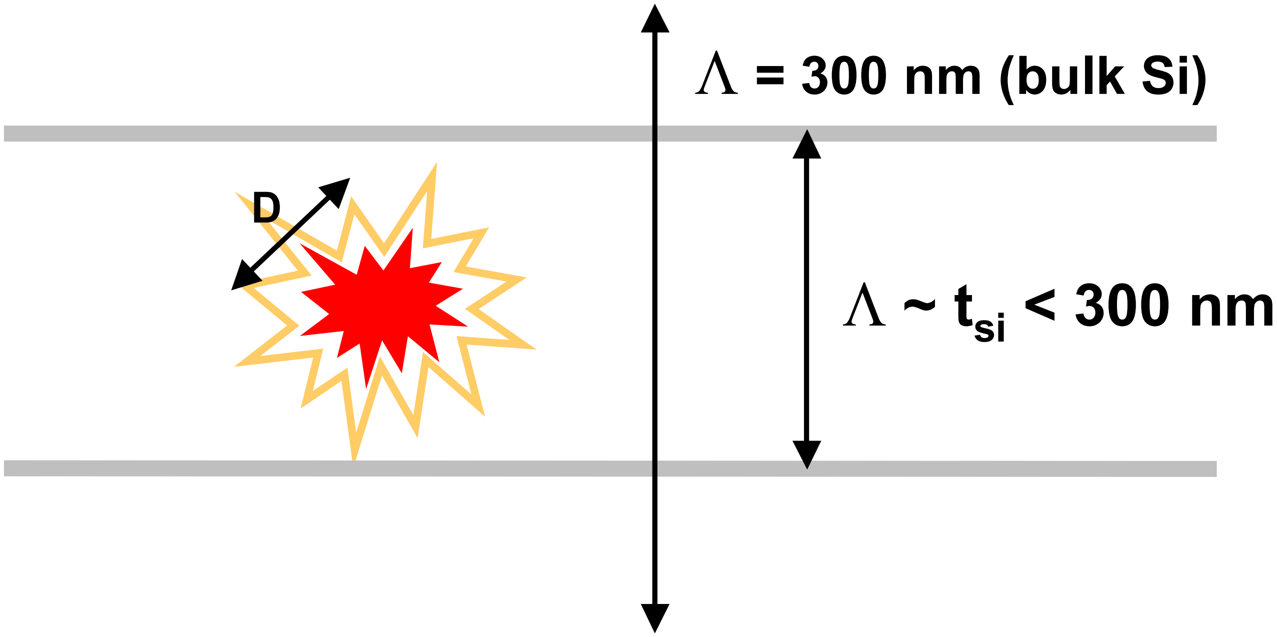
**ITRS Roadmap**

| Year | Feature Size |
|---|---|
| 1999 | 180 nm |
| 2001 | 150 nm |
| 2003 | 130 nm |
| 2006 | 100 nm |

**Λ ~ 300 nm**
**in Silicon at 300 K**

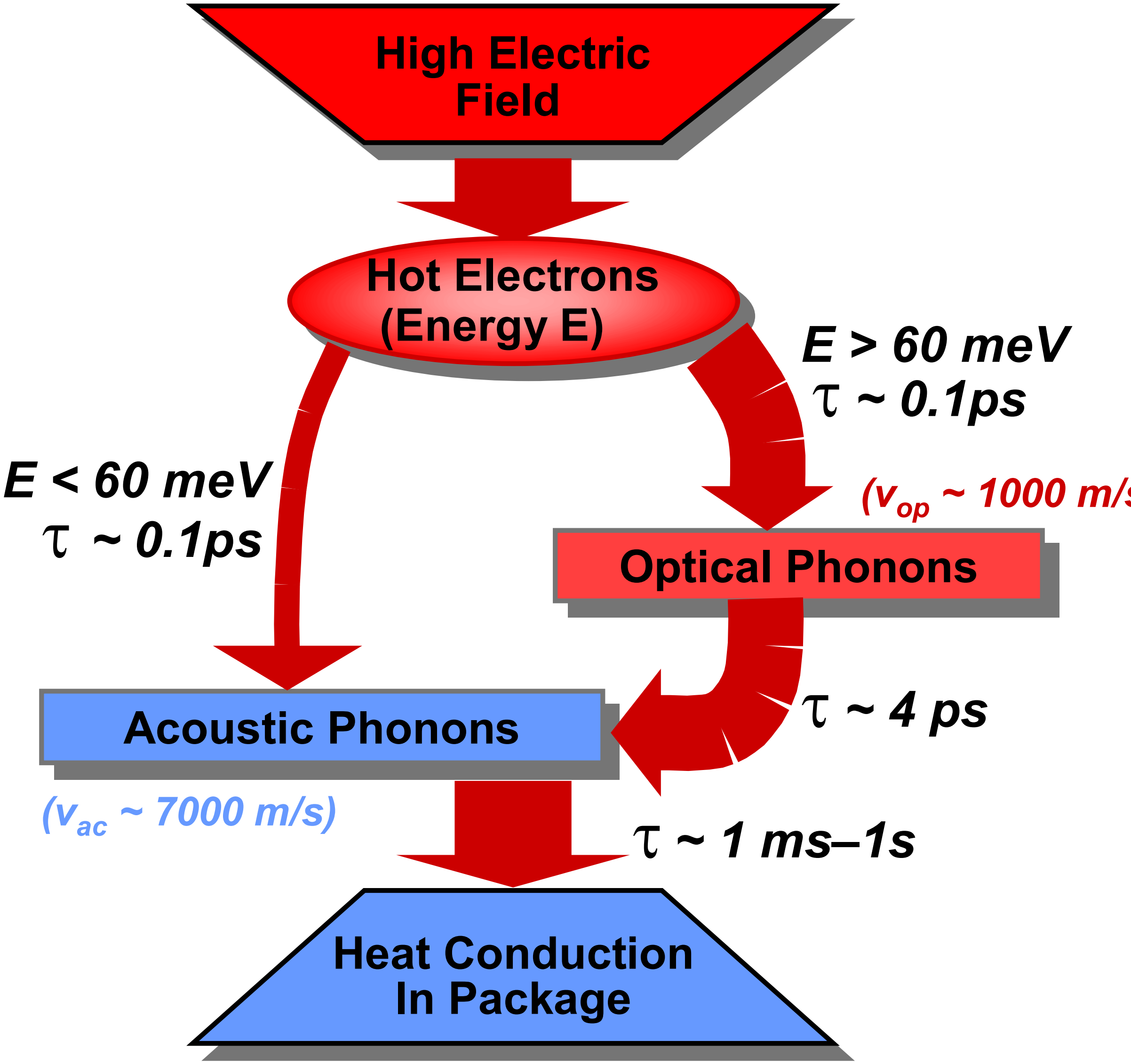
# Sub-Continuum Heat Generation

- Small heat source (D << Λ phonons)



- Reduced number of collisions near small heat source cannot maintain equilibrium, T ↑
- Not all phonons are created equal

# Joule Heating Energy Transfer



**High Electric Field**

**Hot Electrons (Energy E)**

***E > 60 meV***
***τ ~ 0.1ps***

*($v_{op}$ ~ 1000 m/s)*

***E < 60 meV***
***τ ~ 0.1ps***

**Optical Phonons**

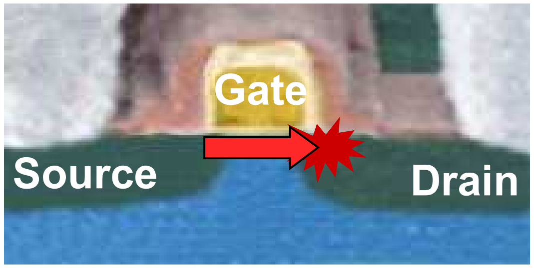
***τ ~ 4 ps***

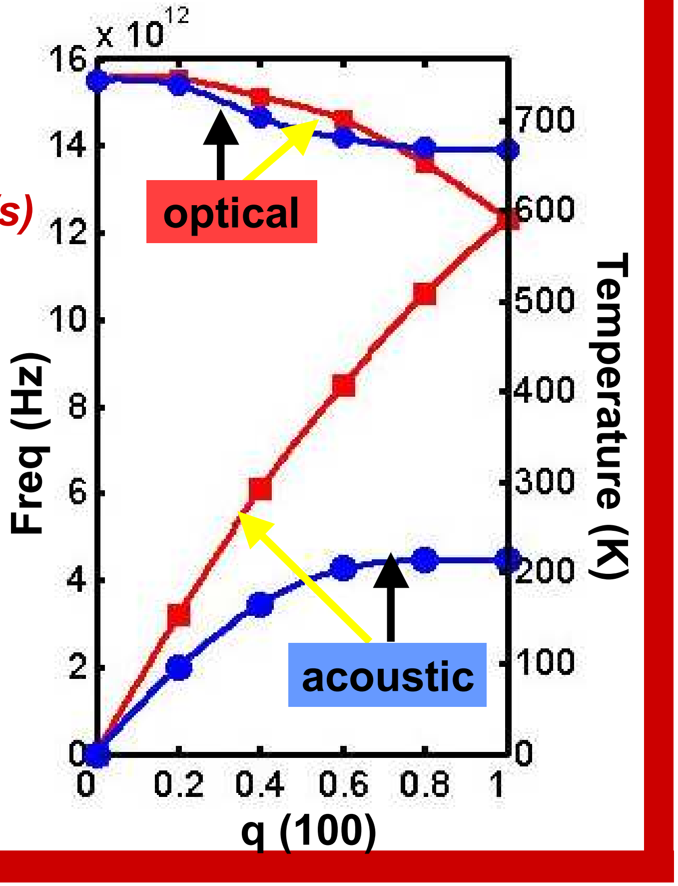
**Acoustic Phonons**

*($v_{ac}$ ~ 7000 m/s)*

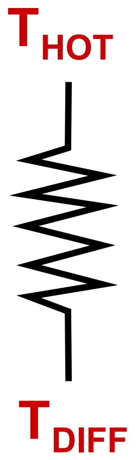
***τ ~ 1 ms–1s***

**Heat Conduction In Package**

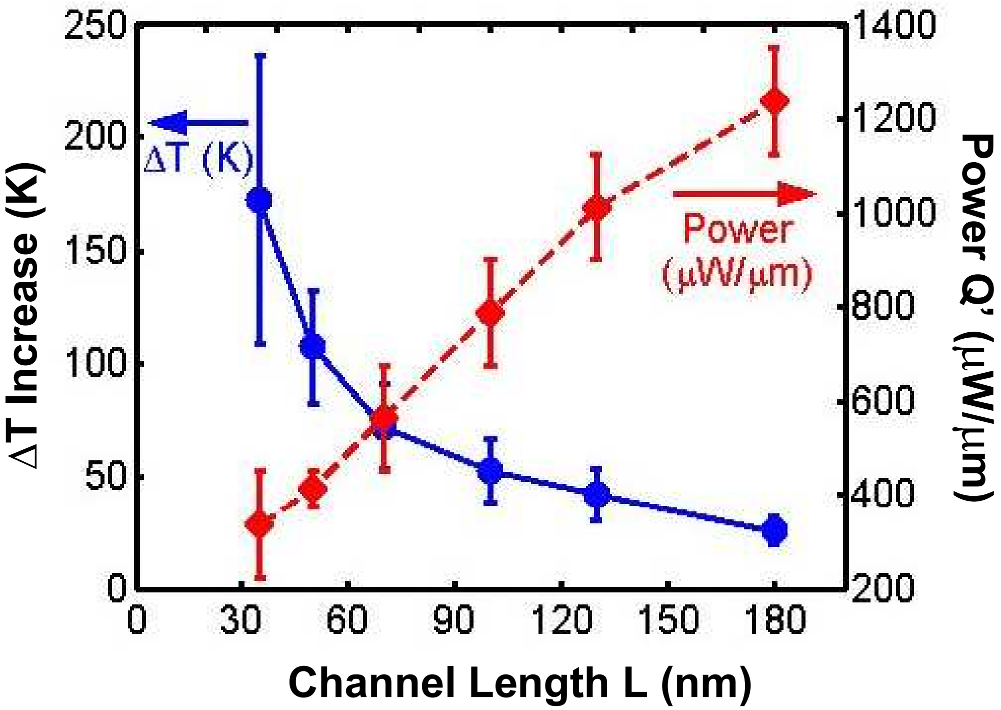




# Peak Device Temperature Scaling



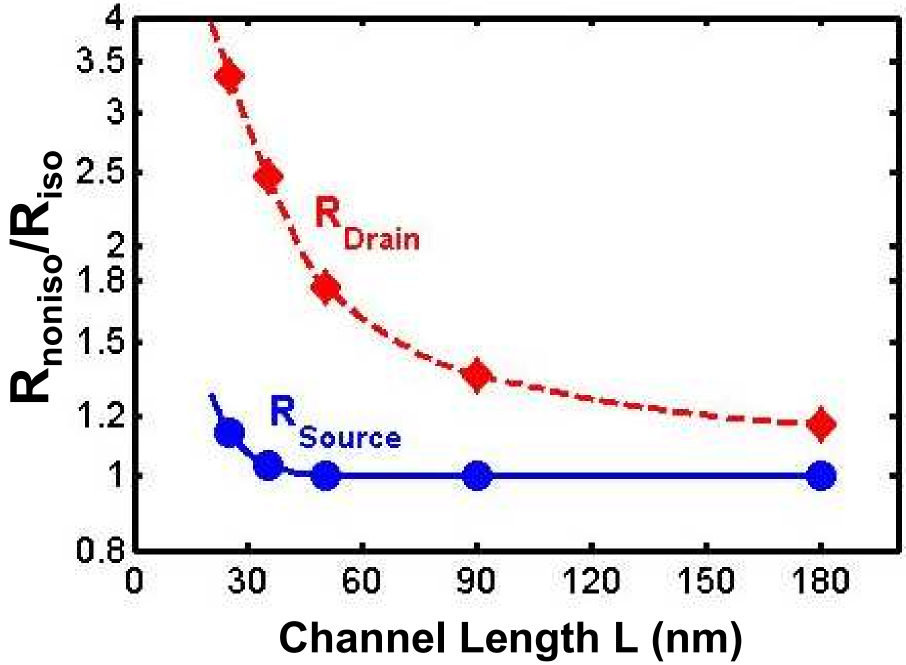
$$\Delta T = \frac{Q' \Lambda^2}{3 A_{eff} k_s}$$

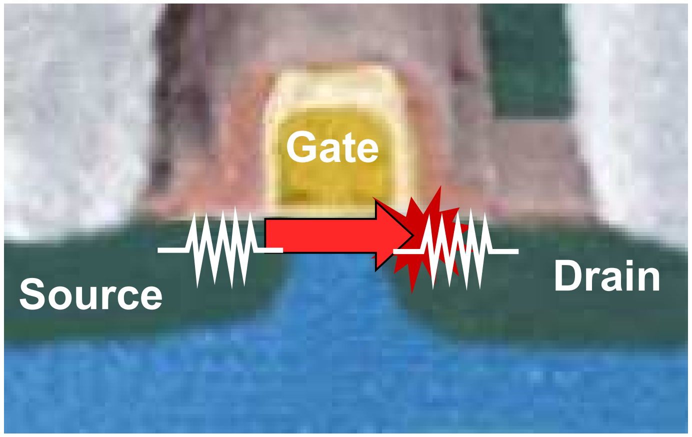


- ***Q' = I•V***
- **simple hot spot T model (Q' → optical phonons)**
- **expect T rise due to localization of power density**

# Series Resistance Scaling

*E. Pop, K. Banerjee, P. Sverdrup, K. Goodson, R. Dutton, IEDM 2001*



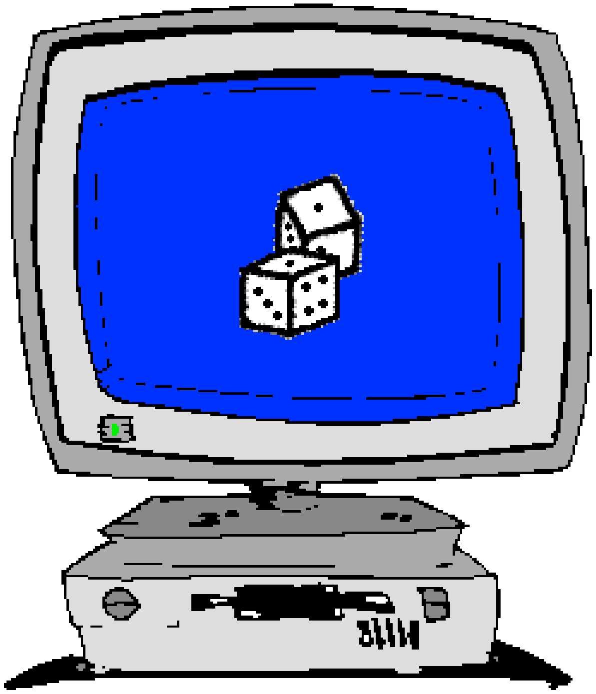


- $R_{Drain}$ ~ 4x, $R_{Source}$ ~ 1.3x at limits of scaling
- $R_{Drain}$ impact: not $I_{DS}$, but ESD, reliability
- $R_{Source}$ impact: $v_{inj}$, $g_m$ and $I_{DS}$

# Heat Generation with Monte Carlo

- Proper accounting of non-equilibrium and non-stationary effects

- Full information about phonon generation (optical vs. acoustic, q, ω)



- Reasonable speed ~ 0.1 msec CPU per particle per psec on modern desktop

# “Fixed-field” MC Implementation

- **Analytic, non-parabolic bands ($V_{dd} \le 1.1$ 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**

$$\Gamma(k)=\frac{2\pi}{\hbar}\left|M(k)\right|^2 g\left(E_k \pm \hbar\omega_q\right)$$

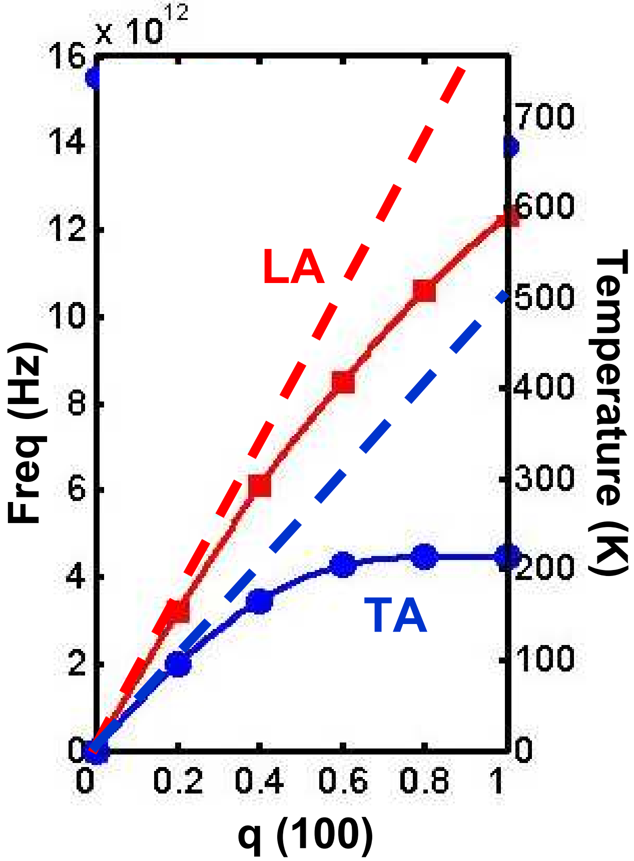
- **20,000 simulated “super-particles”**

  **→ $10^{20}$ ($1/\text{cm}^3$) 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**
- **Deformation potentials** (Herring & Vogt, *Phys. Rev.* 1956)

$$\Xi_{LA} = \Xi_d + \Xi_u \cos^2\theta \qquad \Xi_{TA} = \Xi_u \sin\theta \cos\theta$$

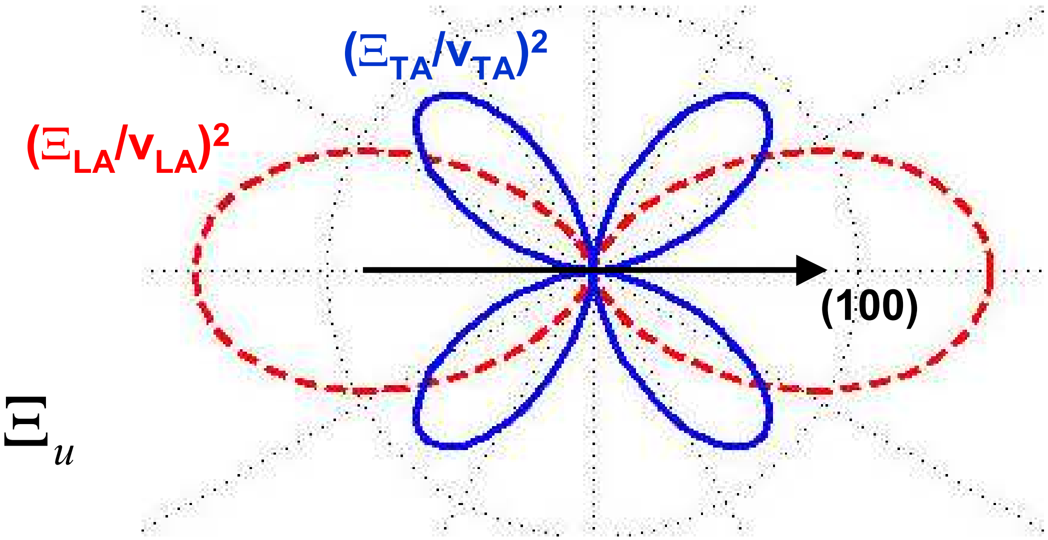
- **... not known with much certainty**

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

**dilation:** $\Xi_d \cong 1 \text{ eV} \ (\text{also } 1.2, 1.13, 5, -11.7 \text{ eV})$

- **Most recent values** (Fischetti & Laux, *J. Appl. Phys*. 1996)

# Average LA, TA Def. Potentials

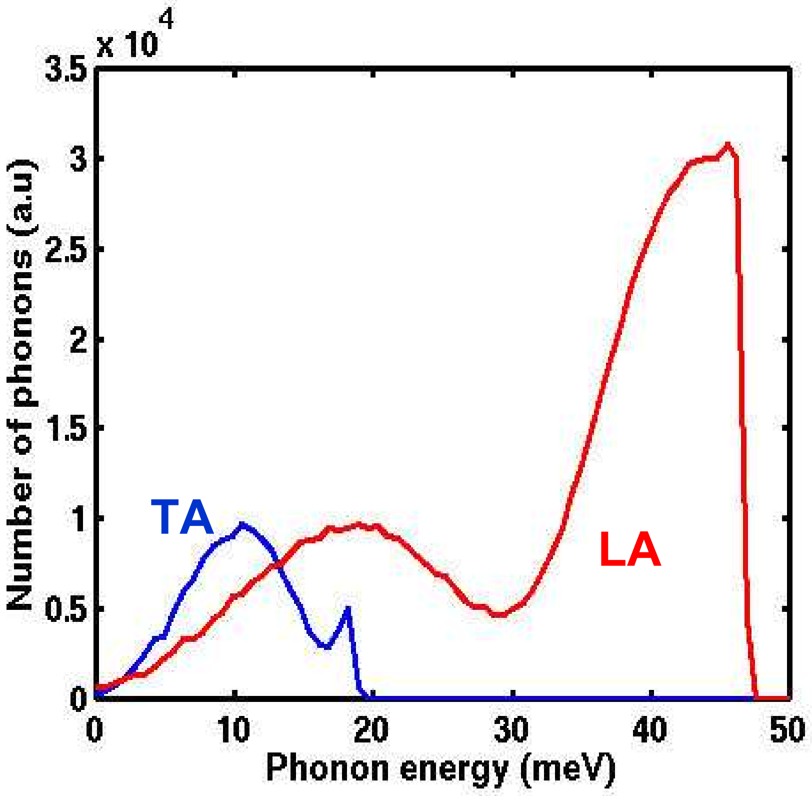


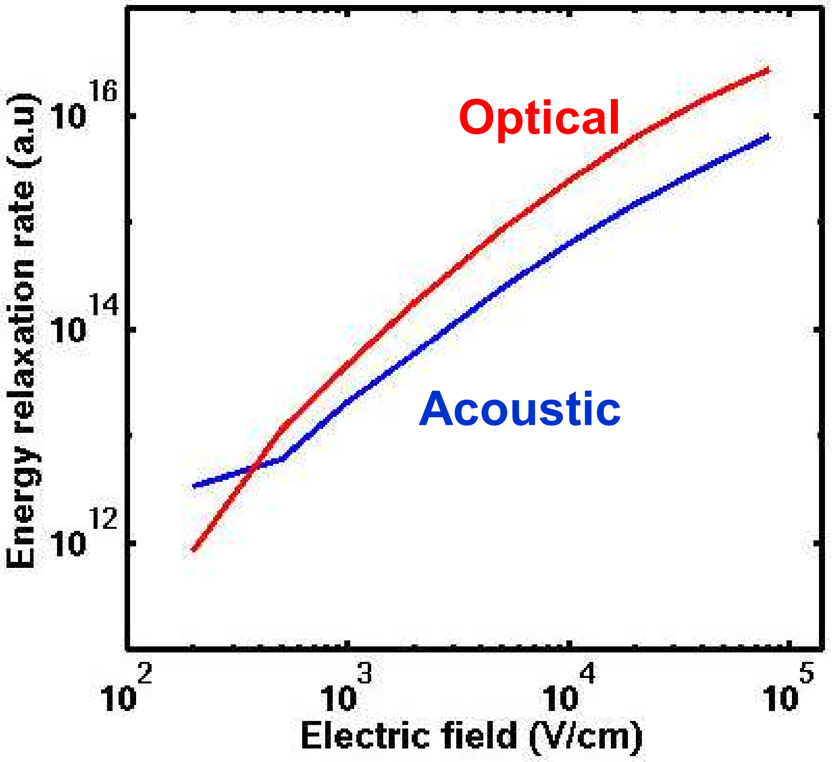
$$D_{TA} = \sqrt{\left\langle \Xi_{TA}^2 \right\rangle\Big|_\theta} = \frac{\sqrt{\pi}}{4}\Xi_u$$

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

- **Averaged** values: $D_{LA}$=8.7 eV, $D_{TA}$=4.4 eV, $v_{LA}$=9000 m/s, $v_{TA}$=5300 m/s

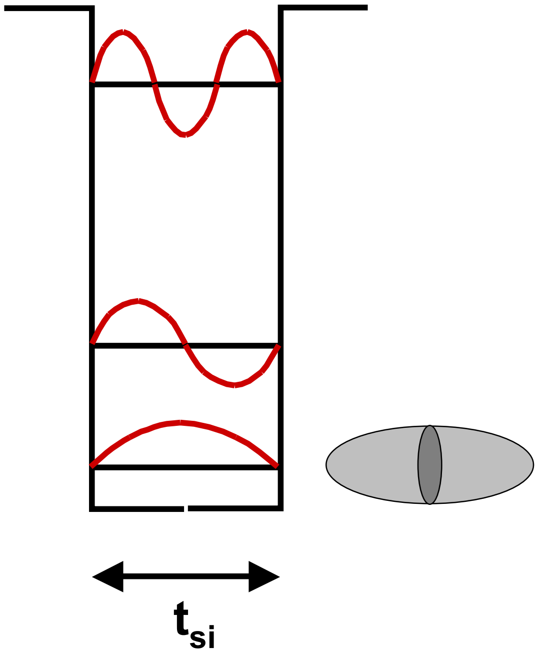
# Computed Phonon Generation

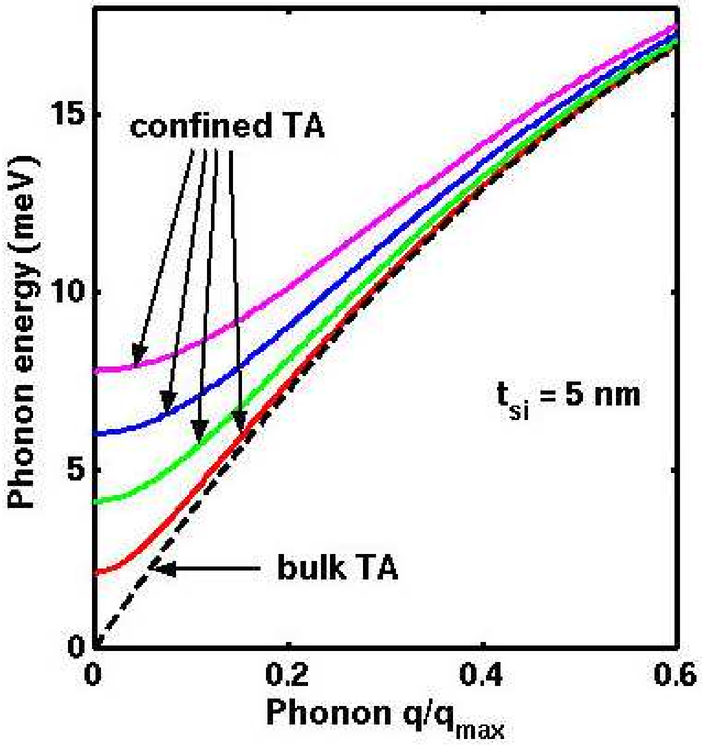




- **Near-full band MC complexity for analytic-band MC speed – towards a device designer’s MC?**

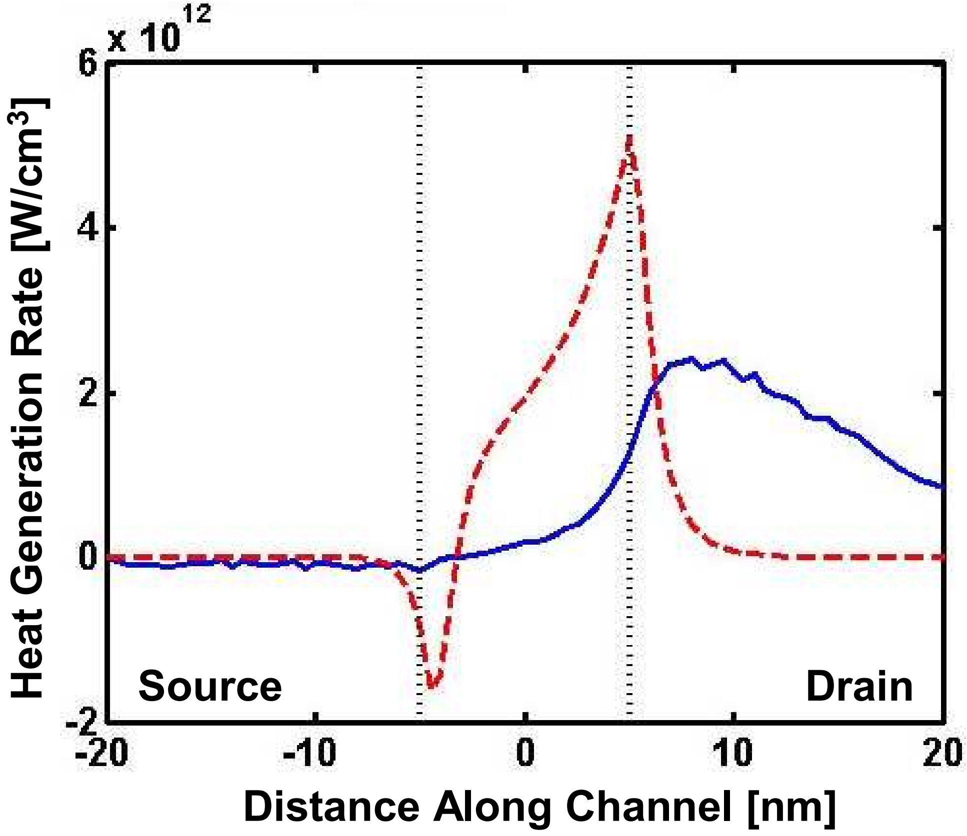
# Confined Electrons  and Phonons





- **Electro-thermal transport in ultra-thin silicon films ($t_{si}$ ~ 5 nm): role of electron and phonon *confinement***

# Heat Generation in 10 nm Device



- Compare W=J·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

# Technology Transfer

- Strong collaboration with IBM
- Share fundamental results and publications (IEDM, IMECE, EDL, APL) with all SRC member companies
- Computer code and manuals to be available online *microheat.stanford.edu* or via Purdue Computational Nanohub