Monte Carlo Modeling of Heat Generation in Silicon Nanostructures

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Project Goals

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

Nanoscale Heat Transport

- **Heat diffusion equation (D » Λ)**

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

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

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

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

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

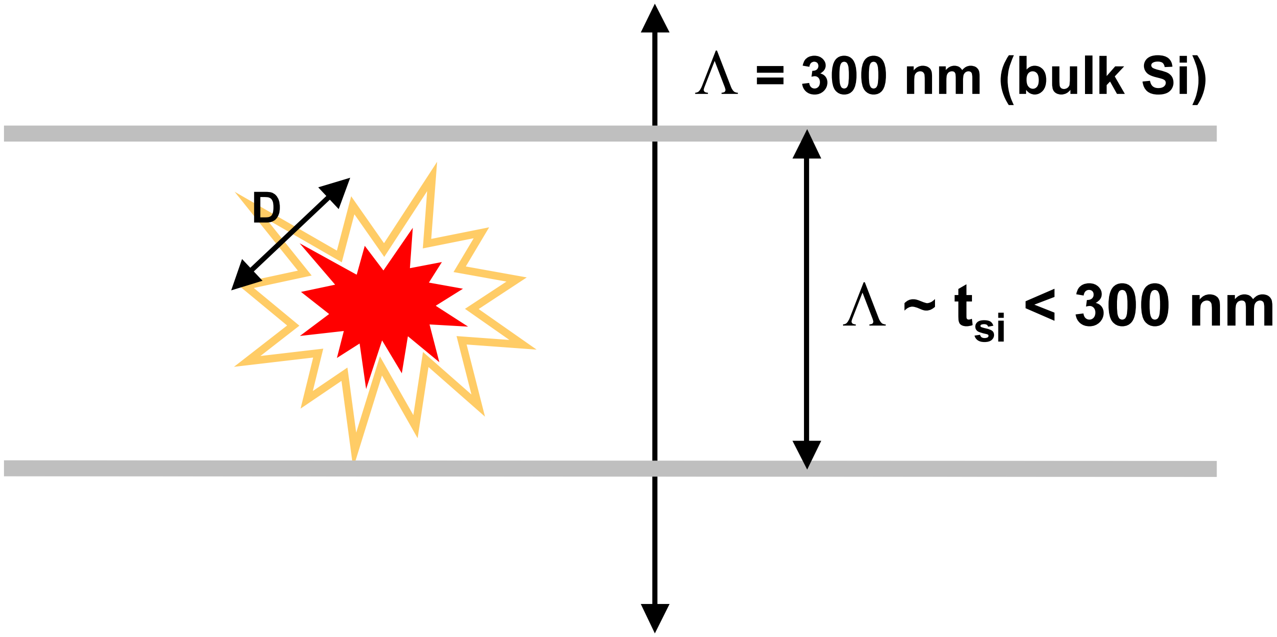
ITRS Roadmap

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 ($D \ll \Lambda$ phonons)



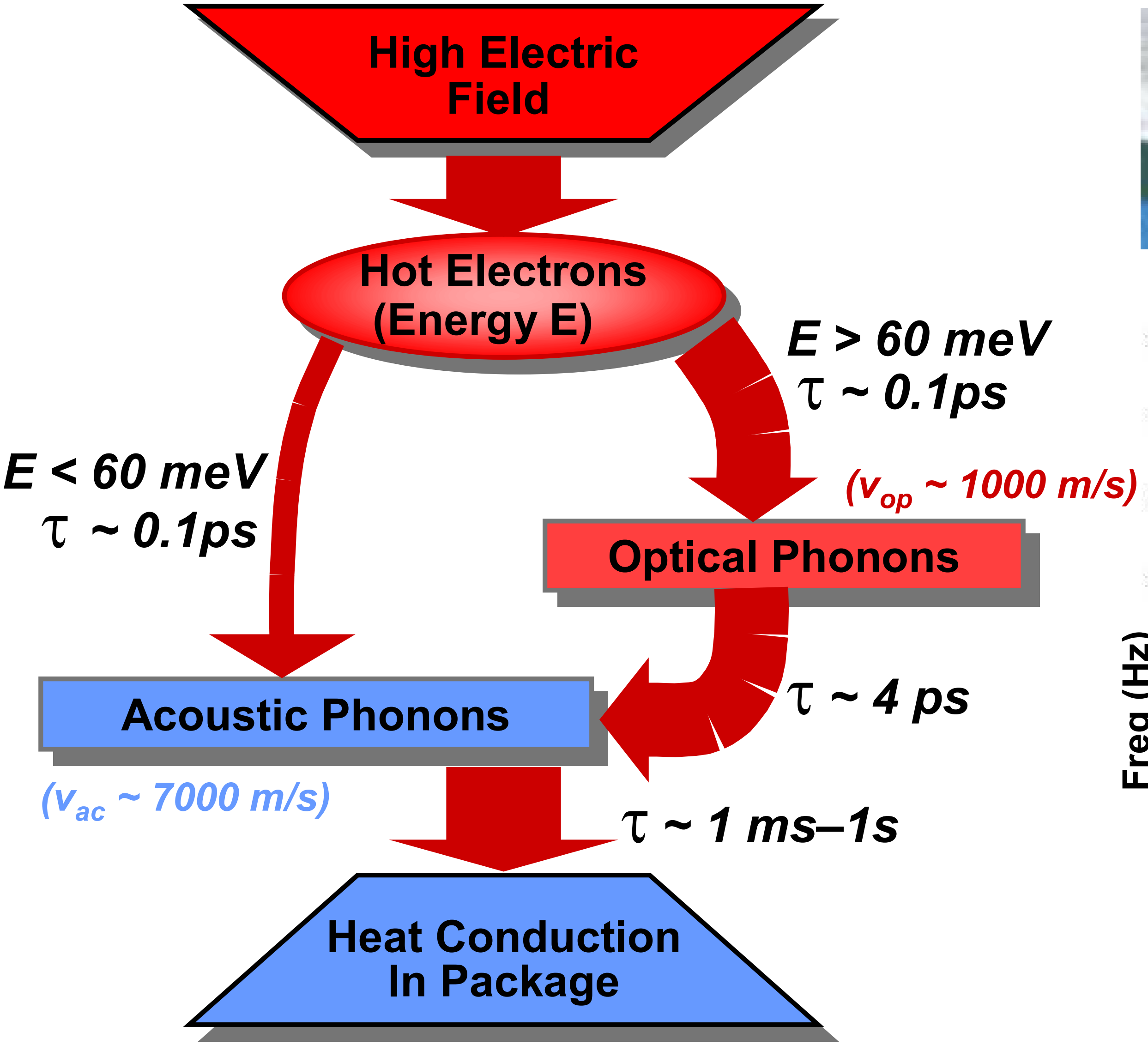
Λ = 300 nm (bulk Si)

D

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

- 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)

Optical Phonons

E < 60 meV
τ ~ 0.1ps

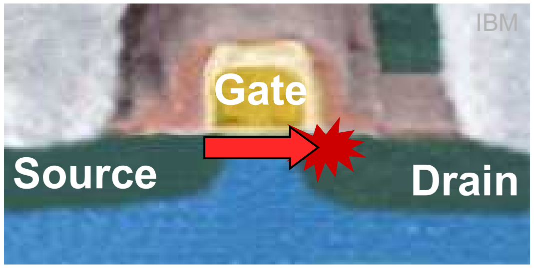
τ ~ 4 ps

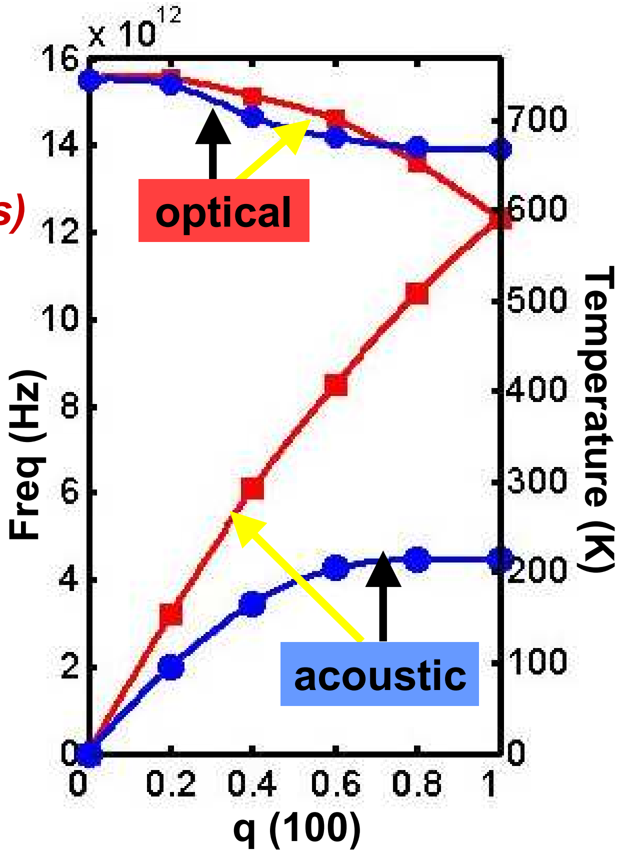
Acoustic Phonons

(v_{ac} ~ 7000 m/s)

τ ~ 1 ms–1s

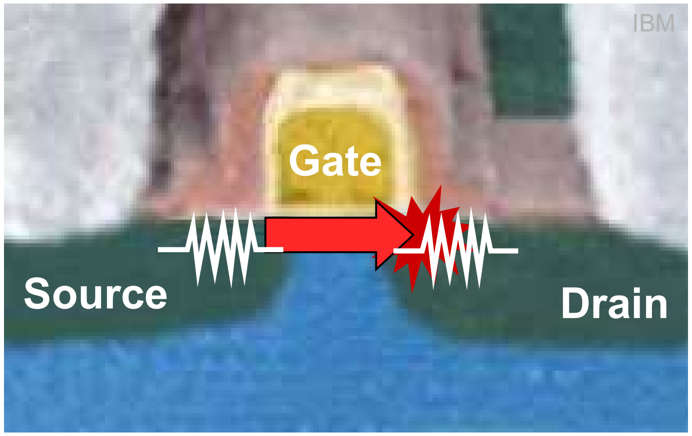
Heat Conduction In Package

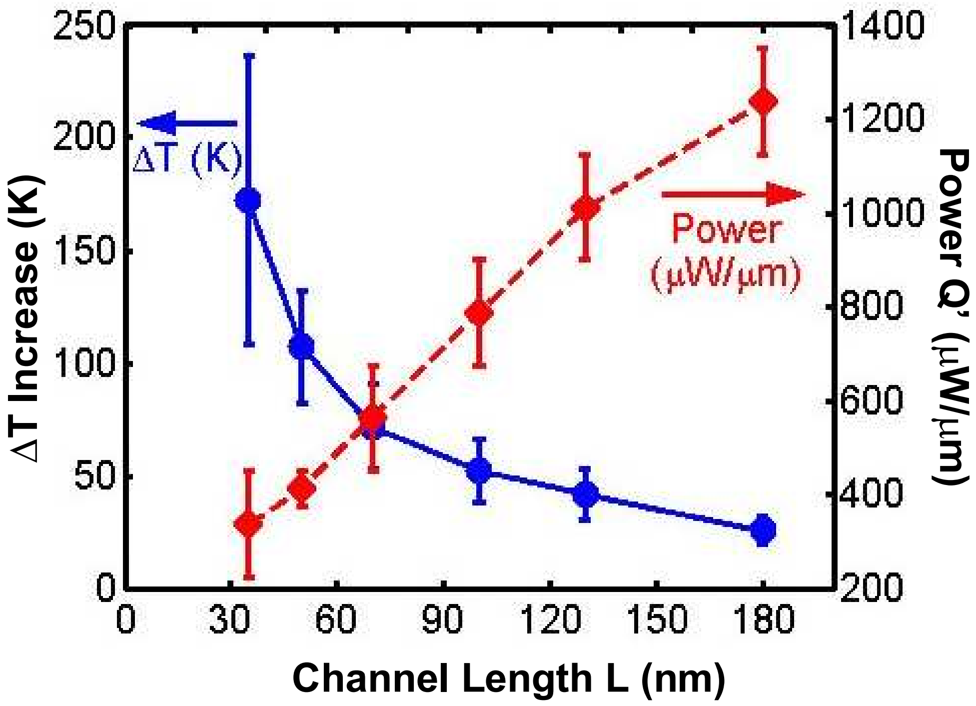




Peak Device Temperature Scaling

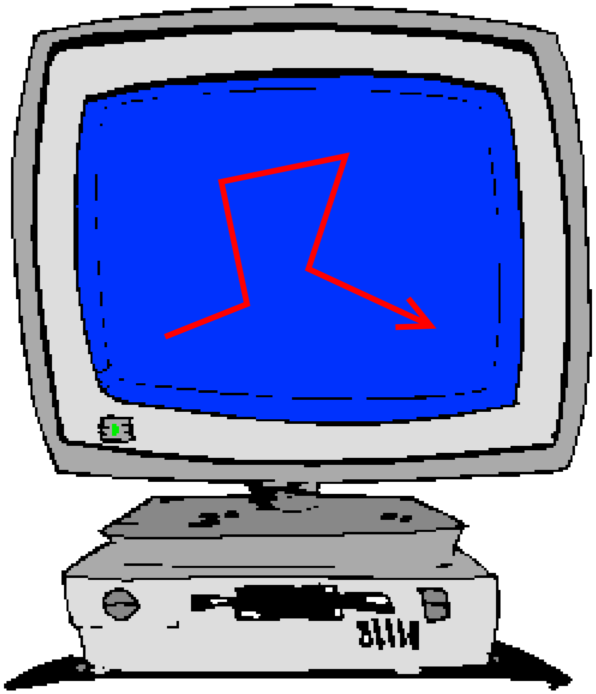
E. Pop, K. Banerjee, P. Sverdrup, K. Goodson, R. Dutton, IEDM 2001





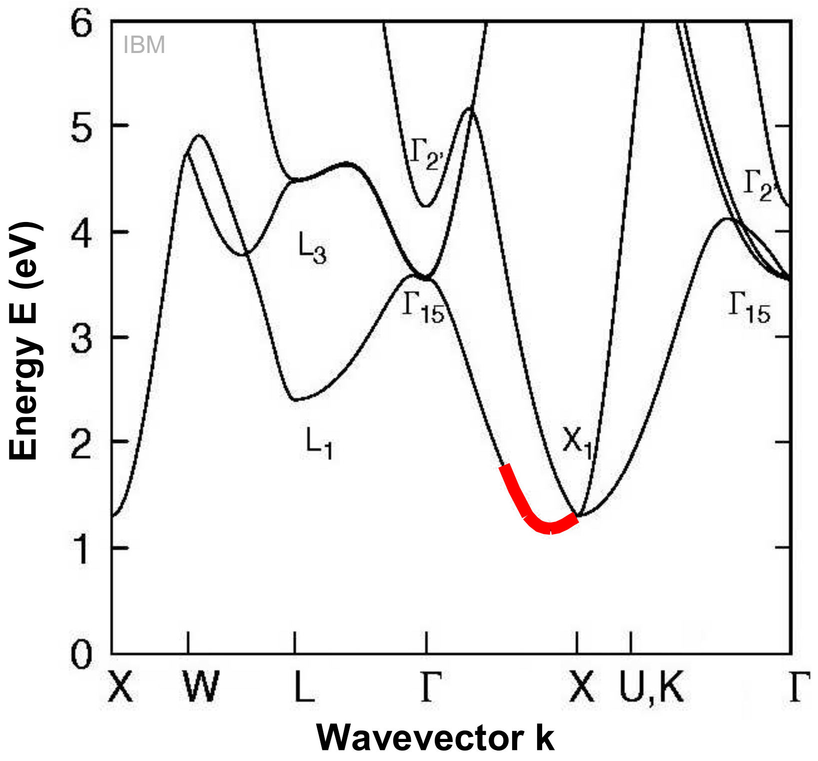
- *Q' = I•V*
- **Simple hot spot T model (Q' → optical phonons)**
- **Decreasing voltage/power as devices scale down**
- **Expect T rise due to localization of power density**

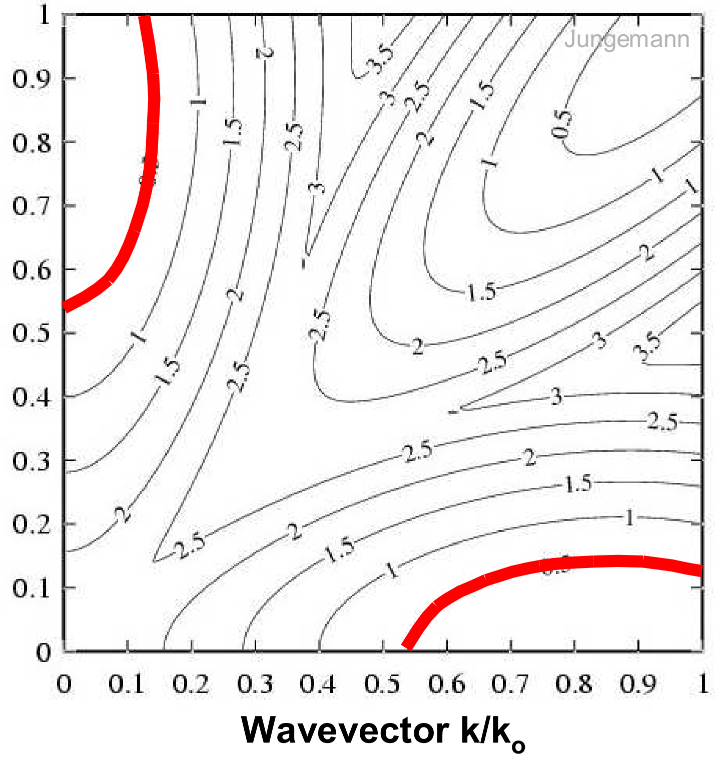
Heat Generation with Monte Carlo



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

Silicon Electron Energy Bands





- **May ignore impact ionization at low V_{dd}**
- **Analytic band approximation below ~ 1 eV**

“Fixed-field” MC Implementation

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

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

- **Inelastic acoustic and optical phonon scattering**

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

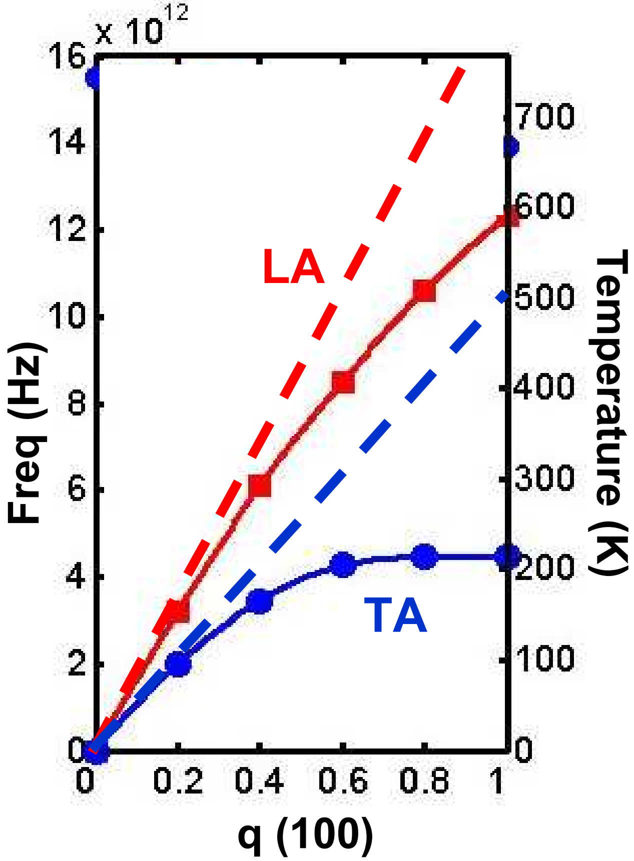
- **20,000 simulated “super-particles”**

  → 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)

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

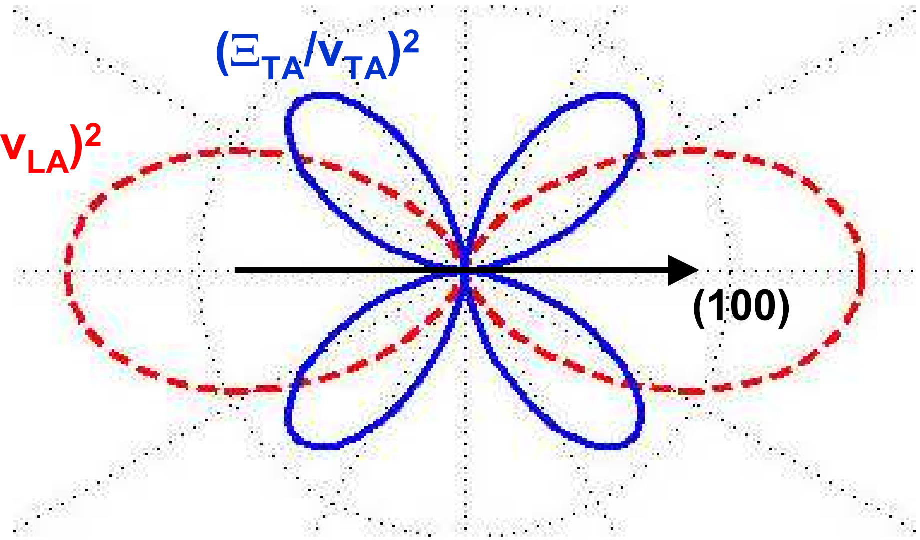
- **... not known with much certainty**

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

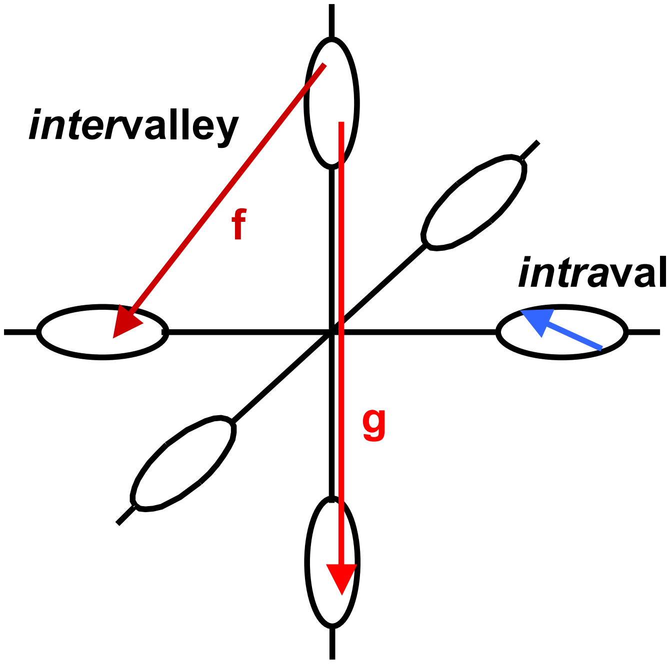


$$D_{TA} = \sqrt{\left.\left\langle \Xi_{TA}^2 \right\rangle\right|_\theta} = \frac{\sqrt{\pi}}{4}\Xi_u$$

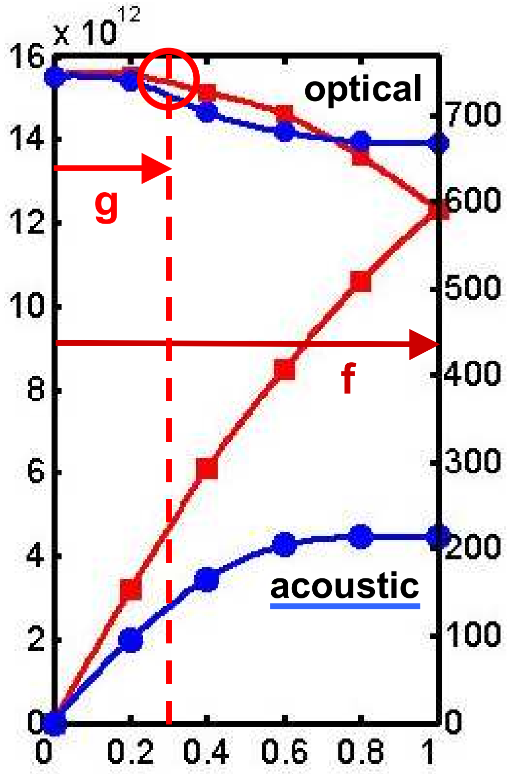
$$D_{LA} = \sqrt{\left.\left\langle \Xi_{LA}^2 \right\rangle\right|_\theta} = \left[\frac{\pi}{2}\left(\Xi_d^2 + \Xi_d\Xi_u + \frac{3}{8}\Xi_u^2\right)\right]^{1/2}$$

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

Intervalley Phonon Scattering

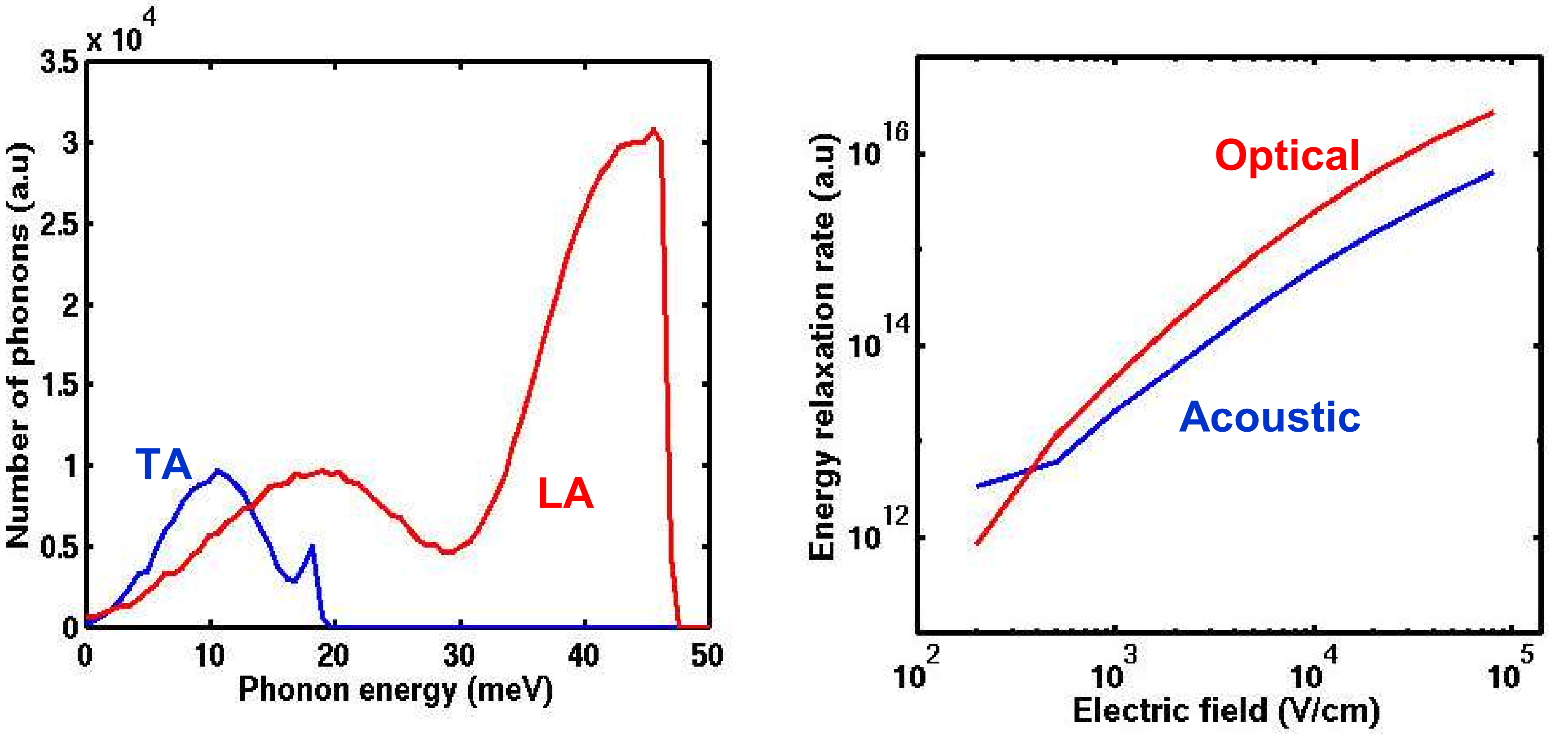


$$\mathbf{k}' = \mathbf{k} \pm \mathbf{q} + \mathbf{G}$$



- ***Intra*valley ~ acoustic, E < 60 meV**
- ***Inter*valley ~ optical (f and g type) inelastic**
- **Does g-phonon at 0.3G (LO 730 K) dominate?**

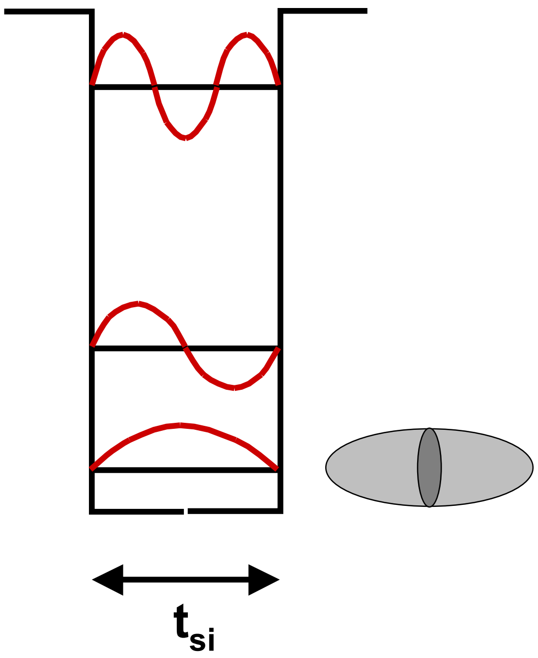
Computed Phonon Generation



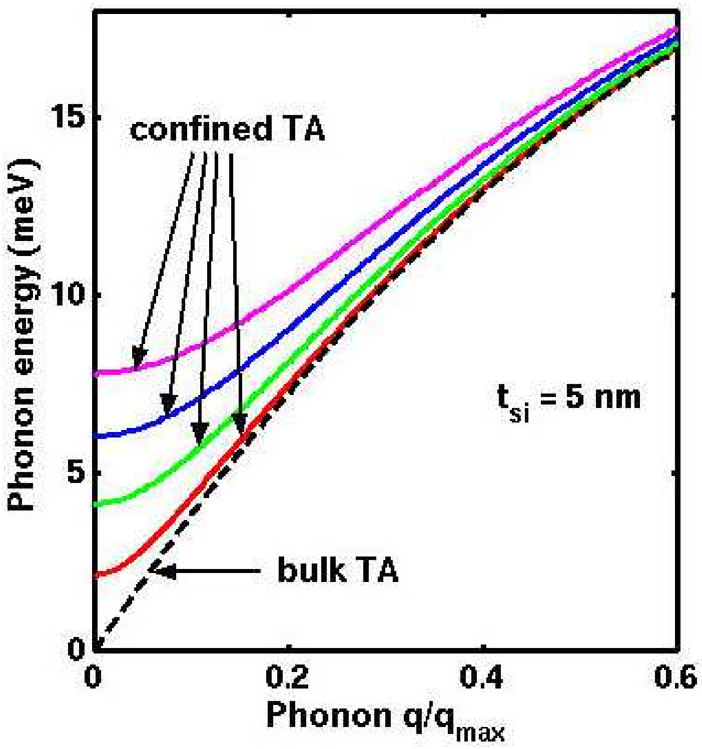
- **Near-full band MC complexity for analytic-band MC speed – towards a device designer’s MC?**

Confined Electrons and Phonons

2-D Electrons

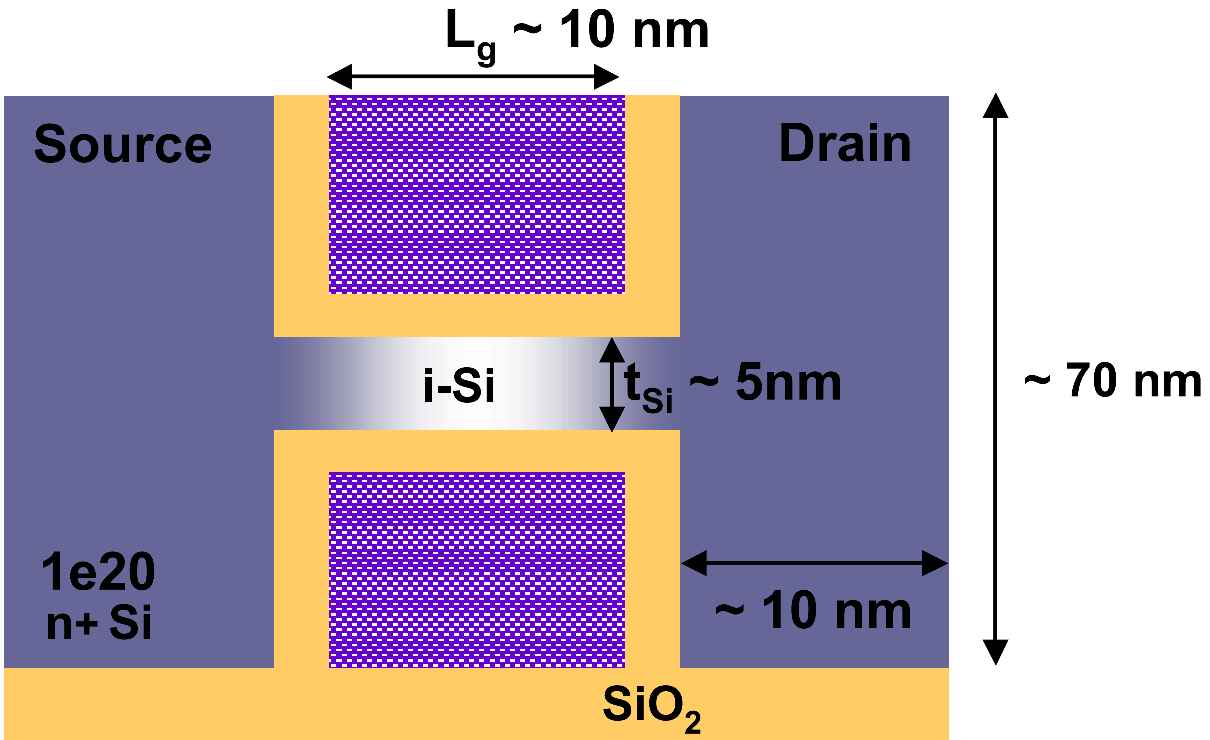


2-D Phonons



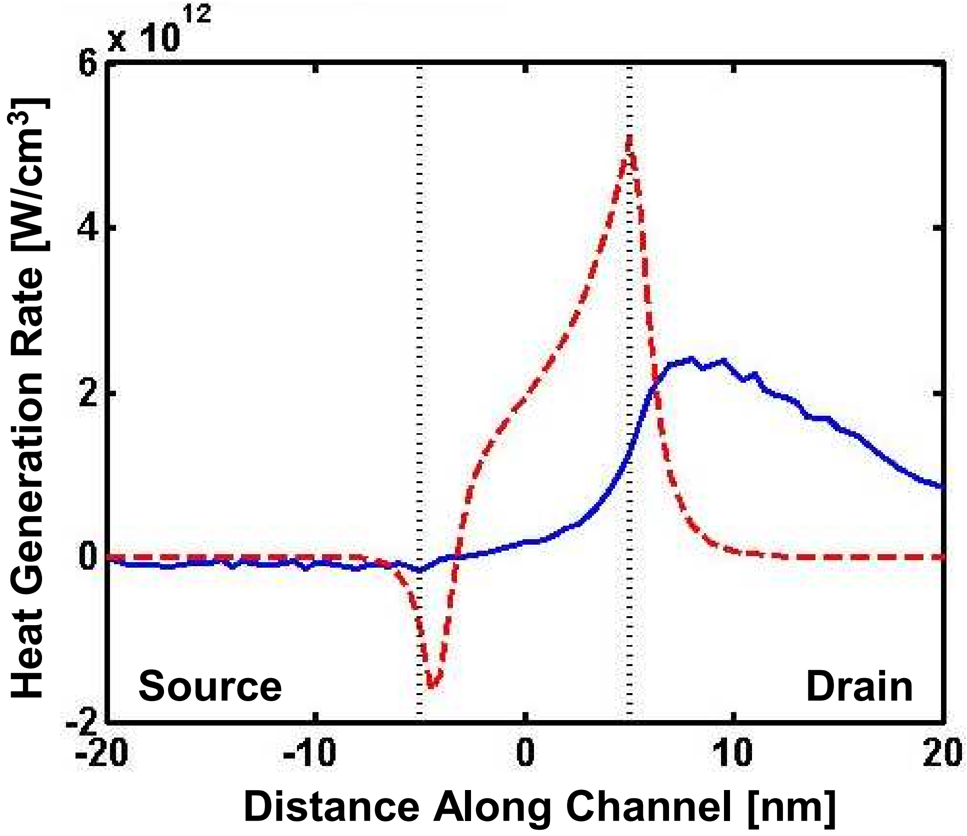
- **Electro-thermal transport in ultra-thin silicon films (t_{si} ~ 5 nm): role of electron and phonon *confinement***

Dual-Gate SOI Transistor



- Great electrostatic channel control
- 1-D electron and phonon transport along channel
- Electron (and phonon!) quantum confinement

Heat Generation in 10 nm Device



- Compare W=J·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