QM: Phonons

Udayan Ganguly
Spring 2024
IIT Bombay

Phonons are collective atomic vibrations

C is spring constant;
u_s is sth atomic position
spring compression i.e. $x=u_s-u_{s-1}$

Force $$F_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s) \ .$$

Using Newton's laws

$$M\frac{d^2u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s)$$

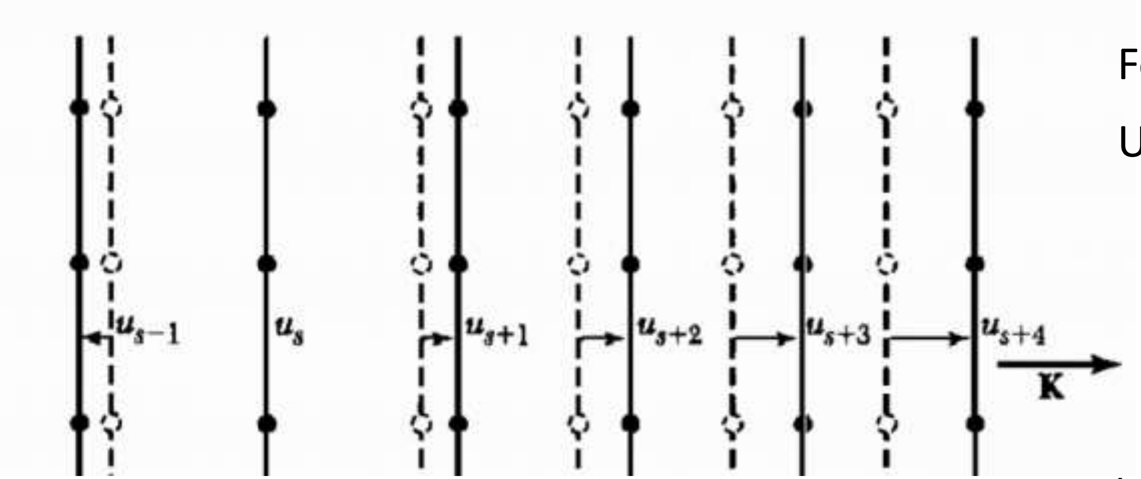


Figure 2 (Dashed lines) Planes of atoms when in equilibrium. (Solid lines) Planes of atoms when displaced as for a longitudinal wave. The coordinate u measures the displacement of the planes.

Assume a plane wave solution
$$\psi = e^{i(kx-\omega t)}$$
where as each site is a lattice point cf. electron where any x is allowed

$$-M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s) \ .$$

Assume $$u_{s\pm1} = u\exp(isKa)\exp(\pm iKa)$$

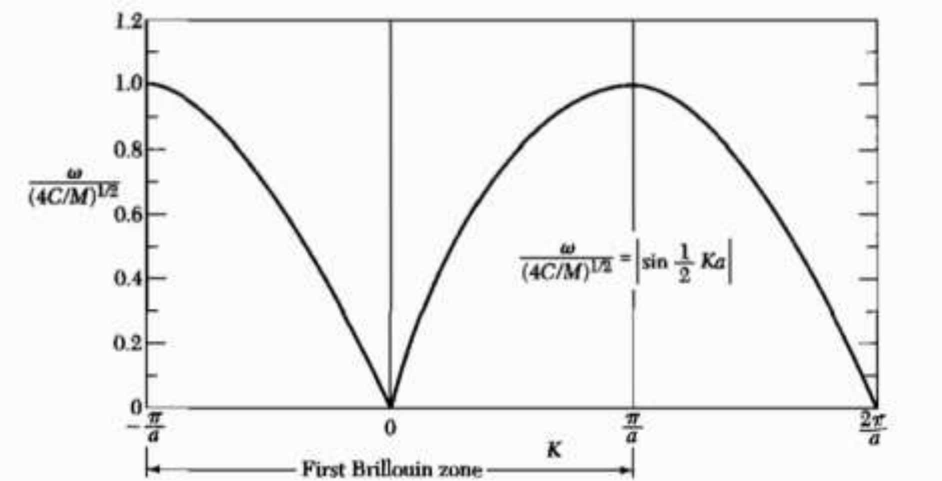
$$-\omega^2 Mu\exp(isKa) = Cu\{\exp[i(s+1)Ka] + \exp[i(s-1)Ka] - 2\exp(isKa)\}$$

We cancel $u\exp(isKa)$ from both sides, to leave

$$\omega^2 M = -C[\exp(iKa) + \exp(-iKa) - 2] \ .$$

$$\omega^2 = (2C/M)(1-\cos Ka)$$

$$\omega = (4C/M)^{1/2}\left|\sin\tfrac{1}{2}Ka\right|$$



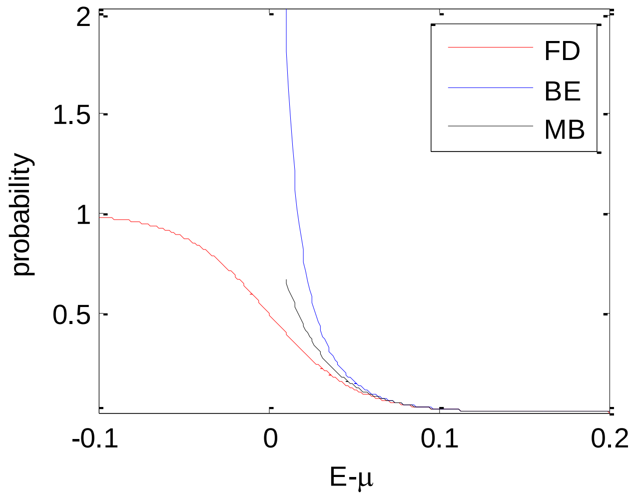
Phonon: A pseudo-particle

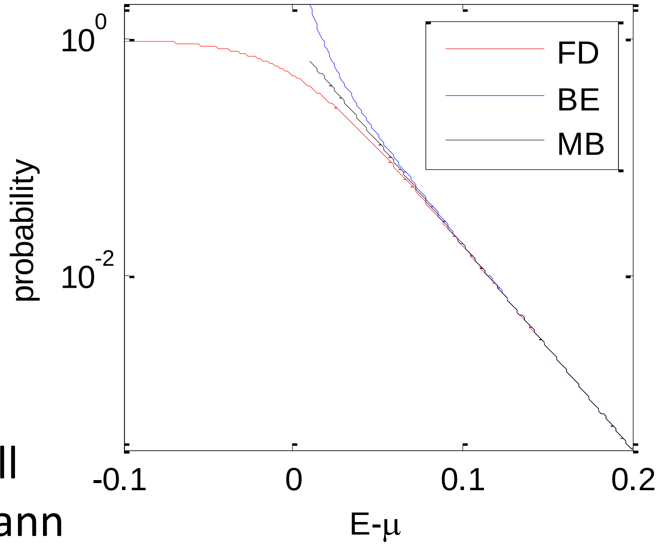
- The ω-k or E-k diagram is shown where $E=\hbar\omega$
- Each k crystal plane wave modes
- Like electrons; pseudo-particle can be generated as wave packets where
  - velocity = group velocity
  - Mass is $\hbar$/curvature
- Note: Electrons are charge waves in a crystal that are treated as particles; phonons are collective atomic oscillations in a crystal that can be treated as particles.

What is the group velocity and mass at k→ 0? As phonons are bosons, most particles are at k→0 or lowest energy

Bose-Einstein Statistics

- Phonons are bosons i.e. they obey Bose Einstein Distribution
- Unlike FD, bosons can occupy the same state (no Pauli's exclusion); Hence μ (chemical potential) is zero and most particle populate lowest energy
- At higher energies, both FD and BE tend to MB distribution





$$f(E) = \frac{1}{exp\left(\frac{E-E_F}{kT}\right) \pm 1} \quad exp\left(-\frac{E-E_F}{kT}\right)$$

Maxwell Boltzmann Distribution

+ Fermi Dirac Distribution
- Bose Einstein Distribution

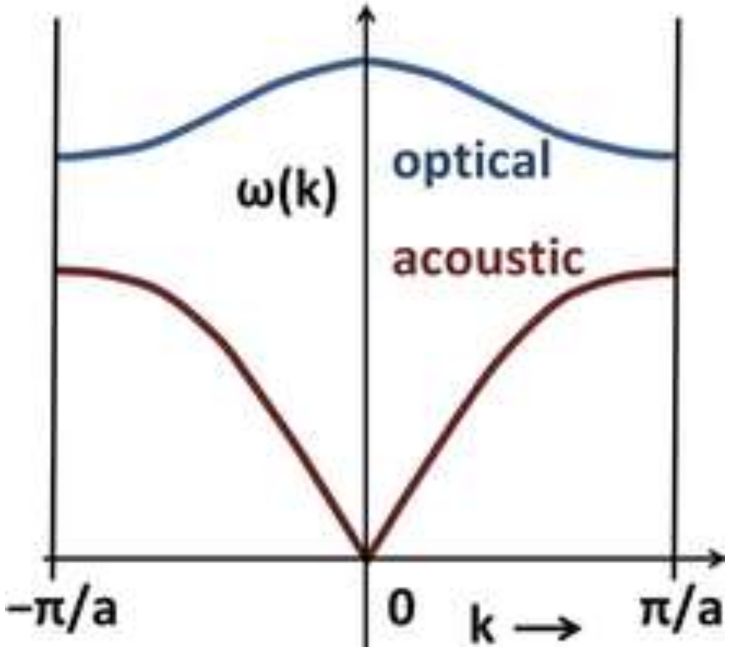
Try this demo
http://demonstrations.wolfram.com/BoseEinsteinFermiDiracAndMaxwellBoltzmannStatistics/

Two types of phonons

- Acoustic phonons: Like sounds waves where adjacent atoms are in phase ➔ generally low energy ➔ causes normal scattering

http://en.wikipedia.org/wiki/Phonon

- Optical phonon: When light moves through an ionic crystal, adjacent ions feel opposite force for same E field due to opposite charge ➔ they move out of phase; High energy ➔ causes velocity saturation



- Which States are primarily filled by phonons?
- Approx. above kT from zero energy

Analogy

- Mobility → terminal velocity like rain drops
- Velocity saturation → drag in a viscous medium (?)

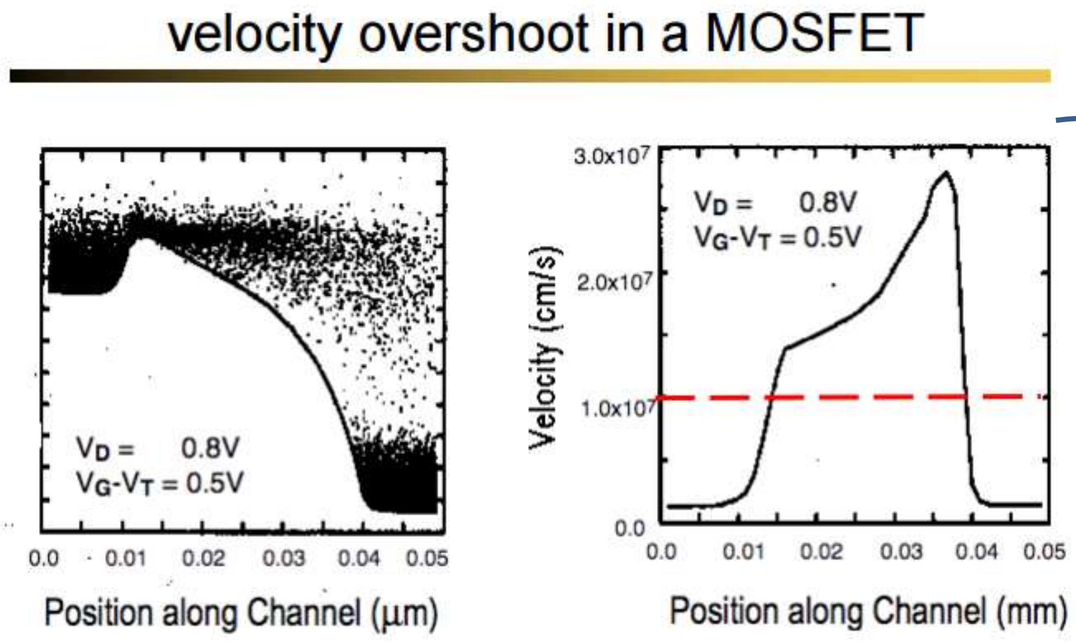
What have we achieved?

- We have an E(k) diagram
- A particle with a mass can be defined : Phonon
- It has high momentum (how is max k_{phonon} related to $k_{electron}$? Think BZ.
- It has low energy compared to electron. Why? How is momentum related to energy? Mass

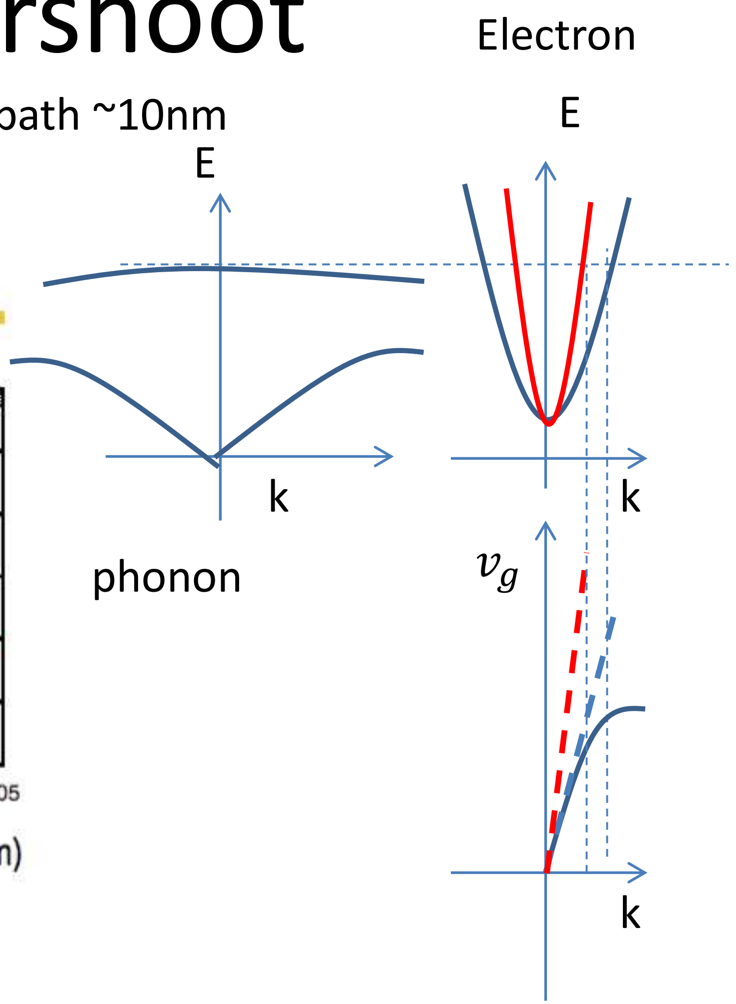
Now both electrons and phonons are particles whose interaction may be treated classically to enable energy and momentum exchange

Velocity overshoot

Optical phonon – mean free path ~10nm



Frank, Laux, and Fischetti, IEDM Tech. Dig., p. 553, 1992



Show electron transport in E-k diagram in time; Why does not matter? Why does v-overshoot occur?

Which crystal property should we engineer?

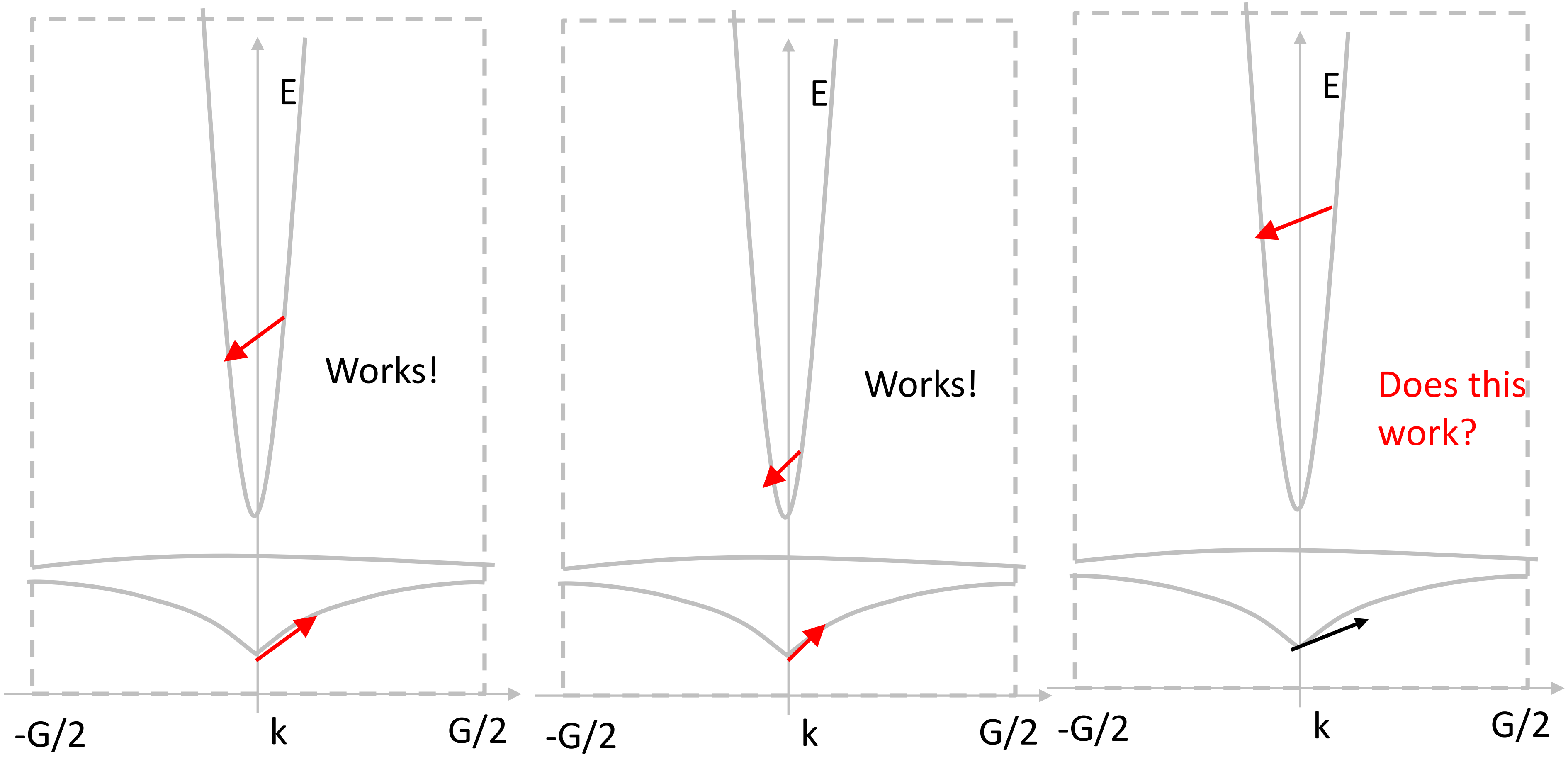
Scattering

Acoustic phonon: has specific relation

For a given (energy difference in electron) equal to ,it also must have correct which is not always possibly. However, can be low as ;
Acoustic phonons can scatter low energy electrons;

Energy balance:

Momentum balance:



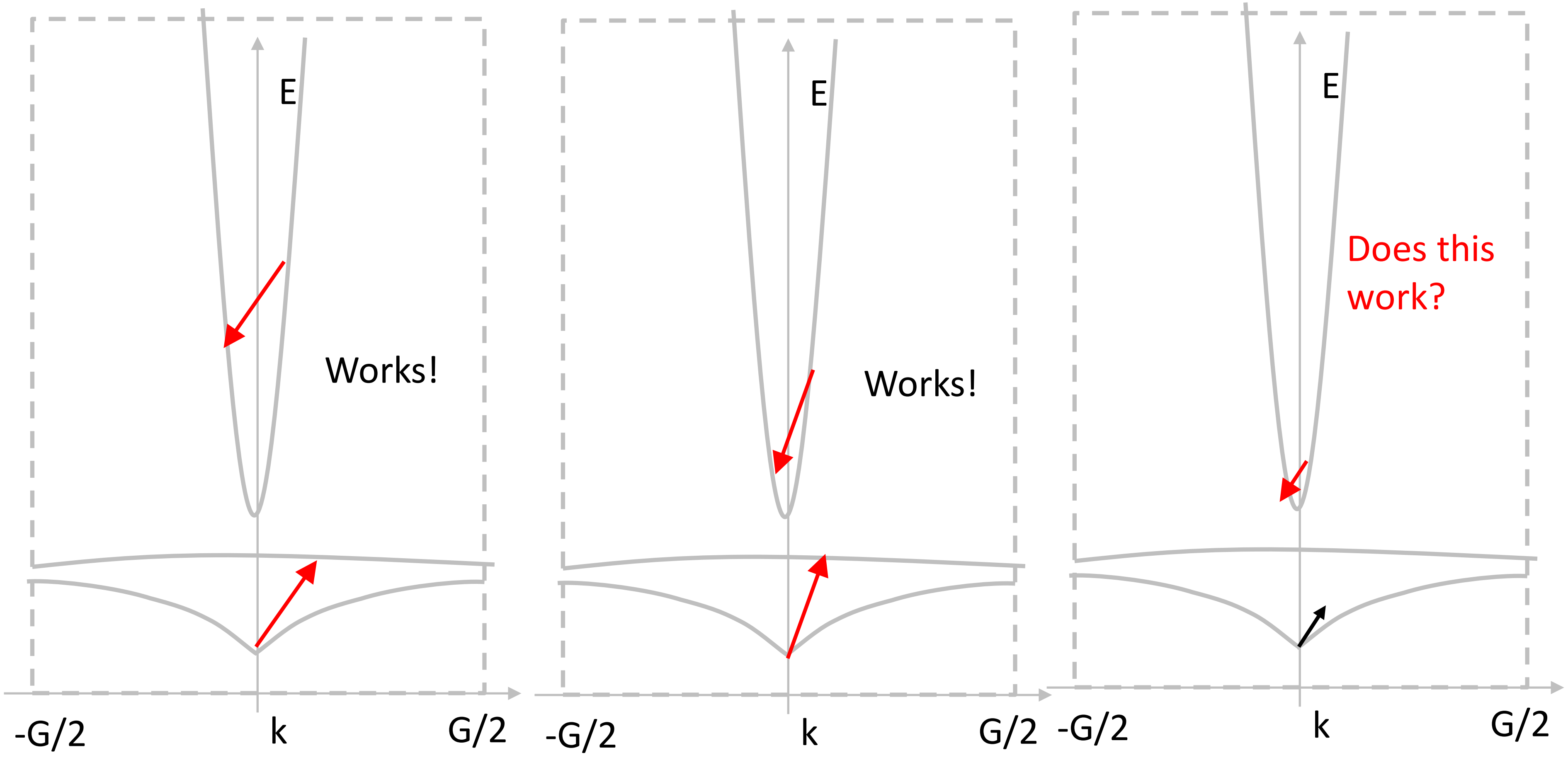
Scattering

Optical phonon:

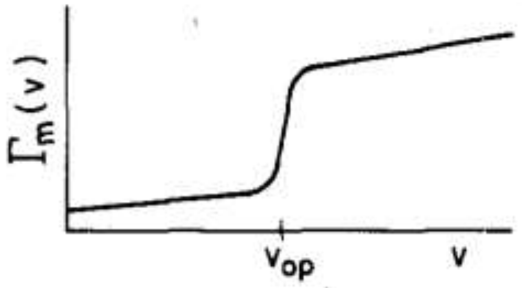
For a given energy difference in electron , we can always find a phonon with the correct ; But ; optical phonons can pnly scatter high energy electrons

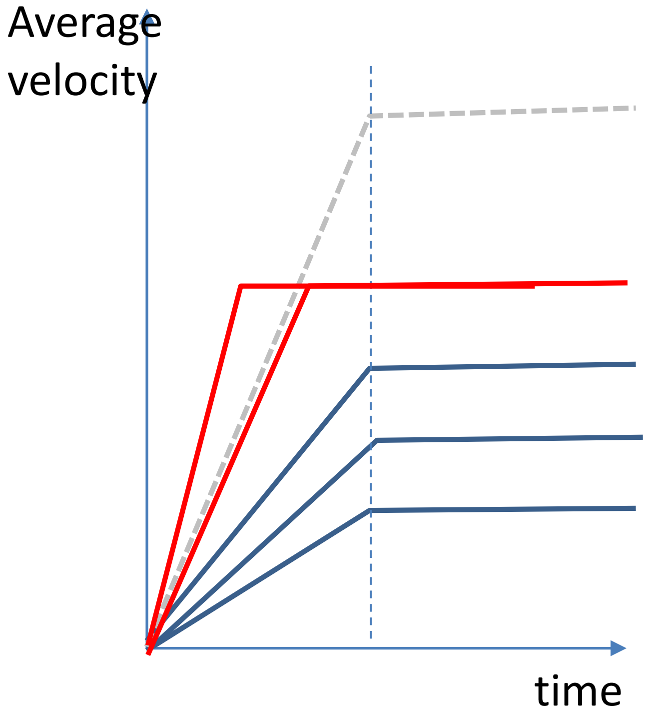
Energy balance:

Momentum balance:



Origin of vsat





<u>1. Scattering vs energy</u>

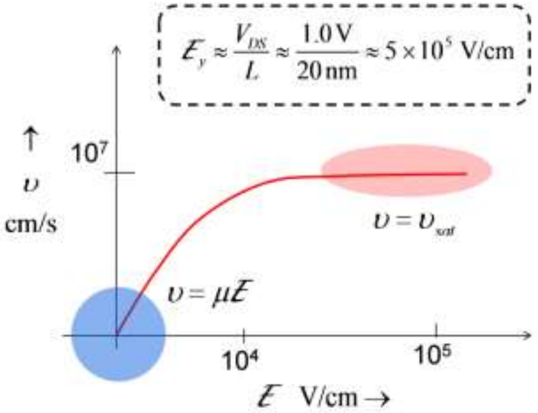
At high energy (scattering rate increases

Scattering time decreases beyond a critical related to optical phonon energy

<u>2. Effect of velocity evolution in time</u>

to enable i.e. velocity increases with E

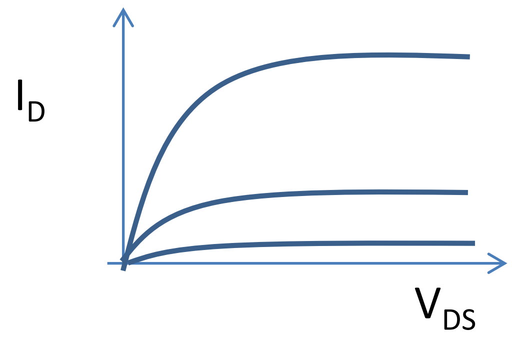
At higher energy to produce

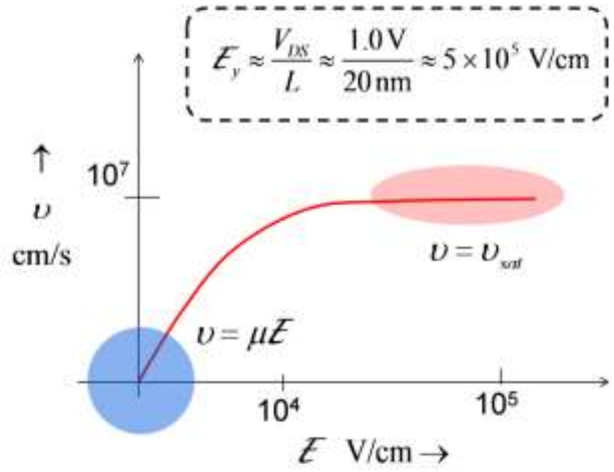


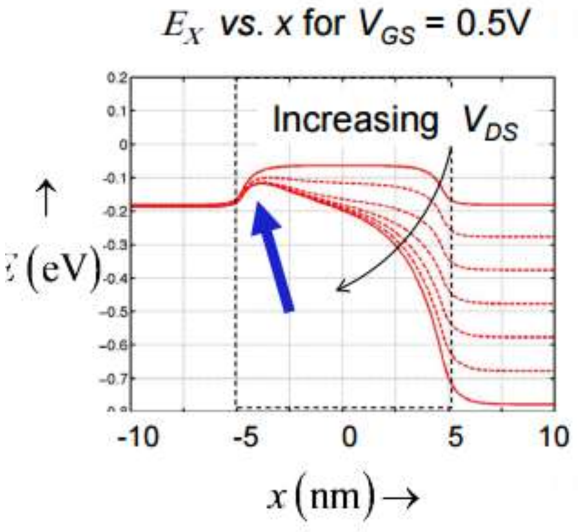
<u>3. Effect of velocity vs field dependence in steady state</u>

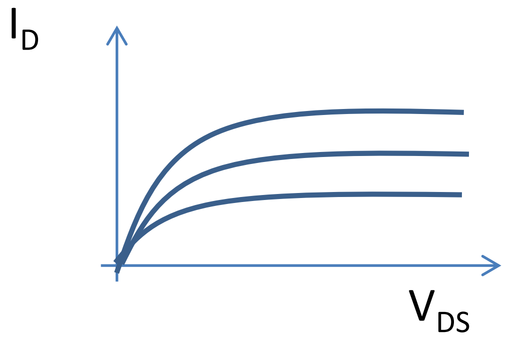
Finally, the following is produced including linear and saturated dependence of https://nanohub.org/resources/17759/download/2013.04.23-Lundstrom-MEXICO.pdf

Velocity Saturation and Overshoot in Nanoscale Devices









Voltage does not scale but is scaled.

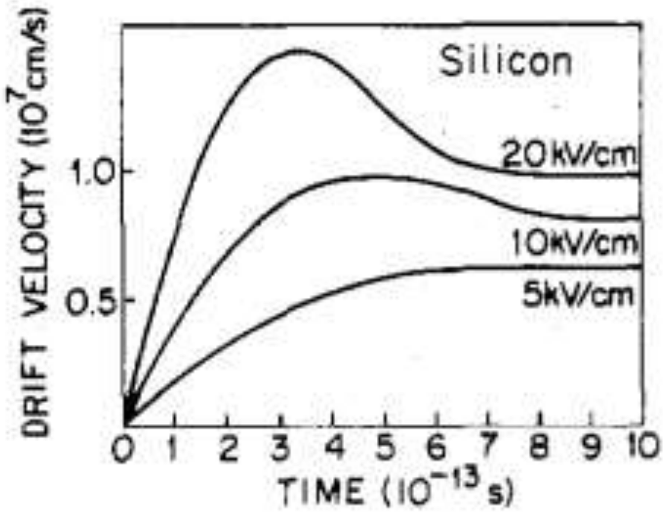
In scaled MOSFETs, which is more critical or mobility ()?

Velocity overshoot

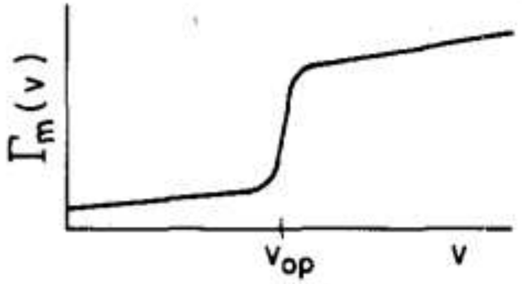
- When momemtum relaxation is faster than energy relaxation
- Initial velocity is higher than final velocity

$$v_i = \frac{qE}{m\Gamma_m(\epsilon_i)}. \qquad v_f = \frac{qE}{m\Gamma_m(\epsilon_f)}.$$

$$v_i > v_f$$

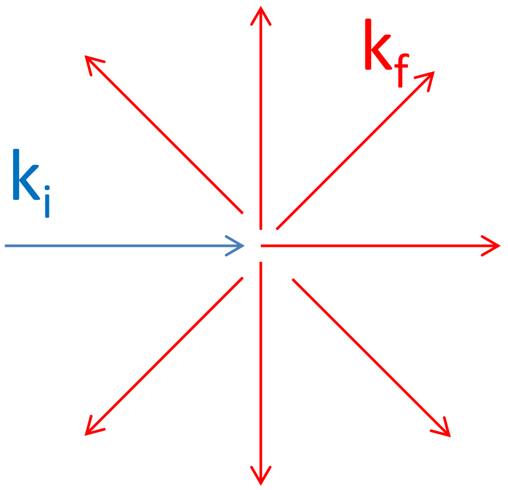


Velocity dependent momentum scattering



http://www.pas.rochester.edu/~stte/papers/IEEE_ED30_150.pdf

Reducing Scattering



$$k_i \xrightarrow{\text{Scattering}} k_f$$

In a 3D solid, scattering is all directions (solid angle) as long as energy is conserved.

Energy is conserved.

$$\text{Rate} = n_i\,(k_i) * n_f\,(k_f) * \,p(k_i, k_f) * \text{freq}$$

n_i : initial state density — Change ➔ 3D-> 2D-> 1D

n_f : final state density — Change ➔ 3D-> 2D-> 1D

$p(k_i, k_f)$: probability of scattering

freq : freq of scattering event

Density of states of electron and phonons drop

So how can we engineer each factor?

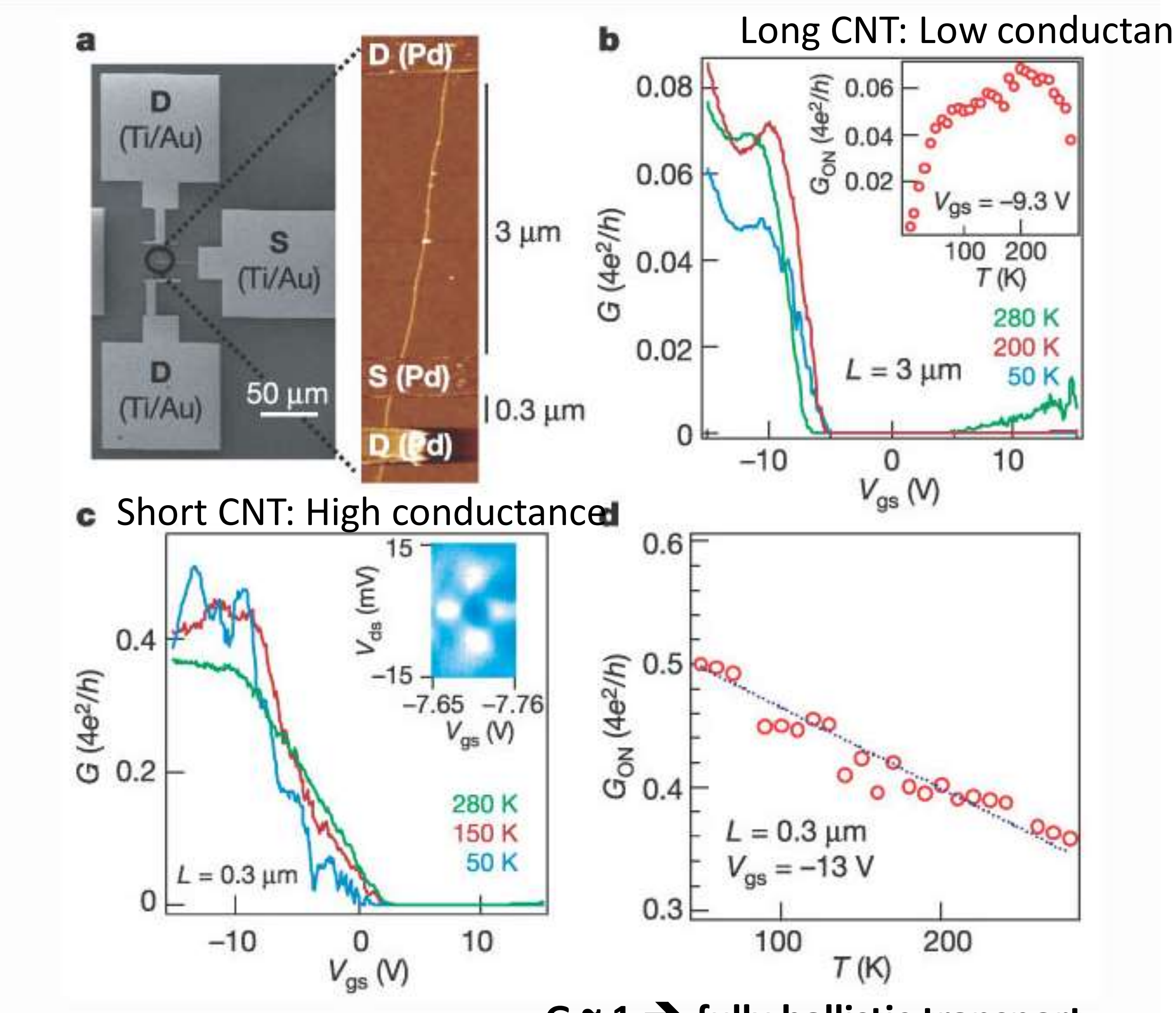
Scattering event could be an impurity Or phonon

Reduce temp; reduce impurity

How can we make scattering improbably without affecting current

Ballistic transport

Long CNT: Low conductance



Short CNT: High conductance

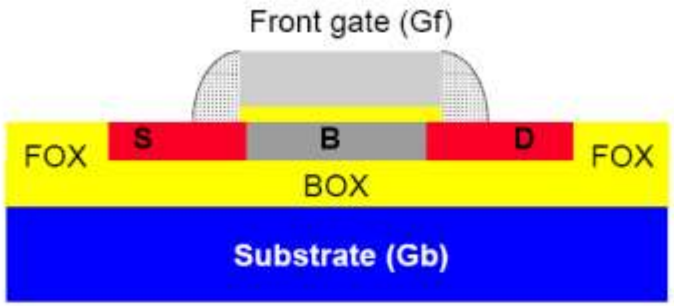
G ~ 1 ➔ fully ballistic transport

doi:10.1038/nature01797

Which is better?
Width scaling or Length Scaling?

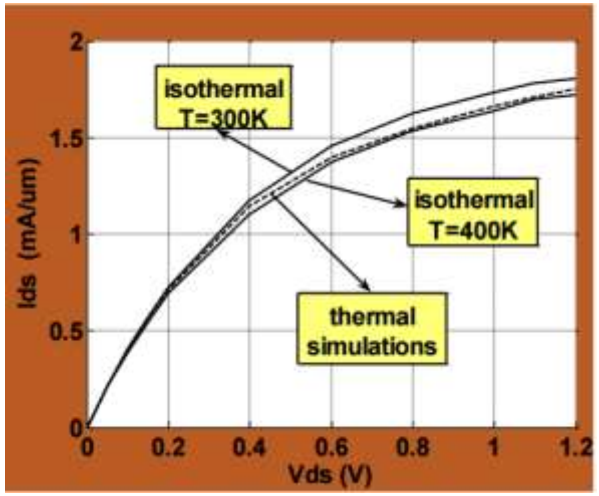
- Length Scaling increases current;

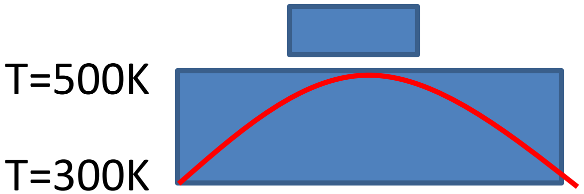
Calculating Temperature in MOSFET mobility & Phonon ➔ heating



Calculate the T (x) if the MOSFET is passing a current I.

Assume 1D





Current → →

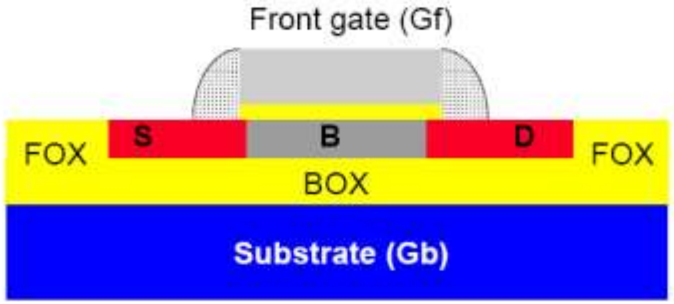
➔ MOSFET performance is degraded

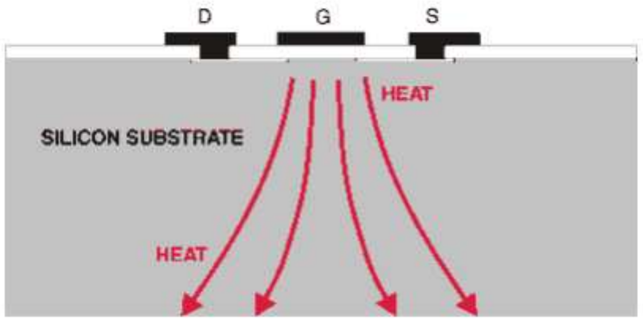
➔ Solution?

Phonons Engineering in CMOS devices

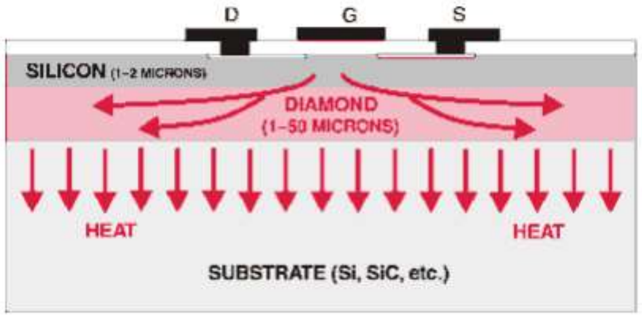
May cause self heating in Nano MOS FETs which causes mobility degradation

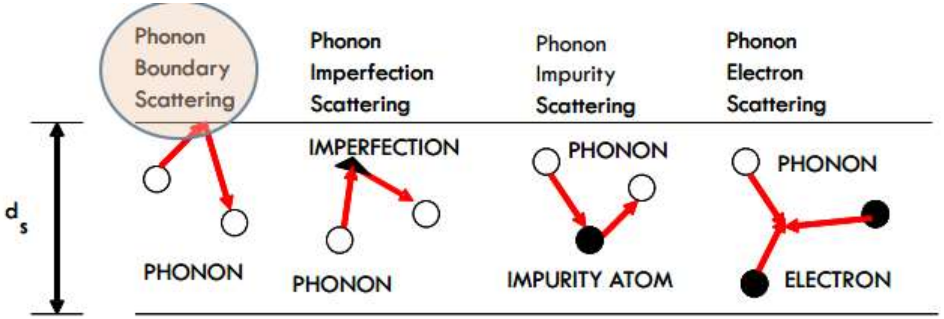
/nanohub.org/resources/18448/download/Self-
g_Effects_in_SOI_Devices_and_GaN_HEMTs.pdf





Standard Si technology

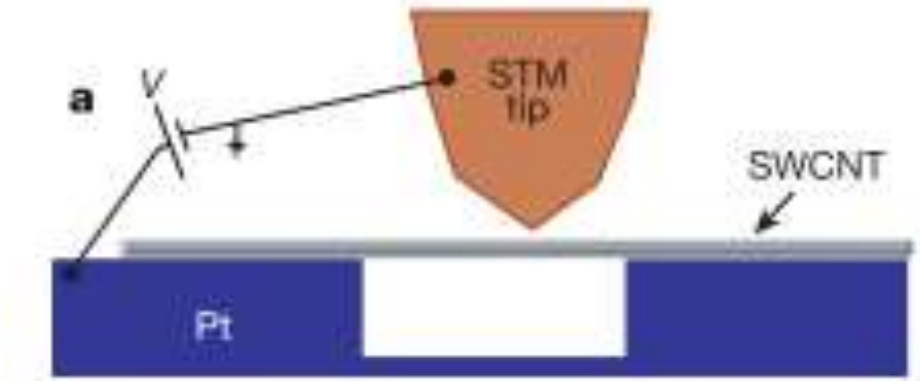




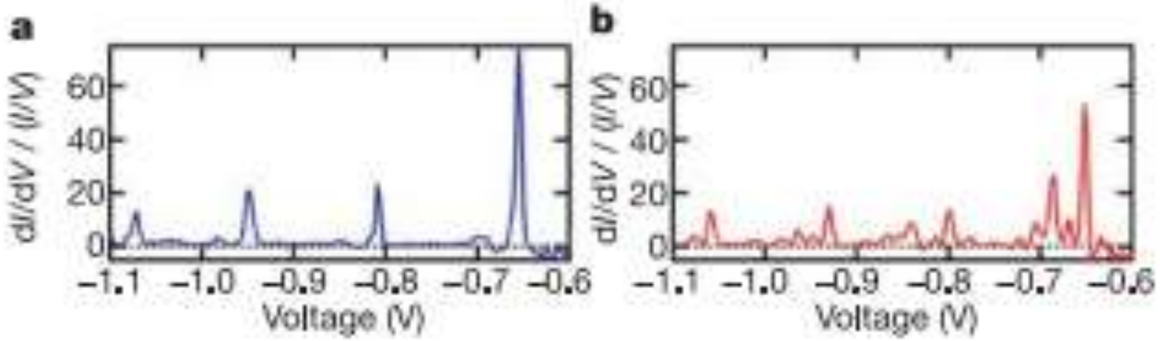
Phonons in Nanoscale devices

http://arxiv.org/ftp/arxiv/papers/0802/0802.3739.pdf

- Nanotubes can be used to reduce phonon modes



http://www.nature.com/nature/journal/v432/n7015/pdf/nature03046.pdf



New Applications: Phonons in Nanoscale devices

- RRAM is based on filament break by heating e.g. like a fuse

http://arxiv.org/ftp/arxiv/papers/0802/0802.3739.pdf