UMass Amherst

Nanophononics: dissipation and thermoelectric energy conversion in nanoscale devices

Zlatan Aksamija

NanoEnergy&Thermophysics lab

University of Massachusetts at Amherst

zlatana@engin.umass.edu

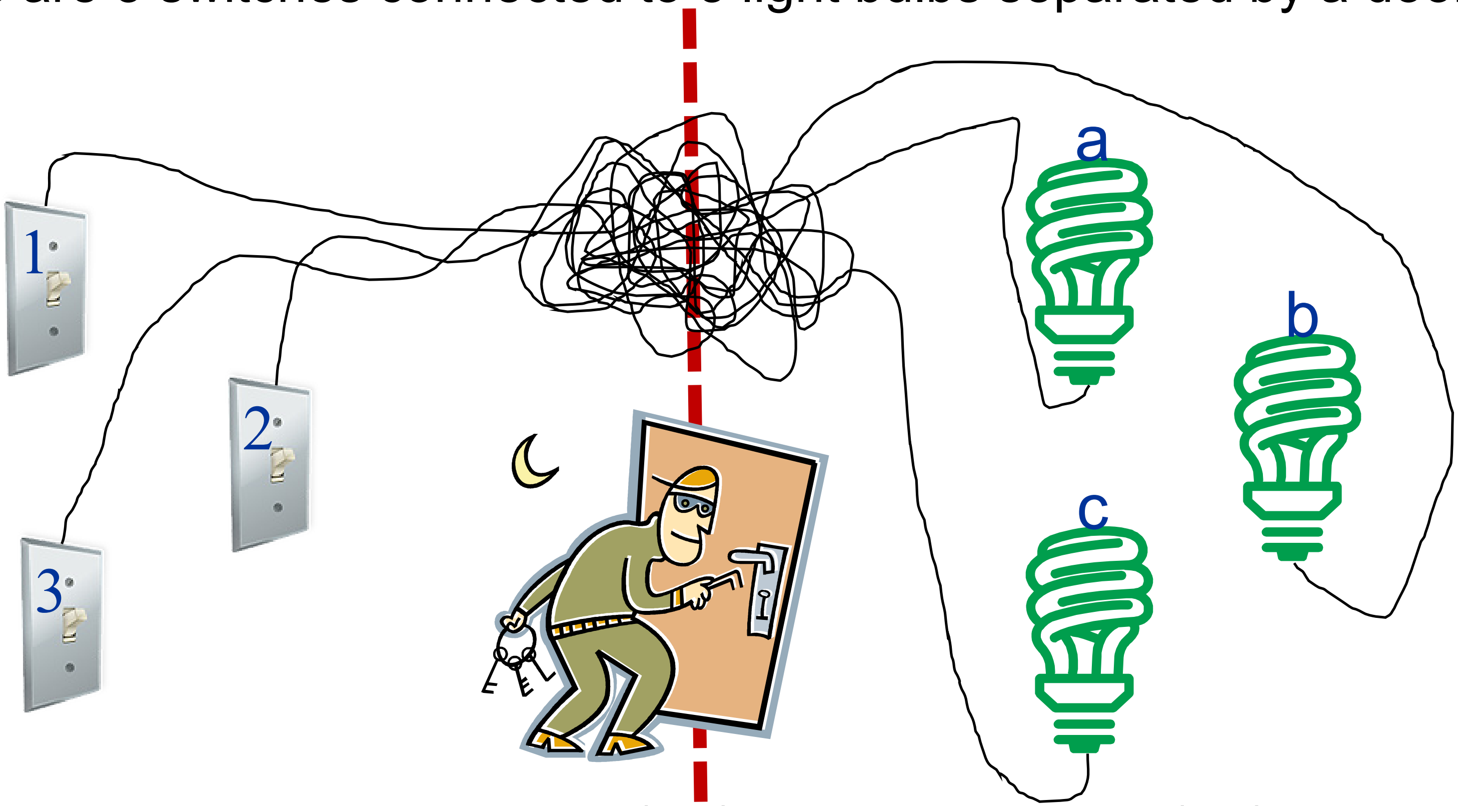
http://netlab.umasscreate.net

PIER, Hamburg 2019

Nanophononics Workshop

Let's start with a thought experiment

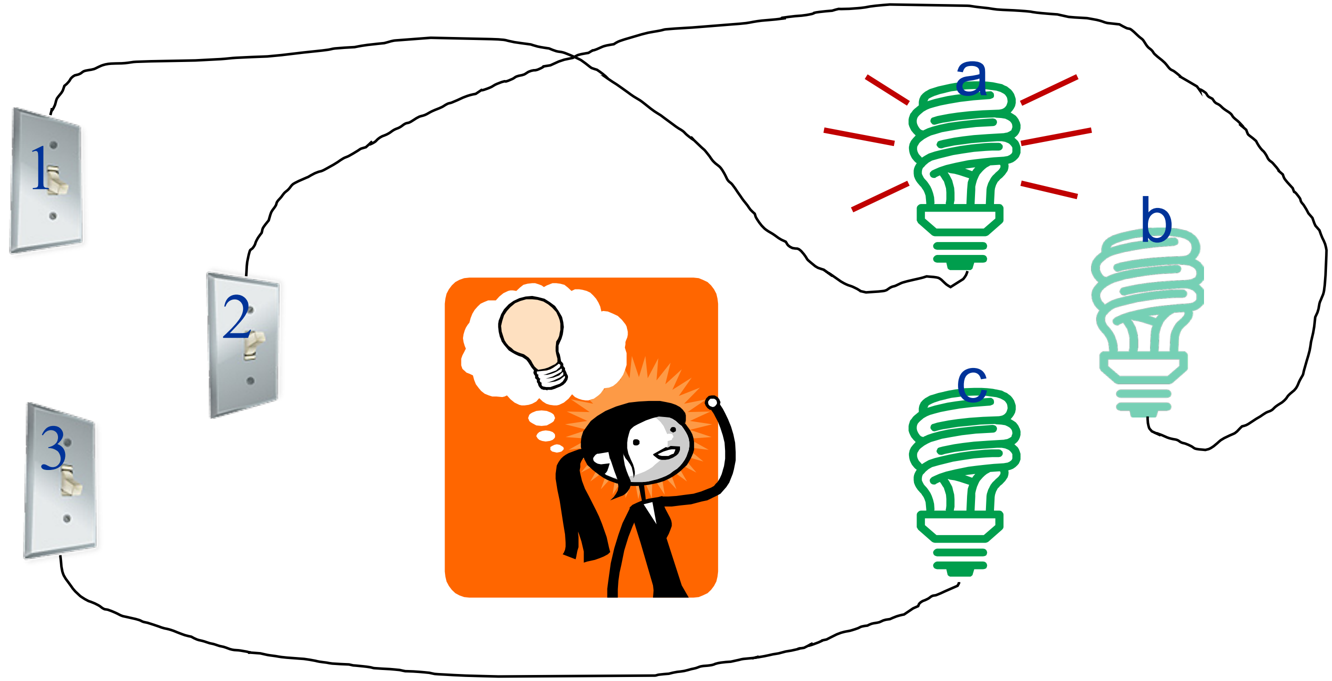
- There are 3 switches connected to 3 light bulbs separated by a door



- **Challenge**: determine which switch (1-3) controls which bulb (a-c) while passing through the door only once (no peeking)!

Answer: use the "thermal signature"!

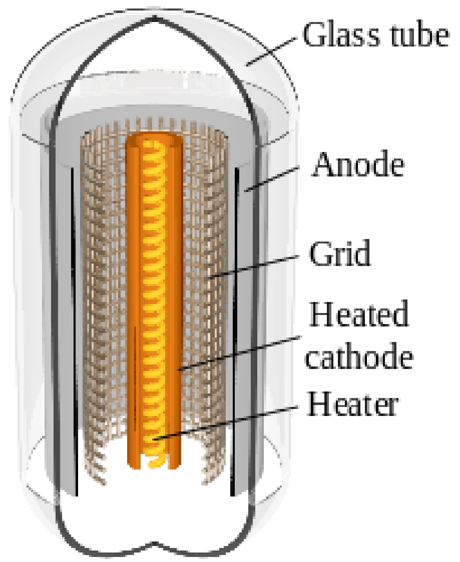
- Flip switch #1, wait 5 mins. Then flip switch #2 and go through
- **Solution:** hot bulb is connected to #1, the lit bulb is connected to #2

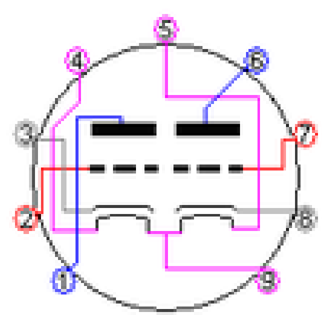


- **Moral**: Heat stores and transmits useful information, a "thermal signature", of a process and is the ultimate destination of all the energy we use!

At the dawn of time…

- First there were vacuum tubes
- Invented in 1904 by John Ambrose Fleming
- Diodes, triodes, pentodes, miniatures
- Still used for extreme environments
  - ex. Viktor Belenko deflected from the USSR to Japan/US with his MIG-25 fighter jet in 1976, all electronics were using vacuum tubes
- Or extreme audiophiles (ex. guitar amps, studio gear)
- Simple operation: heat up a metals and electrons will “boil” off the cathode, add a grid to control them
- Issues: heat/energy, reliability

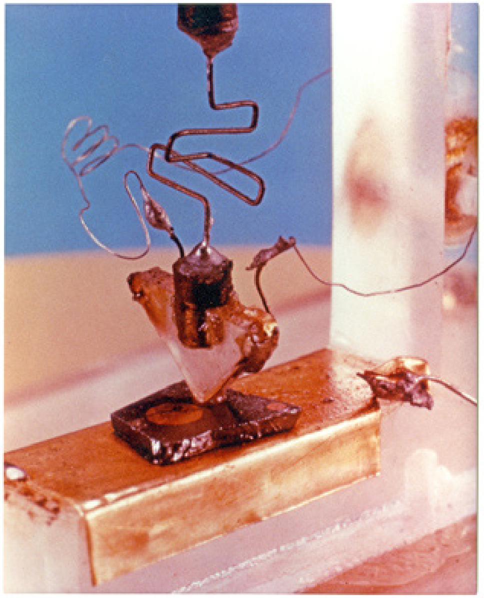


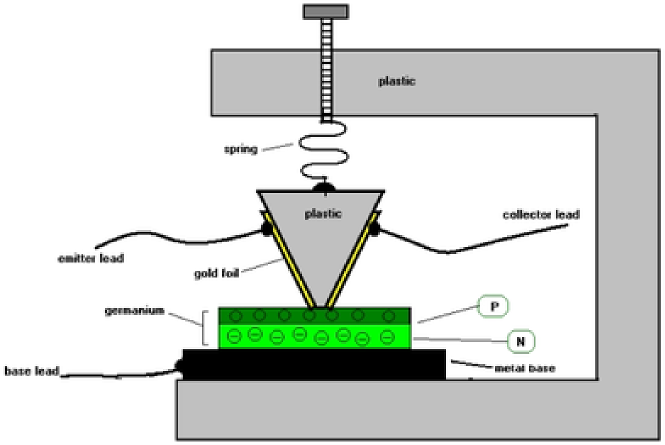


1. Anode Triode Number 2
2. Grid Triode Number 2
3. Cathode Triode Number 2
4. Heater (Triode 2)
5. Heater (Triode 1)
6. Anode Triode Number 1
7. Grid Triode Number 1
8. Cathode Triode Number 1
9. Heater Center tap

Enter the transistor

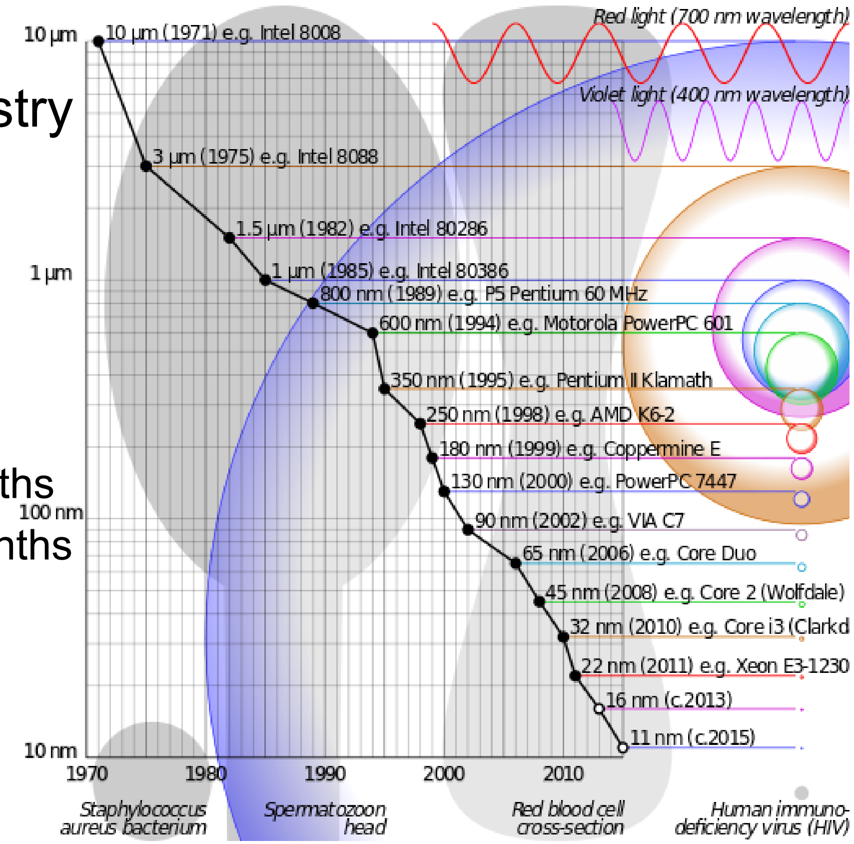
- Invented by 1947 by John Bardeen, Walter Brattain, and William Shockley at Bell Labs
- First transistor was a “point contact” transistor
- Shared the Nobel Prize in Physics in 1956
- One of IEEE milestones in electronics
- Requires no heating
- Can be bipolar (!?!)
- Small, reliable, efficient





Semiconductor Industry today

- Today it is a \$336 billion industry (2014) of that ~\$146 billion in the US
- Employs 250,000 people in the US
- Powers a trillion dollar electronics industry
- Driven by miniaturization
- Moore's law
  - Functionality per cost doubles every 18 months
  - Transistors have to get smaller every 18 months
  - Reach 5 nm by 2020
  - Requires deep understanding of physics
  - Reaching fundamental limits of energy/size



Semiconductor Industry Tomorrow

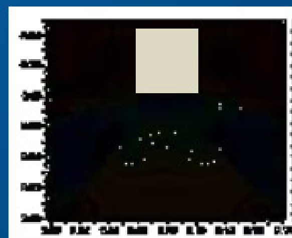
- End of “simple scaling”—no longer can follow Moore’s Law by making transistors smaller
  - Short channel effects—can’t turn transistors off any more due to quantum mechanics
  - Power catastrophe—dissipation limits performance, density, clock frequency
- New materials
  - Seamless integration of compound semiconductors (ex. GaAs channel)
  - **2-dimensional materials: graphene, MoS2, other TMDCs**
- New transistor design/geometry
  - **Tri-gate, nanowire, junctionless,** carbon nanotube, organic/DNA, self-assembled
  - Tunnel FETs, Spin valves
  - Flexible/wearable electronics
- New functionality
  - Optoelectronic integration, on-chip optical interconnects
  - **Energy devices like thermoelectric converters and on-chip cooling**
  - 2-terminal devices such as memristors and neuromorphic (brain-like) computing

NOW

Optimizing Choices for Transistors on Multiple Fronts

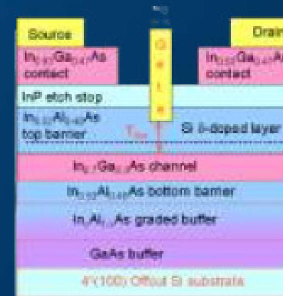
Increasing MOBILITY

(better ON)

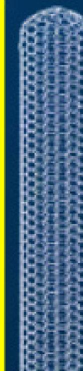


Strain

Ge



III-V

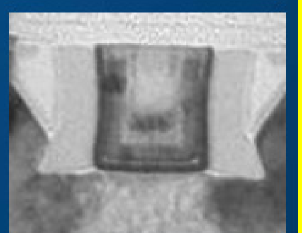


CNT

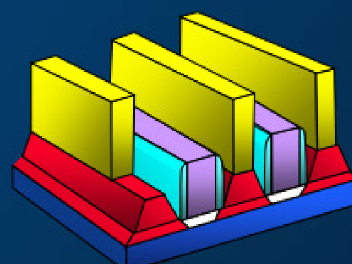
Graphene

Increasing COUPLING

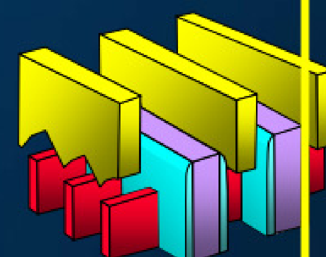
(better OFF)



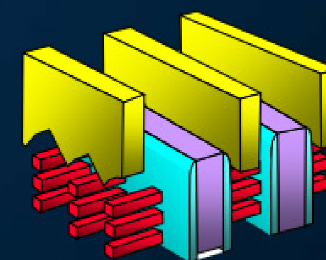
Planar
With High K



UTB SOI
(or QW)

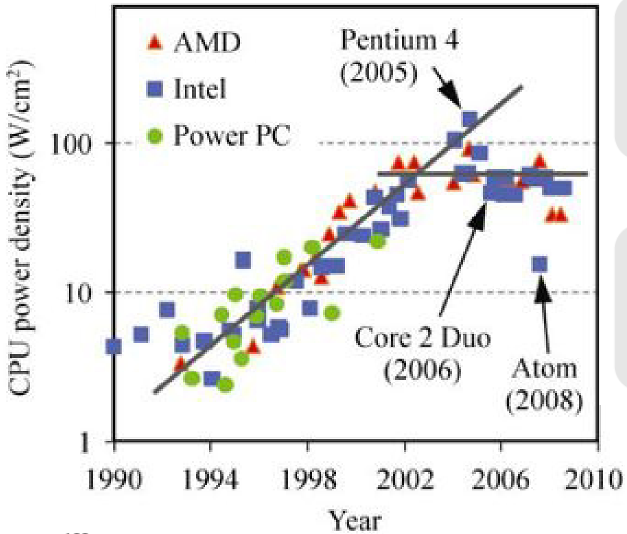


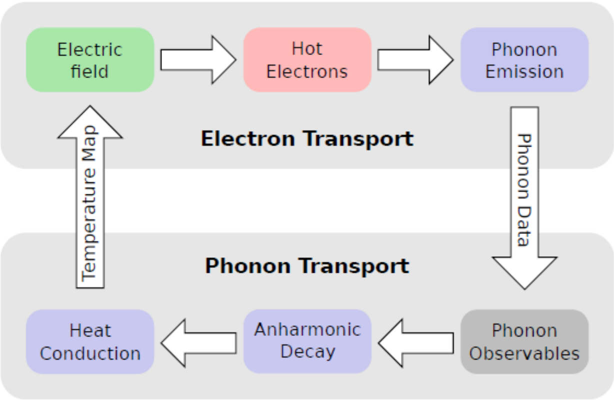
Fins



Wires/Ribbons

Heat dissipation in nanoelectronics





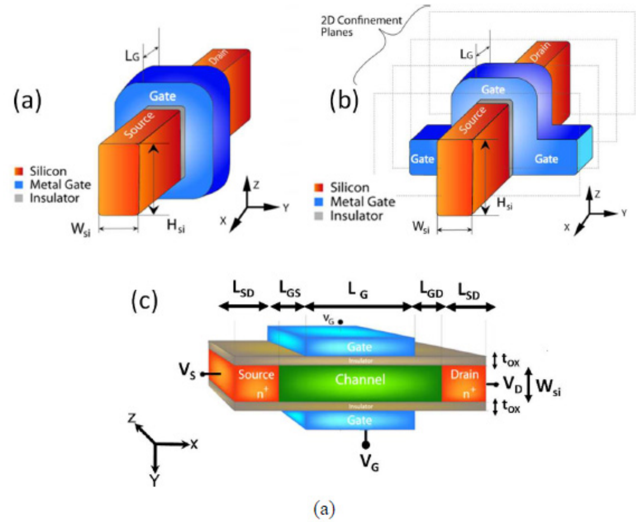
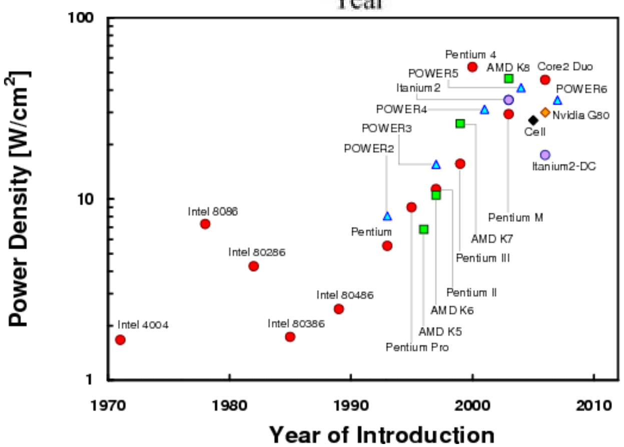
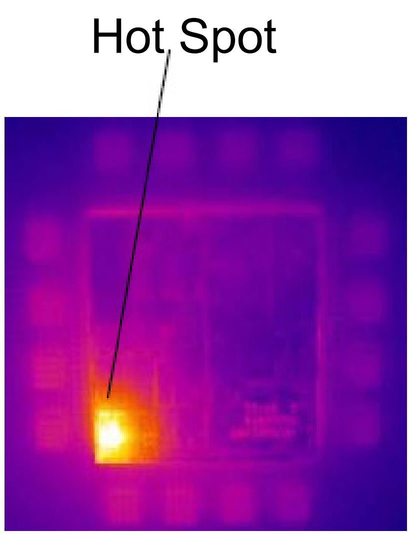
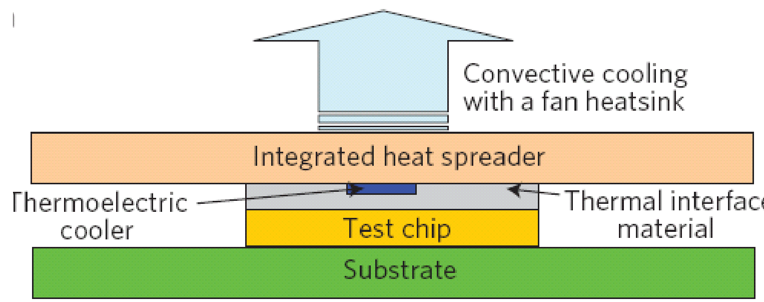


Fig. 4: Schematic of DG,TG and GAA.



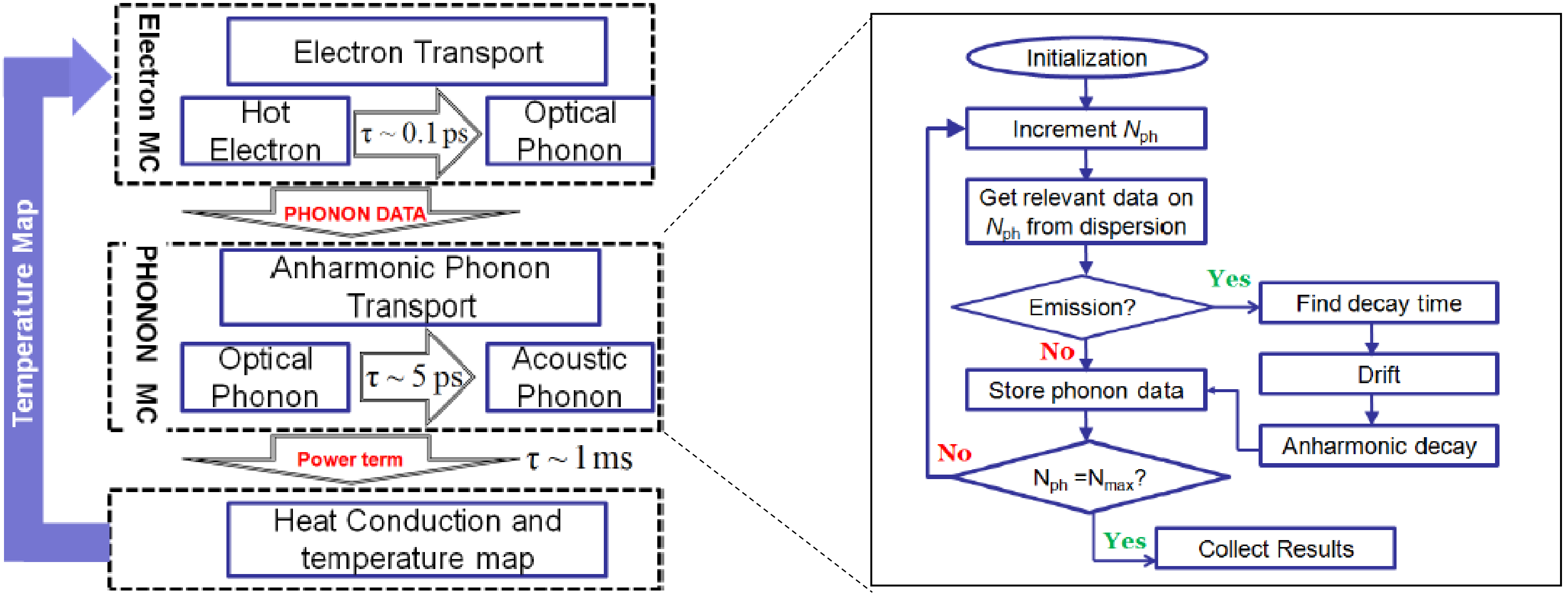




Chowdhury et al., Nature Nano. **4**, 235 (2009)

Electro-thermal simulation of devices

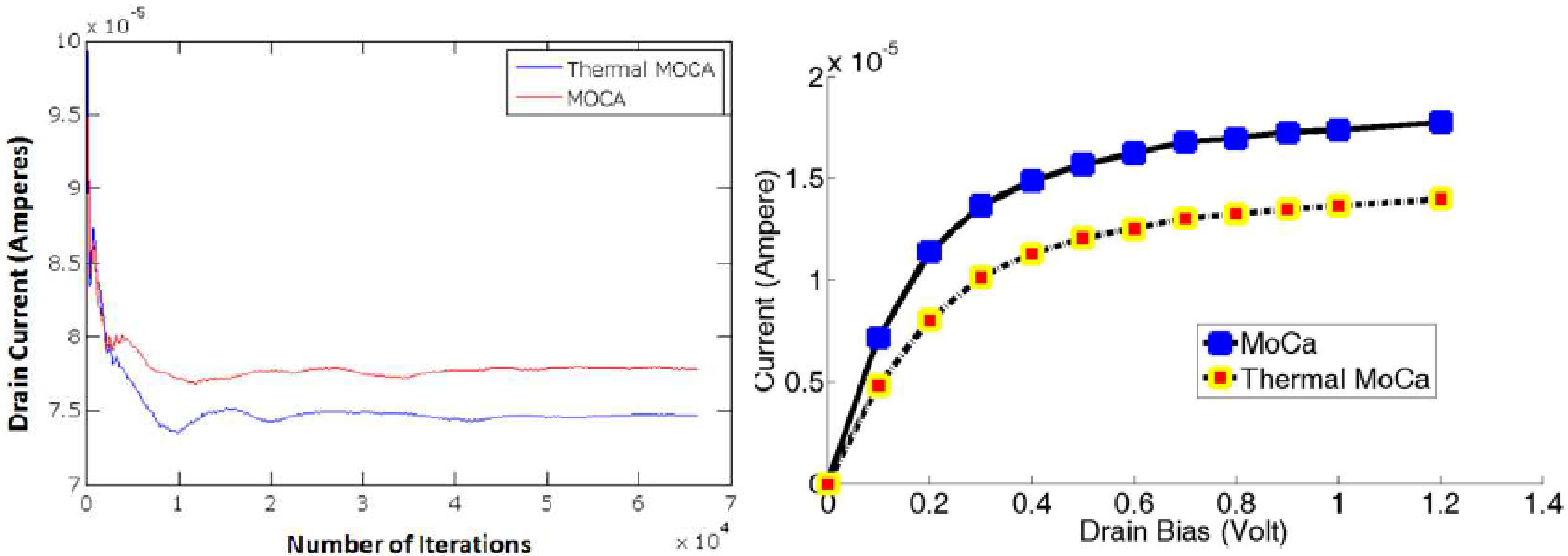
- Basic idea is to solve MC electron transport together with MC for phonons being emitted/absorbed by the electrons



- Also need to solve for heat conduction away from MC region

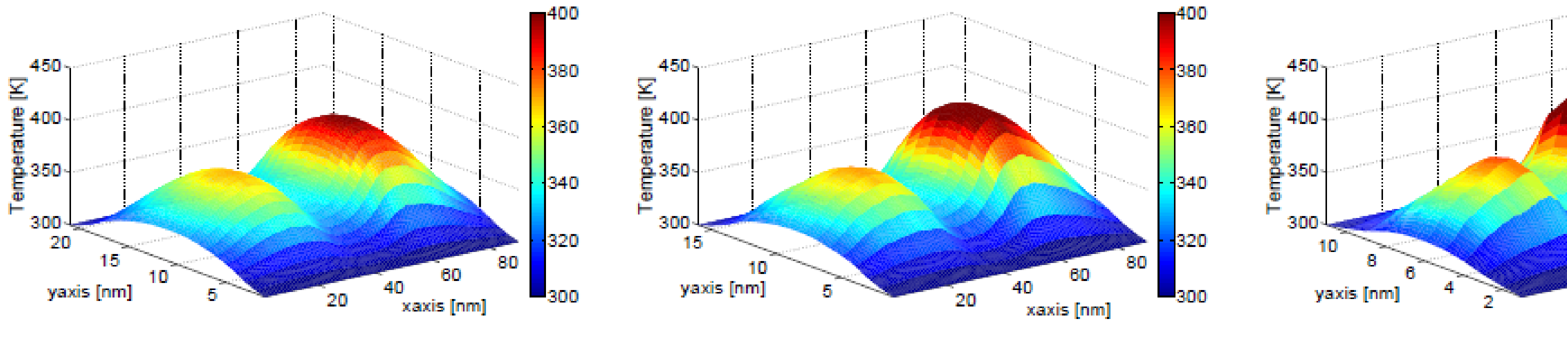
Electro-thermal simulation of devices

- Self-heating in nanoscale MOSFET devices results in current degradation
- We can see the inclusion of thermal effects results in the code converging to lower drain current (left)
- Current degradation is more pronounced at higher bias (right)
- **M. Mohamed et al., IEEE Trans. Elec. Dev. 61, 976 (2014)**



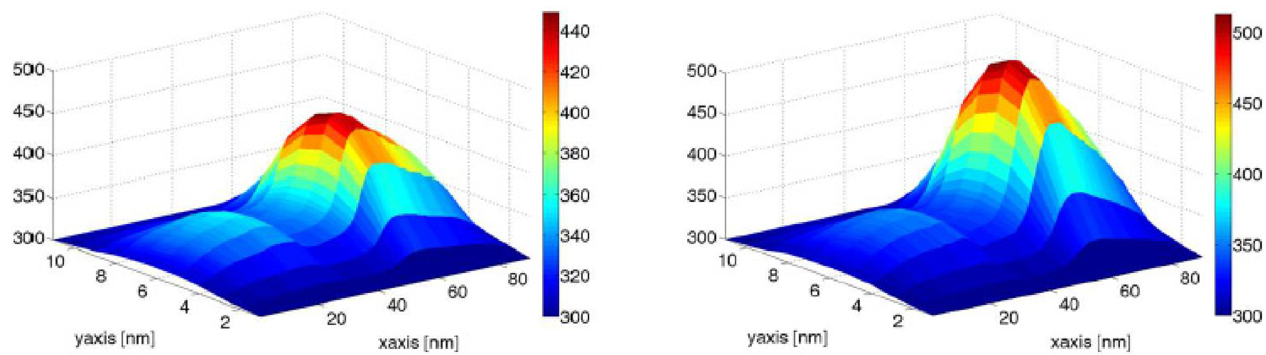
Electro-thermal simulation of devices

- Temperature profiles for GAA (gate-all-around) devices with square cross-section of (a) 20 nm, (b) 10 nm, and (c) 5 nm at $V_G=V_D=0.5$ V



(a) (b) (c)

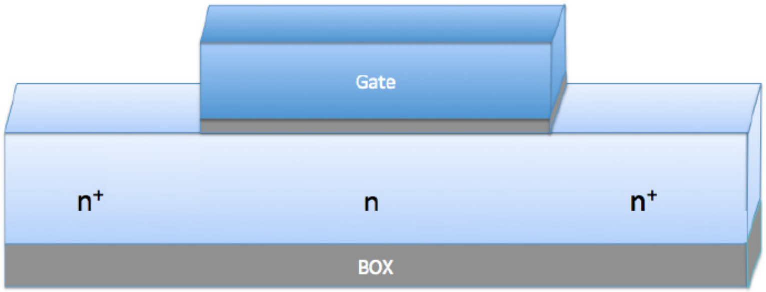
- T profiles for a 5 nm GAA device with $V_G=V_D=0.7$ V (a) and 1 V (b)

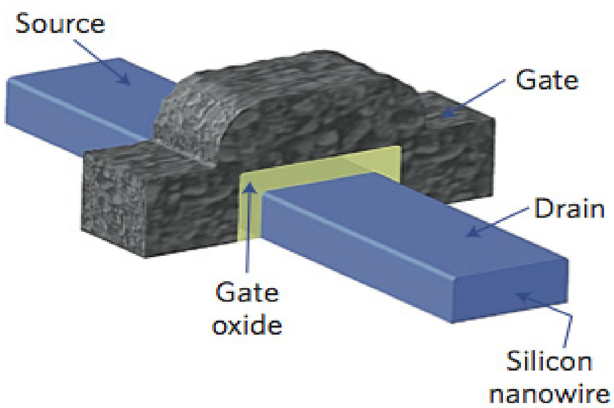


(a) (b)

Dissipation and self-heating in Junctionless MOS

- New type of transistor without junctions.
  - Source, drain and channel all doped with the **same polarity** (dopant type)
  - Easier to manufacture, functionality comparable to inversion mode MOSFETs.
  - JL is **depletion mode device**. The work function difference of silicon wrt the gate material must be large enough to fully deplete the channel when voltage is not applied

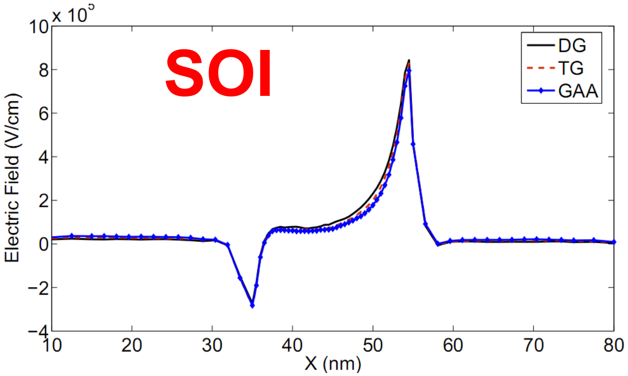


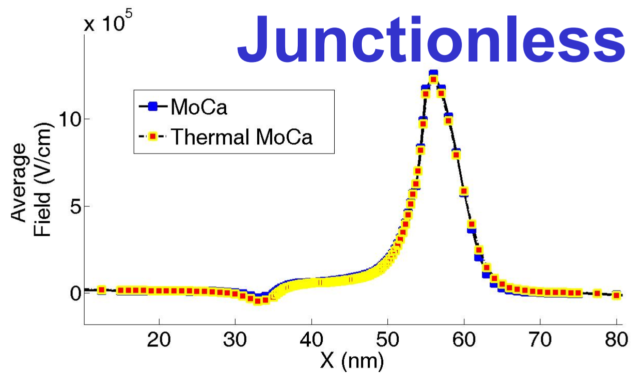


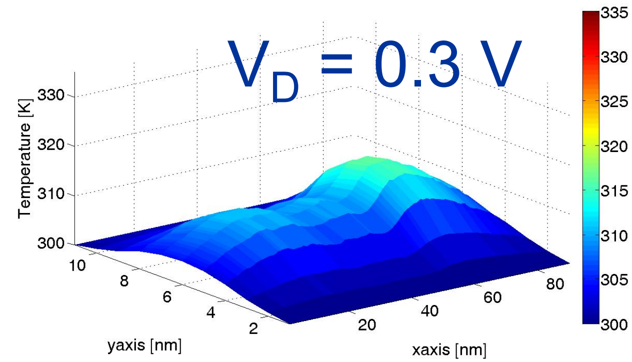
Colinge et al., Nature Nanotech. (5) 2010

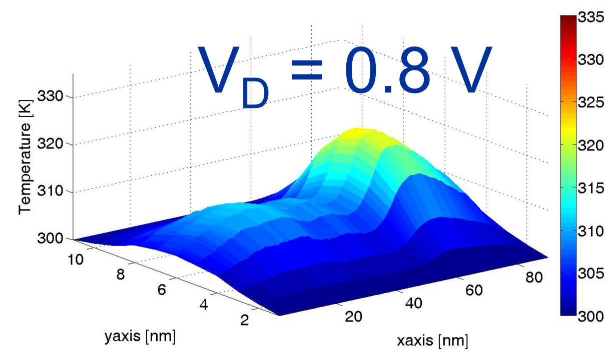
Junctionless vs. Gate-all-around

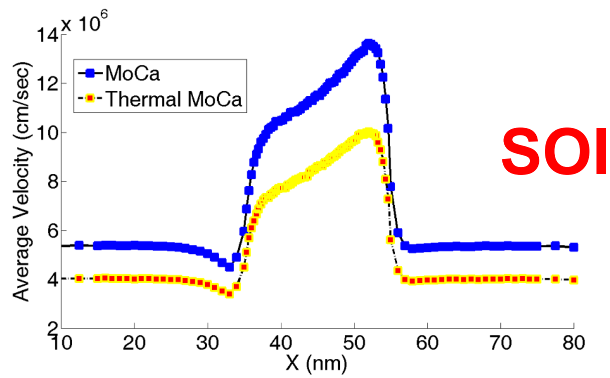
- Much less pronounced self-heating
- Lower peak lattice temperature in the drain
- **M. Mohamed et al. IEEE Nanotechnology Magazine, vol. 13, pg. 6 (2019)**

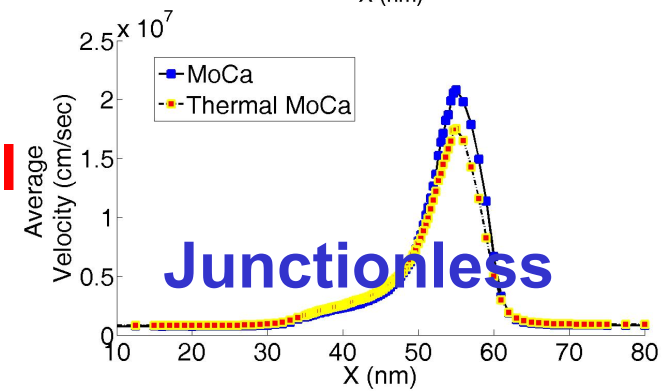


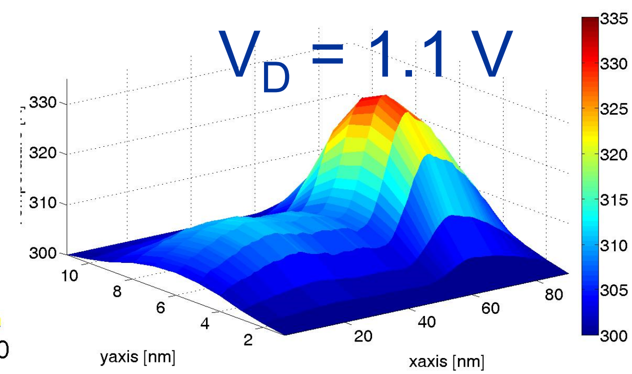






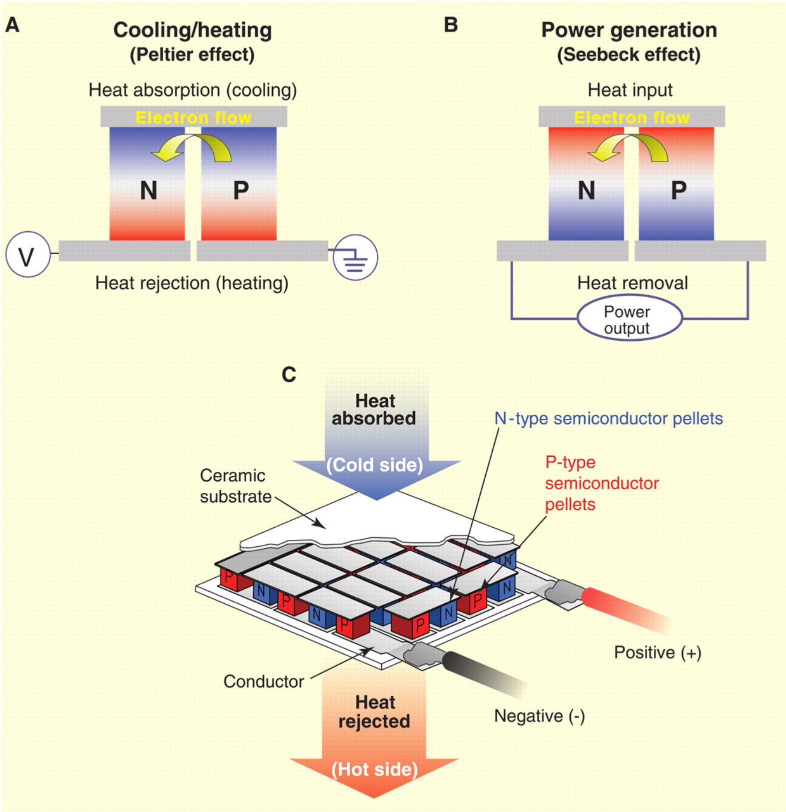




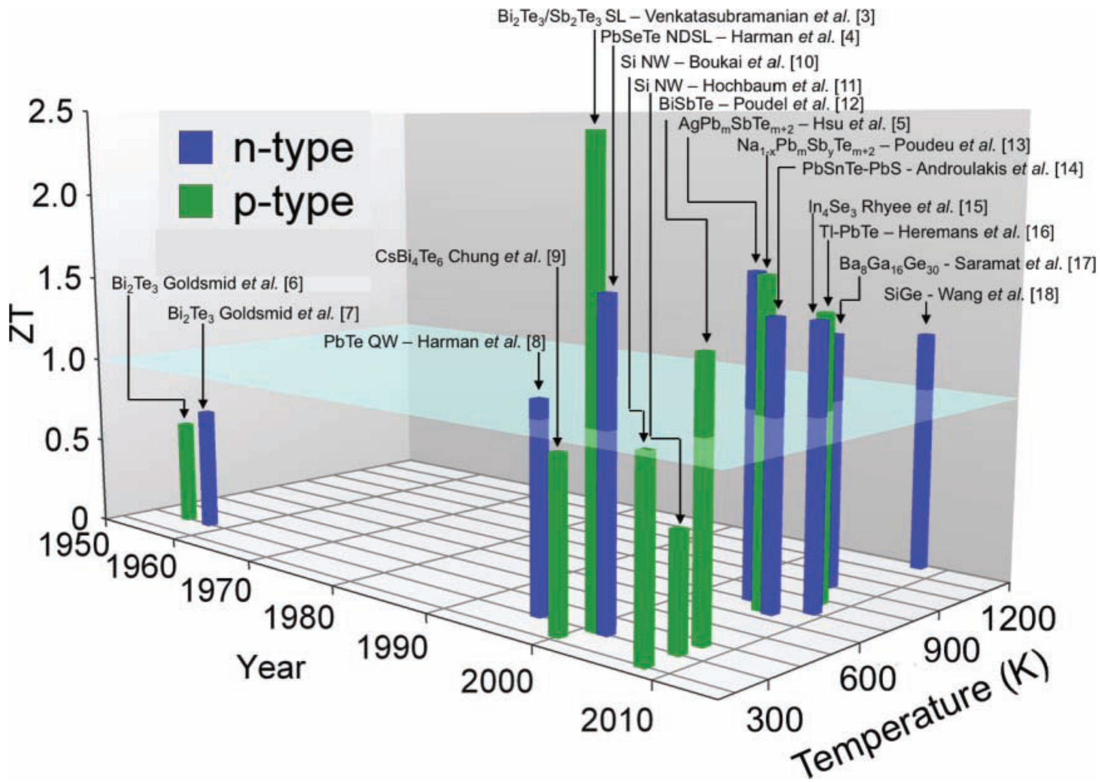


Thermoelectric Energy Conversion

- Semiconductor nanostructures are efficient thermo-electric converters: remove or recycle all that waste heat!



L. E. Bell, Science vol. 321, pp. 1457-1461 (2008)



C. J. Vineis et al., *Adv. Mat.* **22**, 3970-3980 (2010)

Thermoelectric Conversion Efficiency

- Measured by the ratio of energy provided to the load to the heat extracted

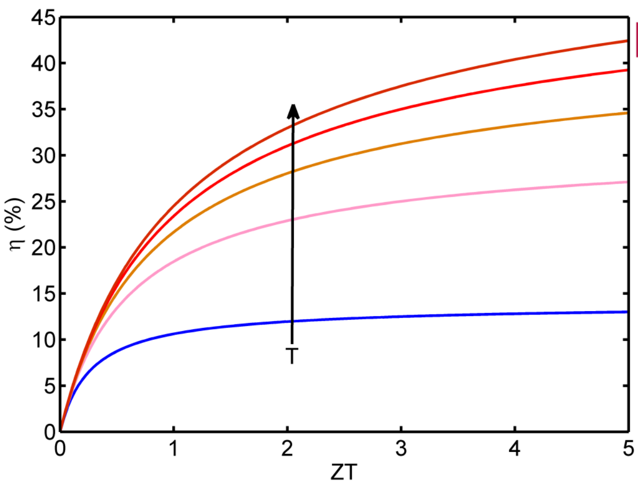
$$\eta = \frac{\text{Energy Produced}}{\text{Heat Absorbed}} = \left(1 - \frac{T_C}{T_H}\right)\frac{\sqrt{Z\overline{T}+1}-1}{\sqrt{Z\overline{T}+1}+{}^{T_C}\!/_{T_H}}$$

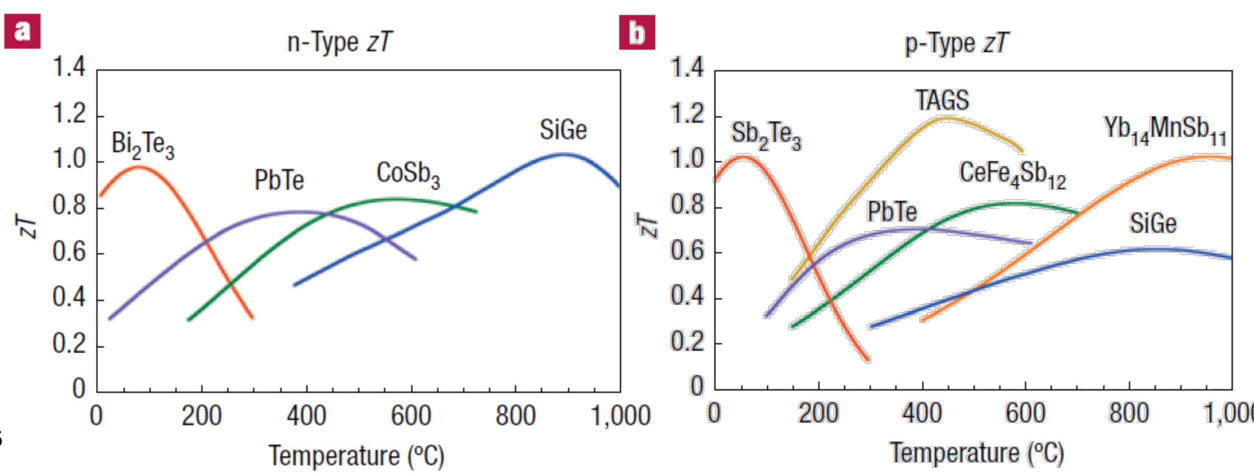
Power factor

$$ZT = \frac{S^2\sigma_{el}}{\kappa_{ph}+\kappa_{el}}T$$

Lattice (phonon)
Thermal conductivity

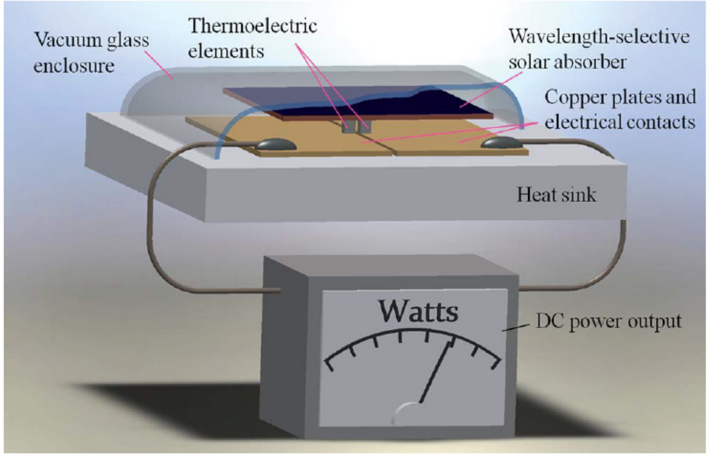
- Increasing ZT causes efficiency to approach the Carnot limit
- Reducing thermal conductivity has tremendous impact on ZT!

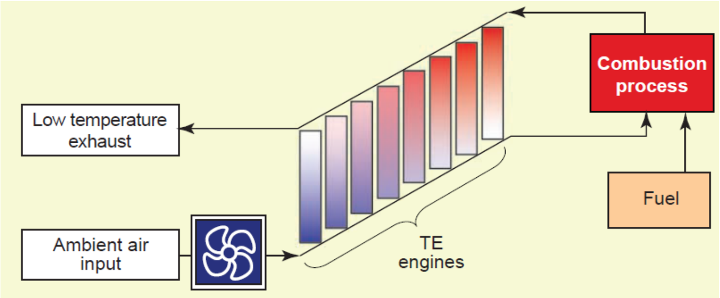


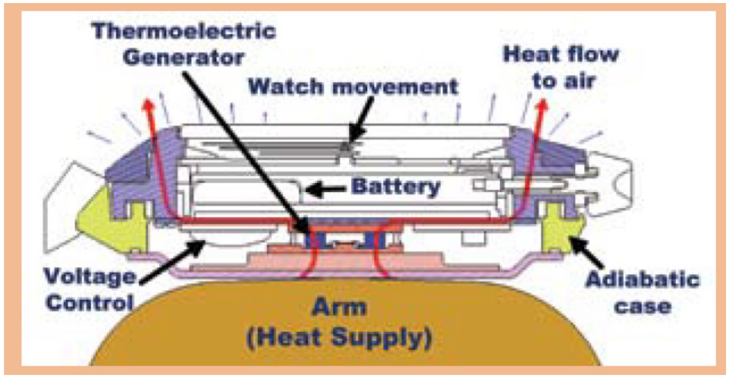


Thermoelectric Applications

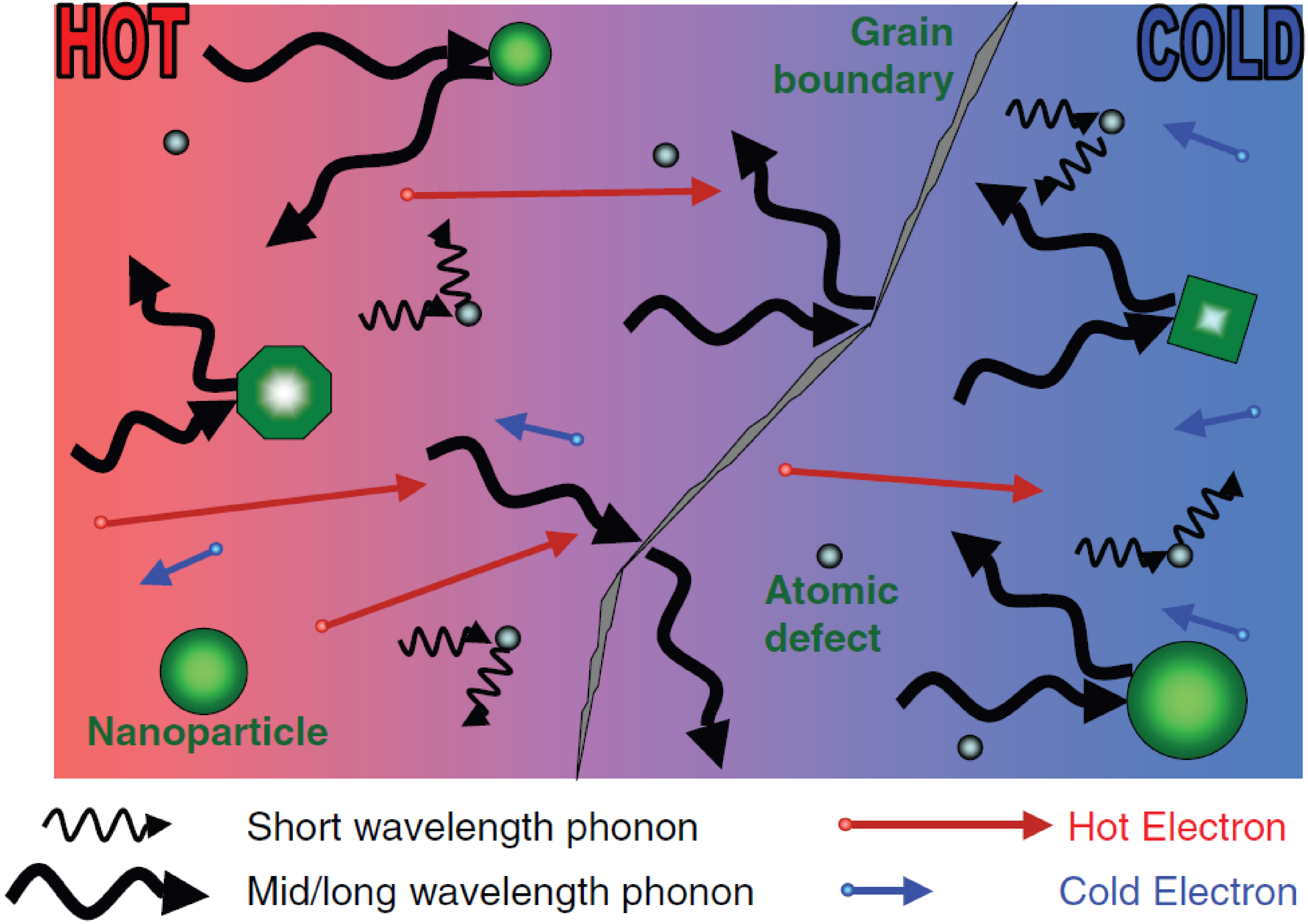
- Car Exhaust Systems
- Wearable Electronics
- Solar-Thermal Generators
- Nanoscale Power Sources





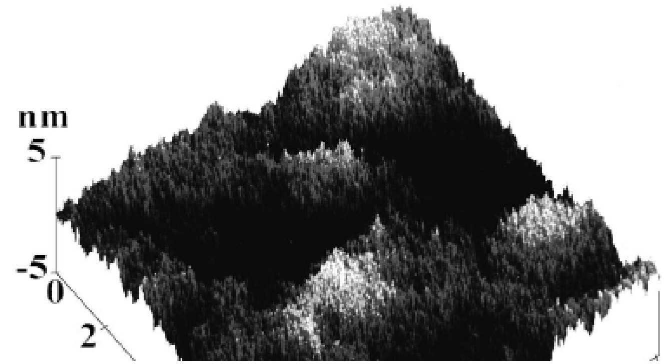


G. J. Snyder, ECS Interface, pp. 54, Fall 2008


HOT
COLD
Grain boundary
Atomic defect
Nanoparticle
Short wavelength phonon
Mid/long wavelength phonon
Hot Electron
Cold Electron

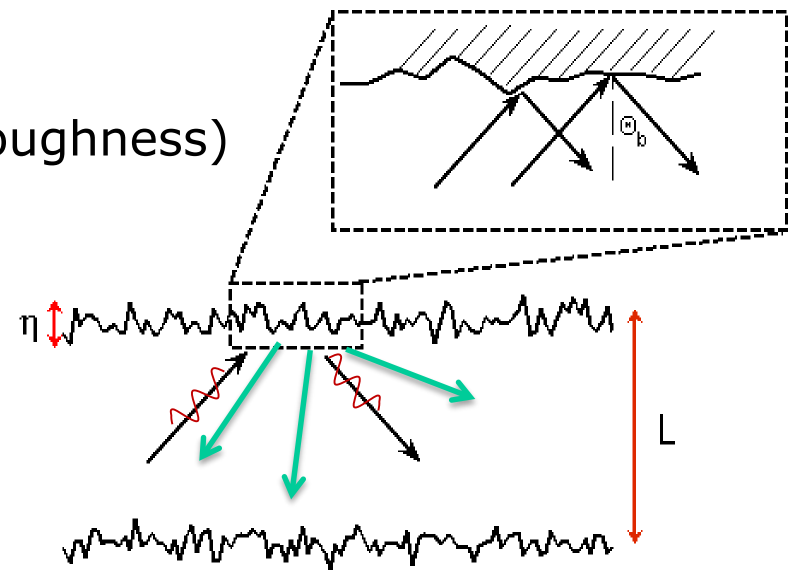
Bouondary/Interface Scattering of Phonons

- Nanostructures have lots of interfaces!
- At a rough interface, phonons can be either reflected or scattered



- If the phonon is large (or surface smooth)
  - The surface variations look small
  - Reflection➔No change in momentum
- Typical phonon is small (wavelength<roughness)
  - The surface variation looks big!
  - Scattered randomly➔Resistance!
- Momentum-dependent specularity:

$$p(\vec{q}) = \exp(-4q^2\Delta^2\cos^2\Theta_B)$$



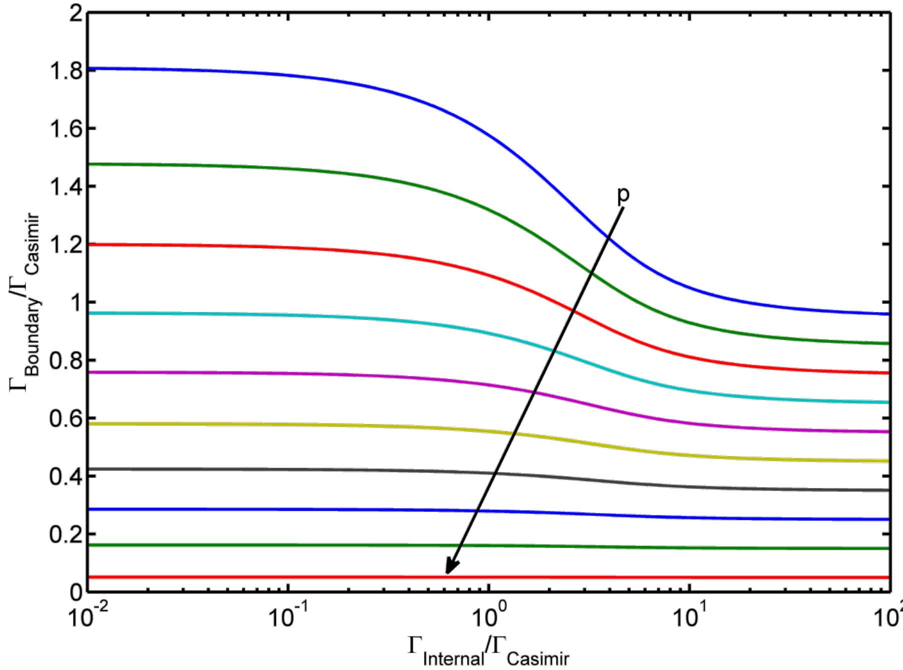
Boundary Scattering Rate

- Final boundary scattering rate:

$$\frac{1}{\tau_B(\vec{q})} = \frac{v_\perp(\vec{q})}{L} \frac{F_p(\vec{q}, L)}{1 - \frac{\tau_{int.}(\vec{q}) v_\perp(\vec{q})}{L} F_p(\vec{q}, L)}$$

- Where F(q,L) is given by:

$$F_p(\vec{q}, L) = \frac{1 - p(\vec{q}) \left[1 - \exp\left(-L/\tau_{int.}(\vec{q}) v_\perp(\vec{q})\right)\right]}{1 - p(\vec{q}) \exp\left(-L/\tau_{int.}(\vec{q}) v_\perp(\vec{q})\right)}$$

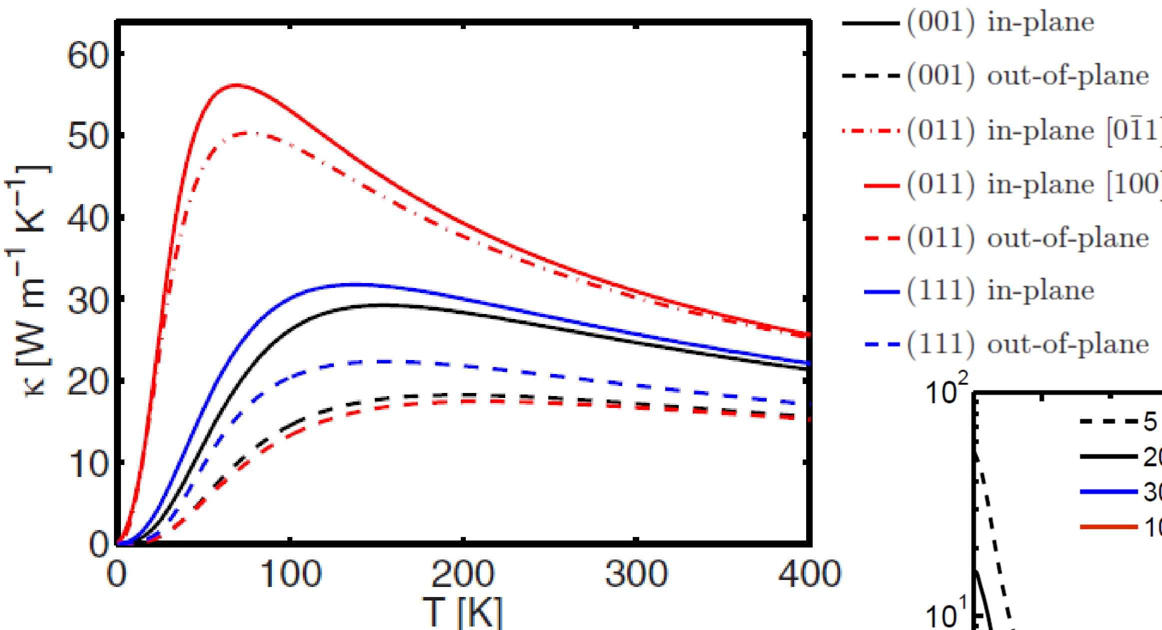


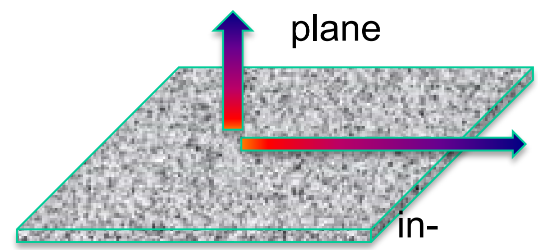
- Two limits to the solution:
  - Weak internal scattering: (1-p)/(1+p)*2*v/L
  - Strong internal scattering: (1-p)*v/L

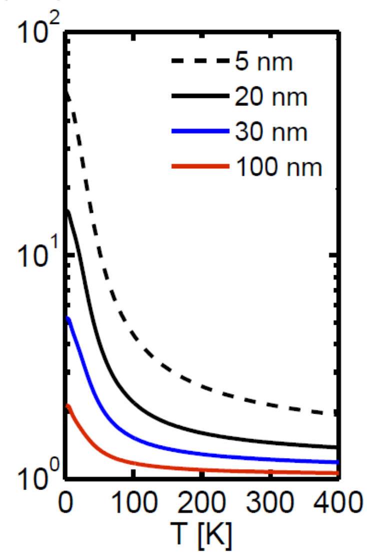
- Weaker boundary scattering rate in the case of strong internal scattering due to competition from internal scattering mechanisms

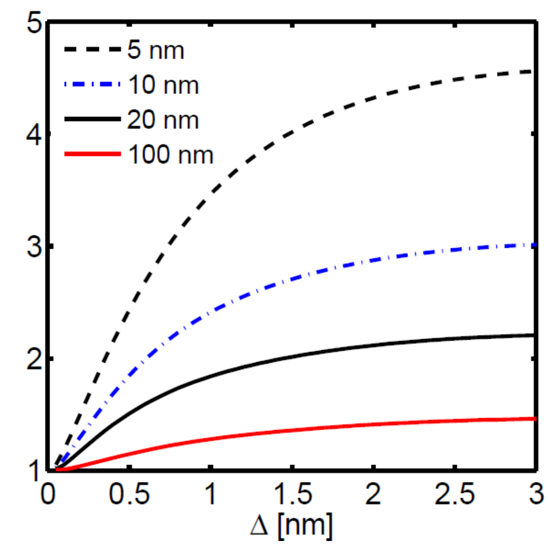
Ultrathin SOI thermal conductivity anisotropy

- Lowest thermal conductivity on a (001), highest on (011) surface







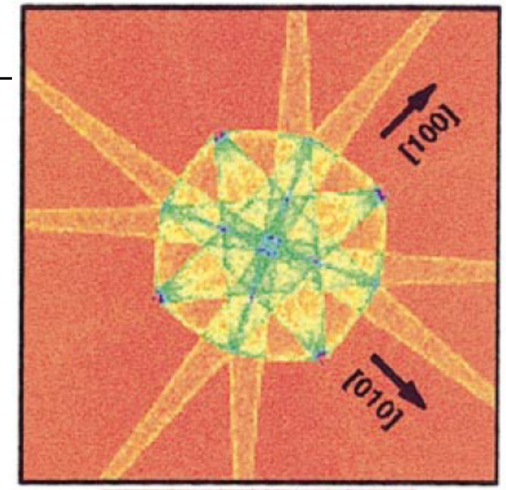


Ratio of highest/lowest in-plane conductivity a factor of >2 at room temp., increases with roughness

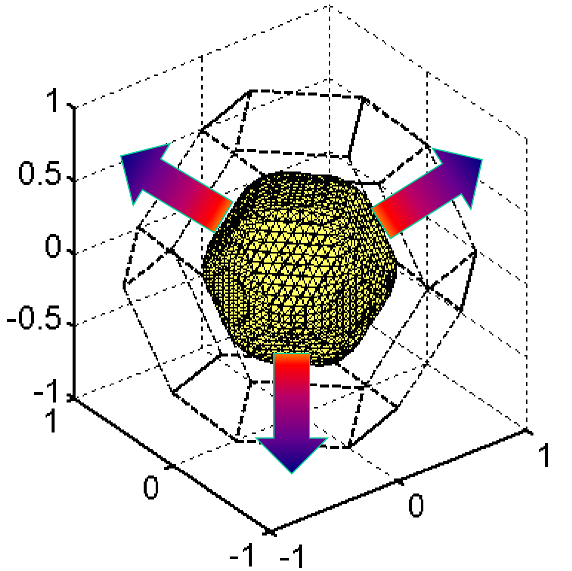
Z. Aksamija and I. Knezevic, Phys. Rev. B **82**, 045319 (2010)

Phonons, Dispersion, and Focusing

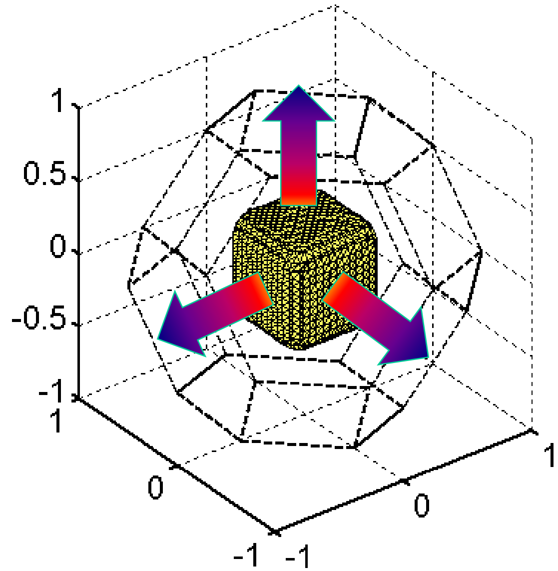
- Phonon isosurfaces show strong anisotropy and phonon focusing [Cahill et al., JAP 93, 793 (2003)]
- LA branch (left) has very flat faces with phonons propagating mainly in the [111] direction
- TA branch (middle) has flat isosurfaces with normal vectors (phonon velocities) in the [100] direction

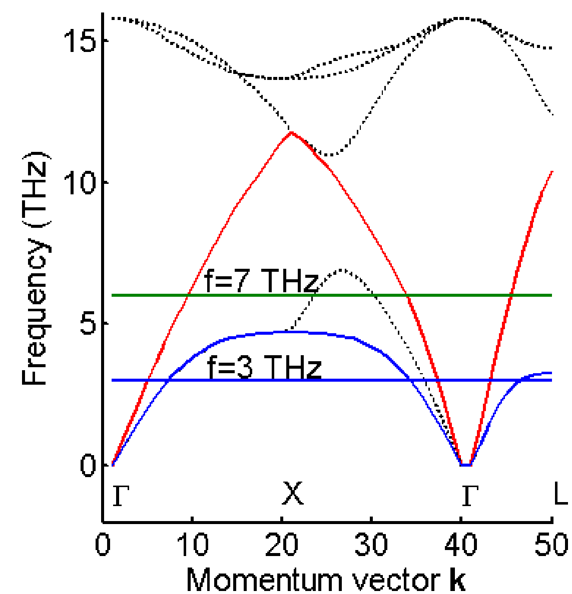


Longitudinal Acoustic (LA) branch



Transverse Acoustic (TA) branch





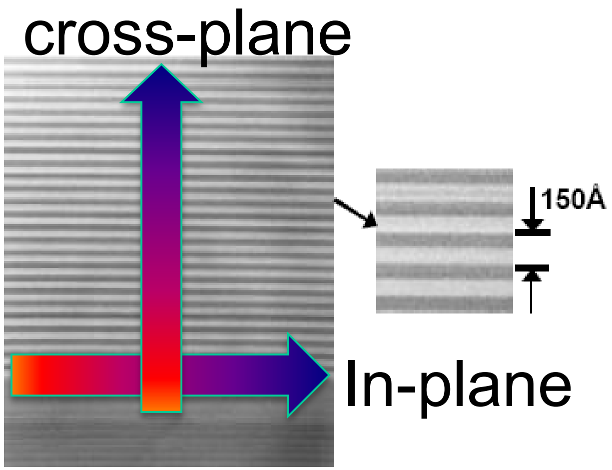
Z. Aksamija and I. Knezevic, Phys. Rev. B **82**, 045319 (2010)

Thermal Transport in SiGe Superlattices

- Superlattices are made up from many thin (few nm) layers of alternating semiconductor materials
- Layers separated by a rough interface with an rms roughness Δ
- Thermal conductivity of the two alternating layers is combined in series for cross-plane transport and in parallel for in-plane transport

$$\kappa_{\text{in-plane}} = \frac{L_1 \kappa_1^{xx} + L_2 \kappa_2^{xx}}{L_1 + L_2}$$

$$\kappa_{\text{cross-plane}} = \frac{L_1 + L_2}{\frac{L_1}{\kappa_1^{yy}} + \frac{L_2}{\kappa_2^{yy}} + \frac{1}{\sigma_1^{AIM}} + \frac{1}{\sigma_2^{AIM}}}$$



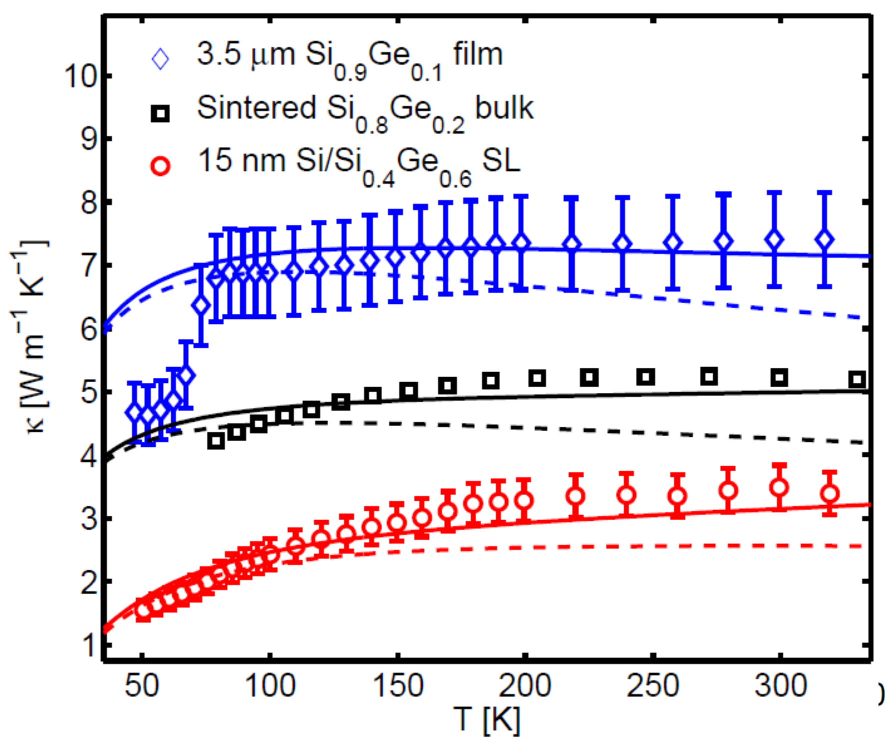
SEM image from S. T. Huxtable, Ph.D. Thesis

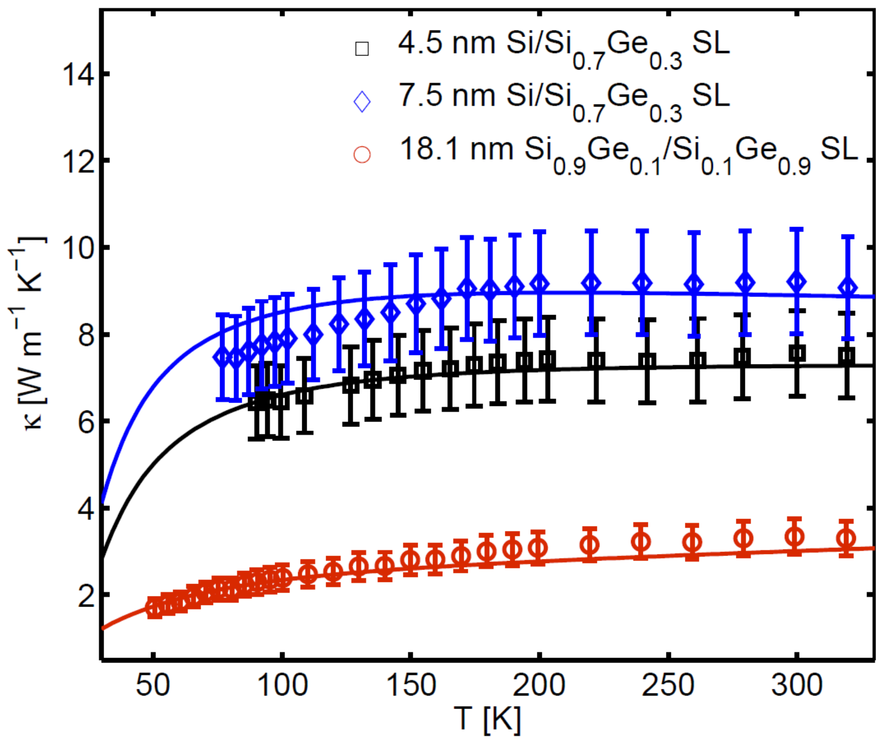
- Additional interface resistance due to acoustic mismatch between dissimilar materials

$$\sigma_i^{AIM}(T) = \frac{1}{2} \sum_{\mathrm{b}} \frac{\sum_{\vec{q}} C\left(\omega_{\mathrm{b,i}}(\vec{q}), T\right) v_{\mathrm{b,i}}^{\perp}(\vec{q}) t_{\mathrm{b}}^{AIM}(\vec{q})}{1 - \langle t_{\mathrm{b}}^{AIM}(\vec{q}) \rangle}$$

Anisotropic thermal conductivity in SiGe alloy SLs

- Strong in-plane/cross-plane anisotropy in 4 nm period Si/Ge SL
- Very low (1~5 W/m/K) cross-plane (through the SL) lattice thermal conductivity in Si/Ge SLs with a wide range of period thickensses (right)
- Thermal conductivity below alloy limit in SiGe alloy SLs!



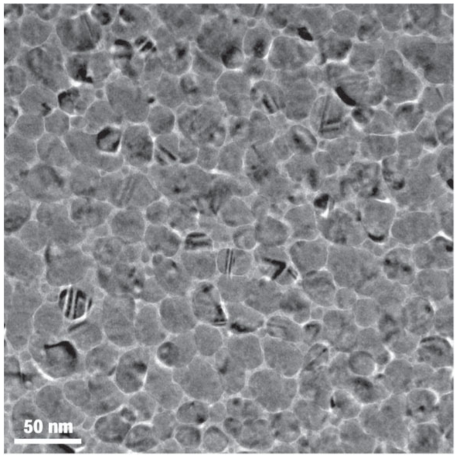


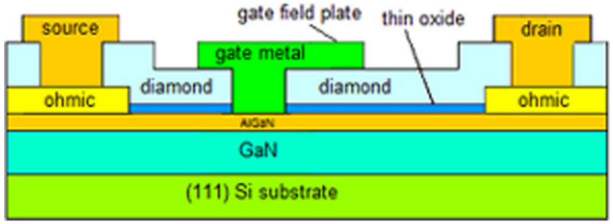
Data from: Huxtable et al. Appl. Phys. Lett. **80**, 1737 (2001)

Theory: Aksamija and Knezevic, Phys. Rev. B 88, 155318 (2013)

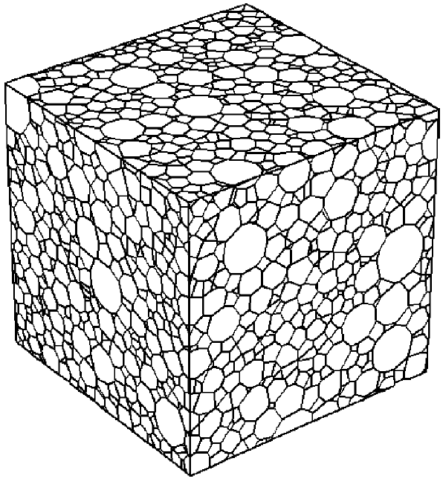
Thermal conductivity in nanocomposites

- Nanocomposites are cheaper to make than SLs
- More difficult problem due to random grain structure

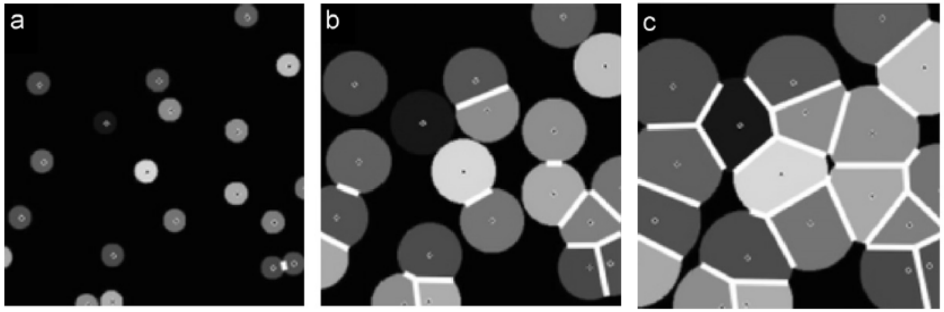


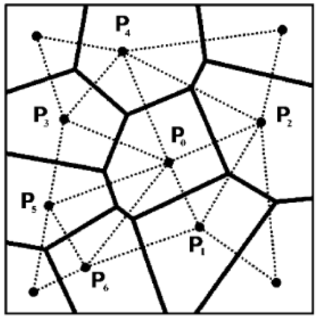


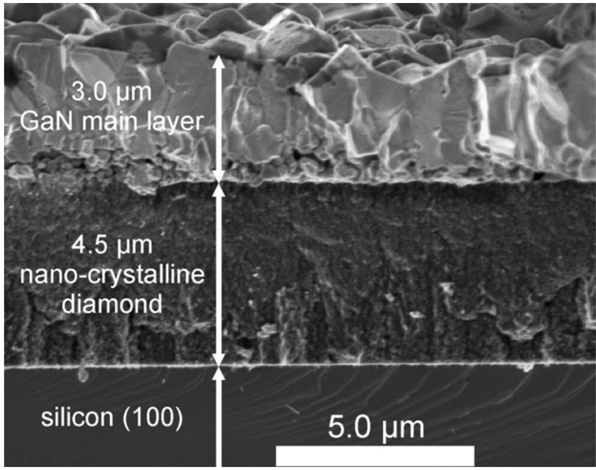
Tadjer et al., IEEE EDL 33, 23-25 (2012)



Nature Materials 3, 668 - 669 (2004)





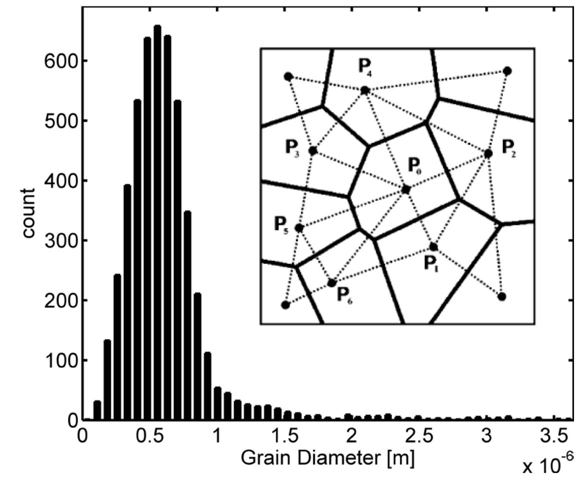


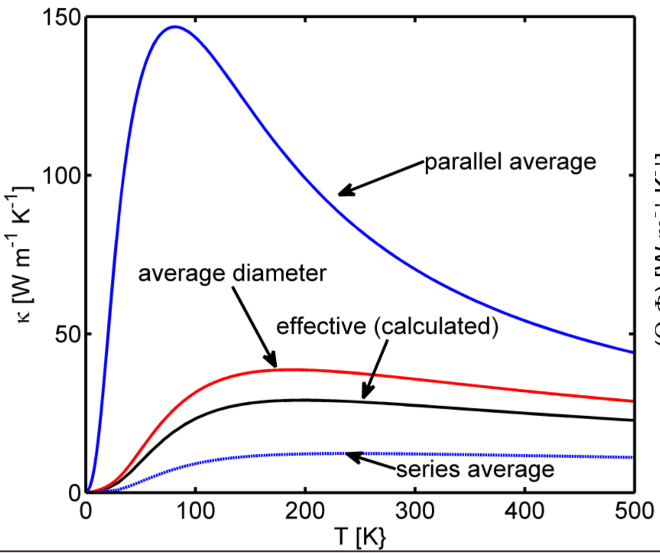
Simulation of thermal transport in nanocomposites

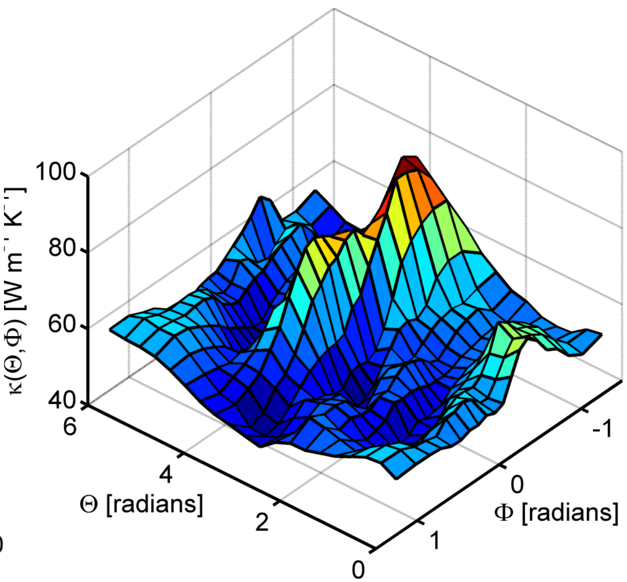
- Pick the grain size from the Voronoi diagram and compute diameter
- Compute the full thermal conductivity tensor of each grain:

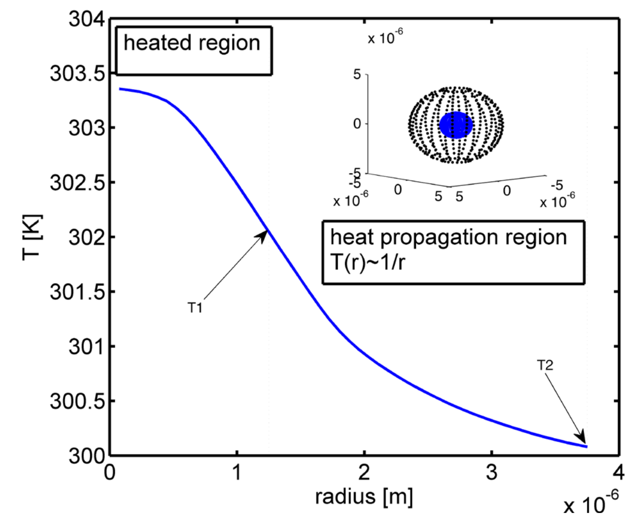
$$\mathbf{K}^{\alpha\beta}(T) = k \sum_{\mathrm{j}} \sum_{\vec{q}} \left[\frac{\hbar\omega_{\mathrm{j}}(\vec{q})}{kT} \right]^2 \frac{e^{\hbar\omega_{\mathrm{j}}(\vec{q})/kT}}{[e^{\hbar\omega_{\mathrm{j}}(\vec{q})/kT} - 1]^2} \; \tau_{\mathrm{j}}(q) v_{\mathrm{j}}^{\alpha}(\vec{q}) v_{\mathrm{j}}^{\beta}(\vec{q})$$

Z. Aksamija, J. Elec. Mater. Vol. 44, pp. 1644-1650 (2015)









Phonon Monte Carlo and the Boltzmann eqn.

- Solve the phonon Boltzmann transport equation:
  - Motion $$\frac{\partial n_\lambda(r,q)}{\partial t} + \nabla_q \omega_\lambda(q)\, \nabla_{\vec{r}} n_\lambda(r,q) = \left[\frac{dn}{dt}\right]_{scat.}$$
  - Scattering $$\left[\frac{dn}{dt}\right]_{scat.} = -\sum_{\vec{k}'}\left[P(q,q')n_\lambda(r,q) - P(q',q)n_\lambda(r,q')\right]$$
- 7-dimensional (3+3 phase space + time)➔use MC technique
- Top eqn. is the classical equation of motion
- Bottom is the collision integral from quantum-mechanical perturbation theory (Fermi's Golden Rule)
- Sample scattering probability at random from Poisson process: $$P_{\text{scat}} = 1 - \exp\left(\frac{-\Delta t}{\tau_{NU}}\right)$$

2- (elastic) and 3-phonon (anharmonic) collisions

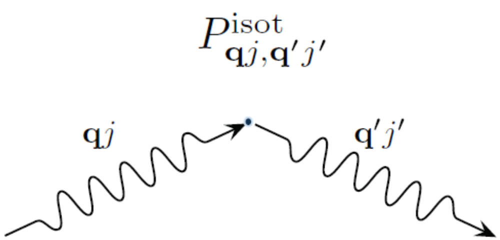
- Only energy is conserved in elastic scattering processes

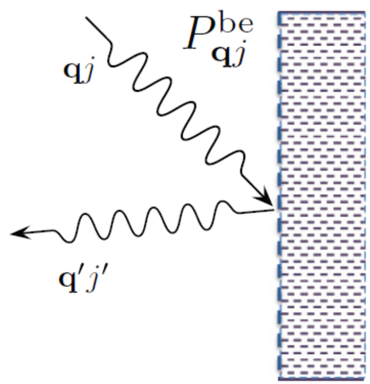
Mass-difference (isotope, impurity, alloy) randomizes momentum

Rough boundaries of the nanostructures also scatter phonons

Correlated Surfaces only partially randomize momentum/direction

Energy conservation: $\omega_\lambda = \omega_\lambda{}'$

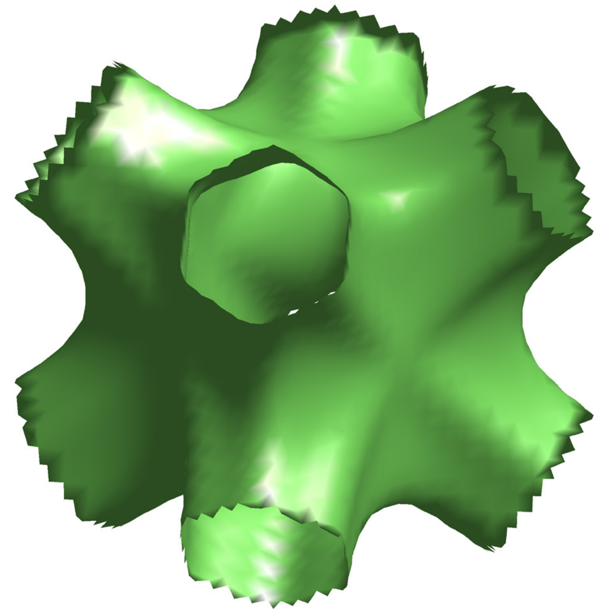




Elastic (2-phonon)

Fugallo et al., Phys. Rev. B 88, 045430 (2013)

Final State After Elastic Scattering



- Rejection algorithm for final state selection:

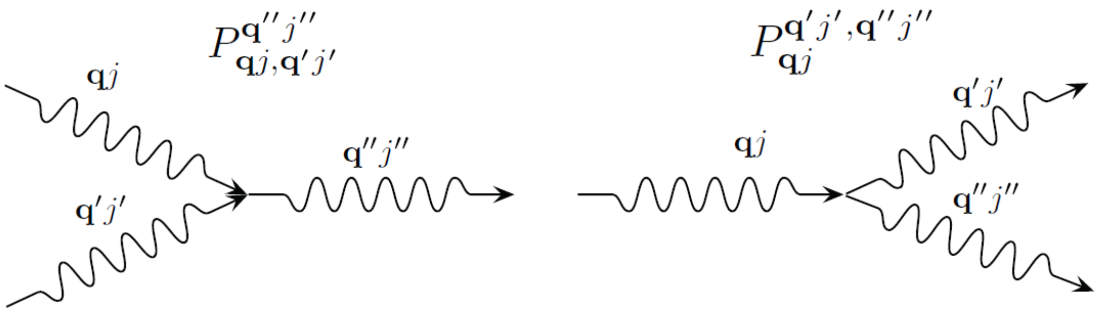
  1. Select a candidate final state
     - Uniformly sample the constant energy surface
     - Discretize the 1st BZ into small cubes

     - Compute the size of the intersection of the constant energy surface with the cube
     - Use rejection method to select a cube, pick a final state uniformly on the constant energy surface in that cube

  2. Compute the change in (crystal)momentum between initial and final state $\Delta q = q_{init} - q_{final}$; reduce to 1st BZ if necessary!
  3. Compute the autocorrelation function $S(\Delta q)$ and compare to a rand
  4. If $S(\Delta q) < r_{rand}$ then keep the final state candidate q_{final}

2- (elastic) and 3-phonon (anharmonic) collisions

Both energy and momentum are conserved in inelastic scattering process



Inelastic (3-phonon)

$$P(q,q') = \frac{2\pi}{\hbar}\left|V^{(3)}\right|^2 n_\lambda \left(n'_\lambda + \frac{1}{2} \mp \frac{1}{2}\right)\left(n_\lambda'' + 1\right)\delta_{q\pm q',q''+G}\,\delta\left(\omega_\lambda \pm \omega_\lambda' - \omega_\lambda''\right)$$

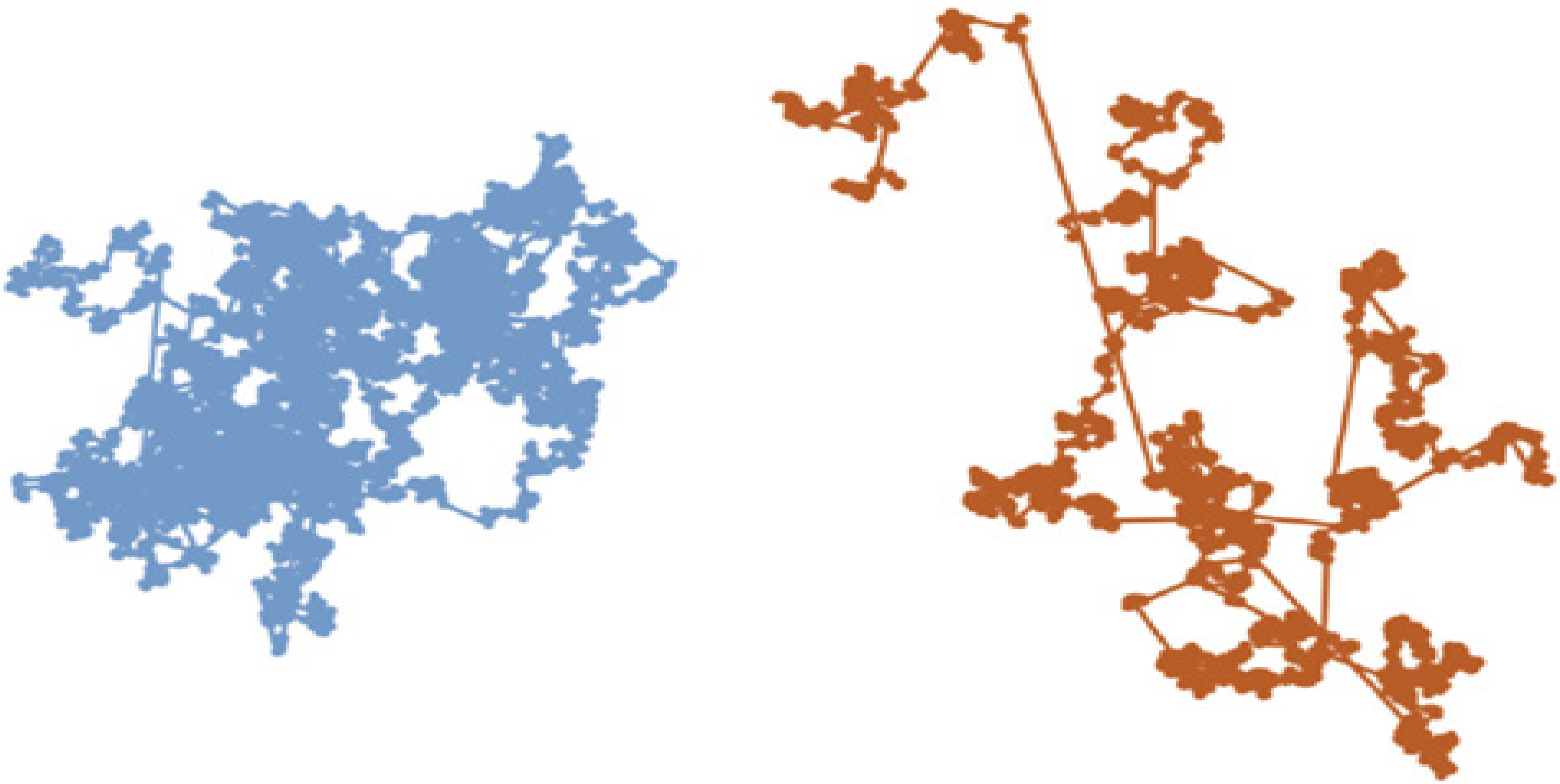
Energy conservation: $\omega_\lambda \pm \omega_\lambda' = \omega_\lambda''$

Normal process: $q \pm q' = q''$

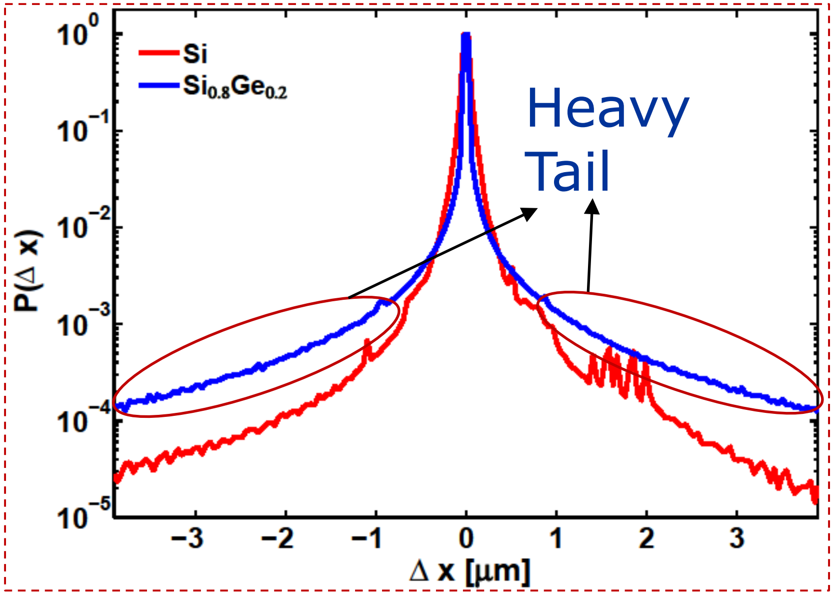
Non-randomizing
Infinite conductivity
Hydrodynamics

Umklapp process: $q \pm q' = q'' + G$

Superdiffusive phonons in Si-Ge alloys

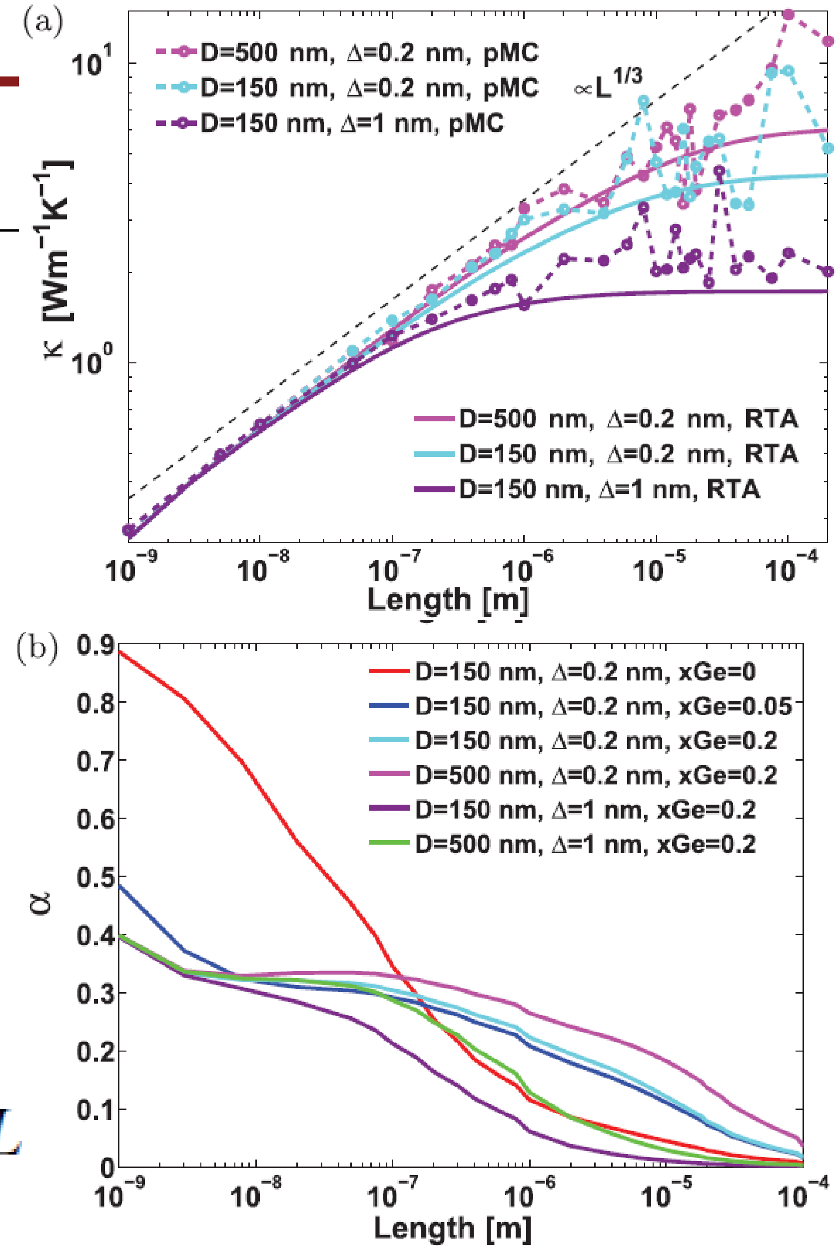


Length scaling in Si-Ge NWs



Histogram of the flight lengths in Si (red) and SiGe NWs (blue). The broad spectrum of MFPs in SiGe NWs leads to a heavy-tailed distribution.

$$\alpha(L) = d \ln \kappa(L) / d \ln L$$



(Super) Diffusion Coefficient

- The mean square energy displacement (MSD),

$$\sigma^2(t) = \langle \Delta x^2(t) \rangle \propto t^{\beta}$$

- Diffusion coefficient,

$$\frac{\sigma^2(t)}{2t} \propto t^{\alpha}, \qquad 0 < \alpha < 1$$

- $\alpha = \beta - 1$
- Normal diffusion:

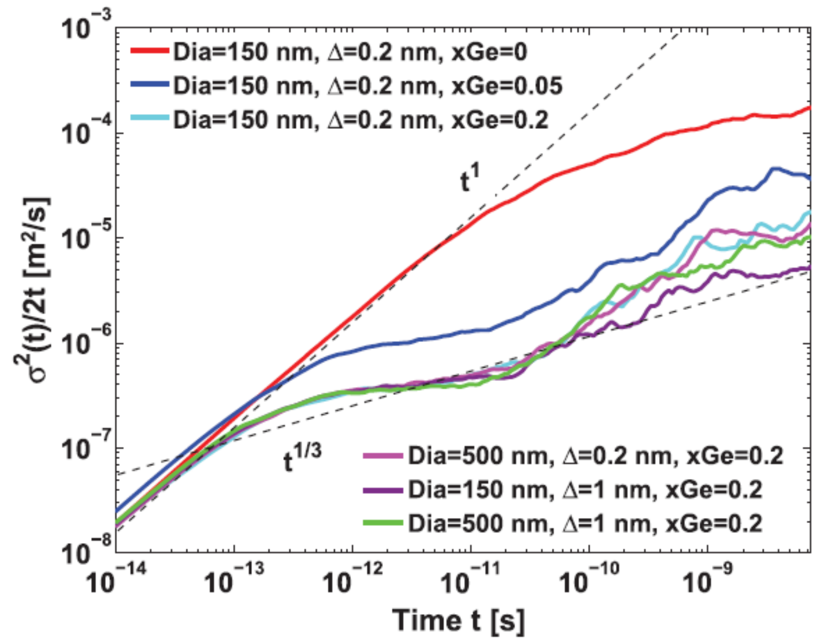
$$\beta = 1, \qquad \sigma^2(t) \propto t \text{ and } \alpha = 0$$

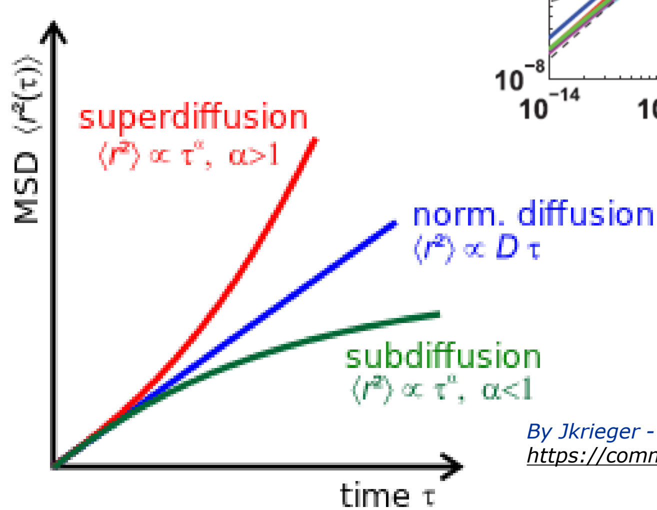
- Ballistic transport:

$$\beta = 2, \qquad \sigma^2(t) \propto t^2 \text{ and } \alpha = 1$$

- Super-diffusive transport:

$$1 < \beta < 2, \qquad \text{and } \ 0 < \alpha < 1$$

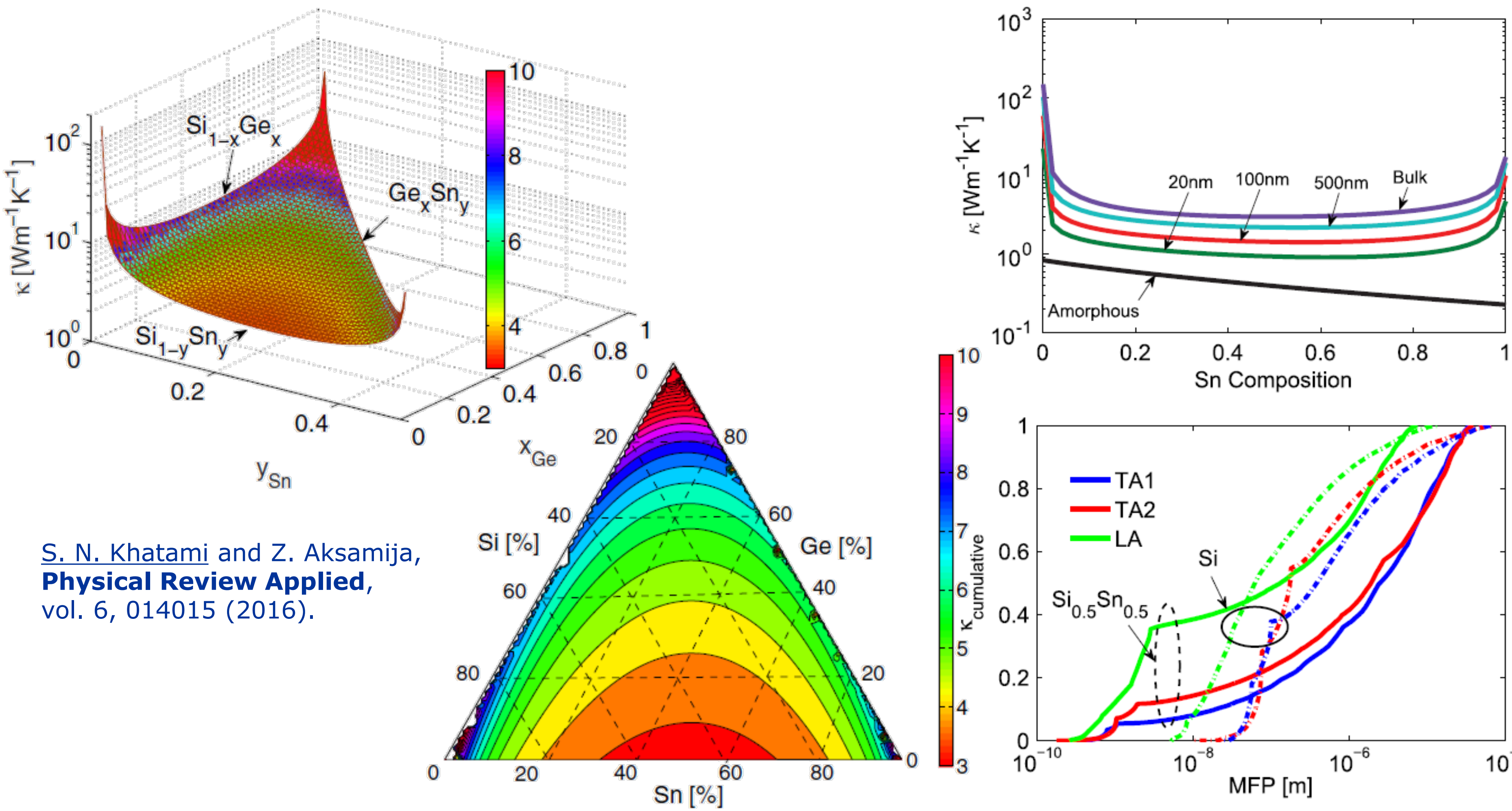




By Jkrieger - Own work, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=22631162

M. Upadhyaya, Z. Aksamija, "*Non-diffusive Lattice Thermal Transport in Si-Ge Alloy Nanowires*", **Physical Review B**, vol. 94, 174303 (2016).

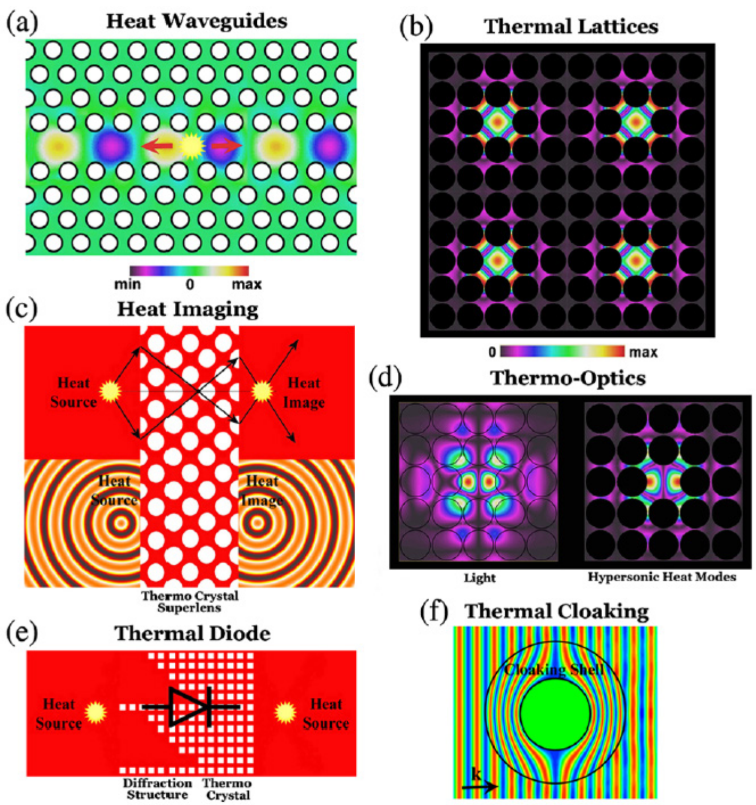
Ultralow thermal conductivity in Si-Sn



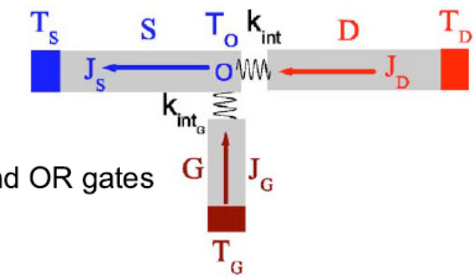
S. N. Khatami and Z. Aksamija, **Physical Review Applied**, vol. 6, 014015 (2016).

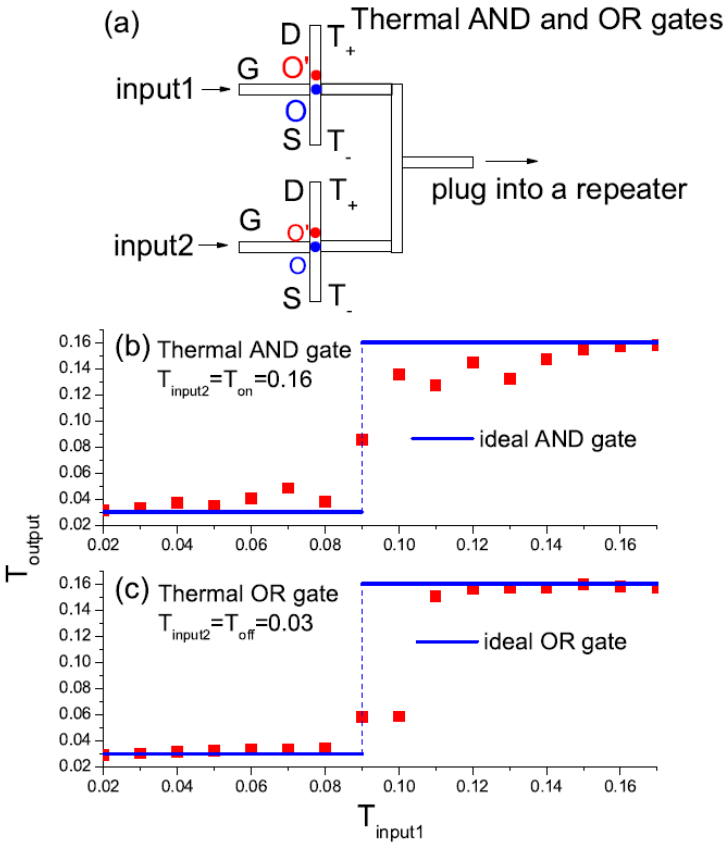
Directional Energy Transfer using Nanostructures

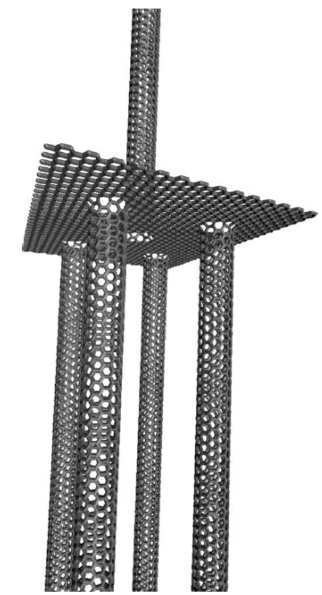
- Nanoscale control of heat propagation
- Thermal devices, logic, memory, thermal cloaking



M. Maldovan, PRL 110, 025902 (2013)







Thank you for your attention!

- This work has been supported by the National Science Foundation through:
  - NSF Award 1542864, **EFRI 2-DARE**
  - NSF Award 1449418, **CI TraCS**

- Questions?