Thermal and Electric Conduction in Nanostructures

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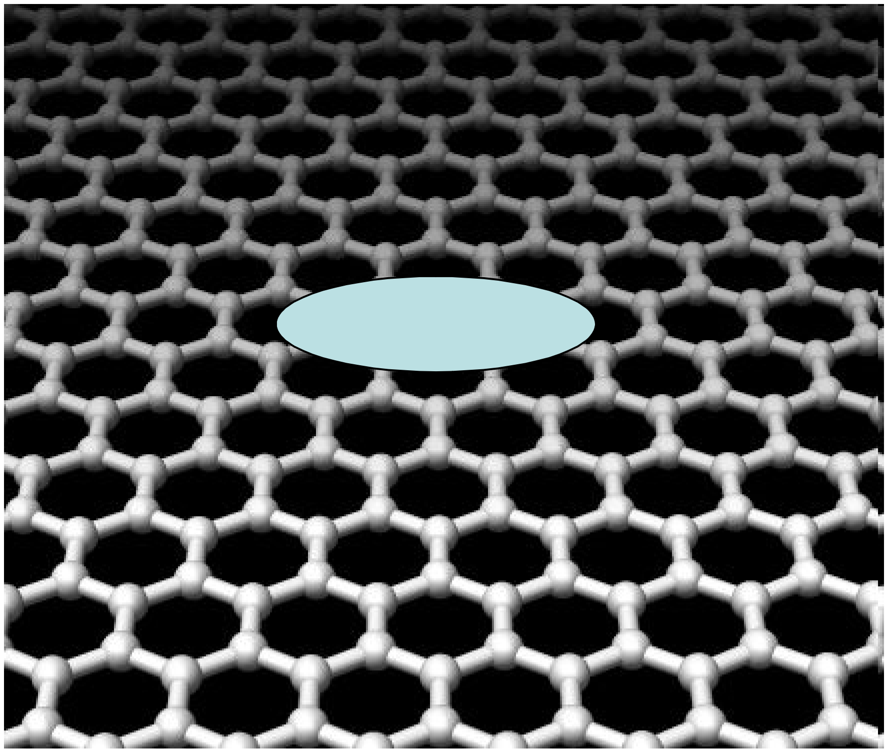
Course Website: **nanoHUB.org**
Compass.illinois.edu

First Midterm

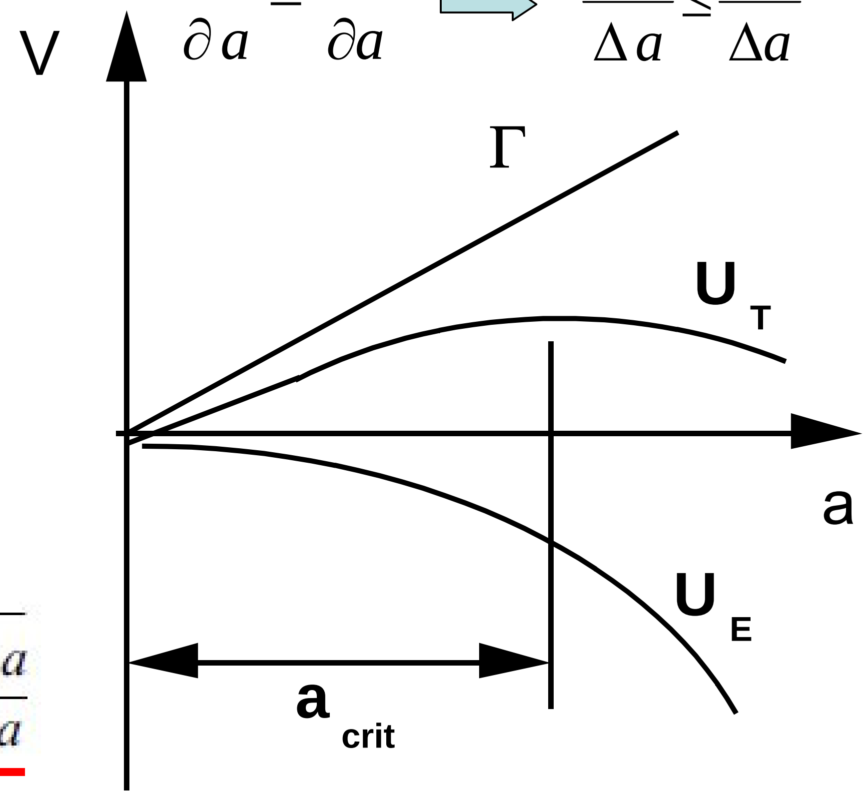
- Friday, Sept 25 1-2PM
- Coverage:
  - Scaling
  - Quantum Effects
  - Molecular Dynamics of Transport
  - Nanoscale Solid Mechanics
- A Review Lecture on Monday, Sept 21

Quantum Fracture Mechanics



Applying Griffith's approach to atomic lattices, e.g. graphenes:

$$\frac{\partial U}{\partial a} = \frac{\partial \Gamma}{\partial a} \quad \Rightarrow \quad \frac{\Delta U}{\Delta a} \leq \frac{\Delta \Gamma}{\Delta a}$$

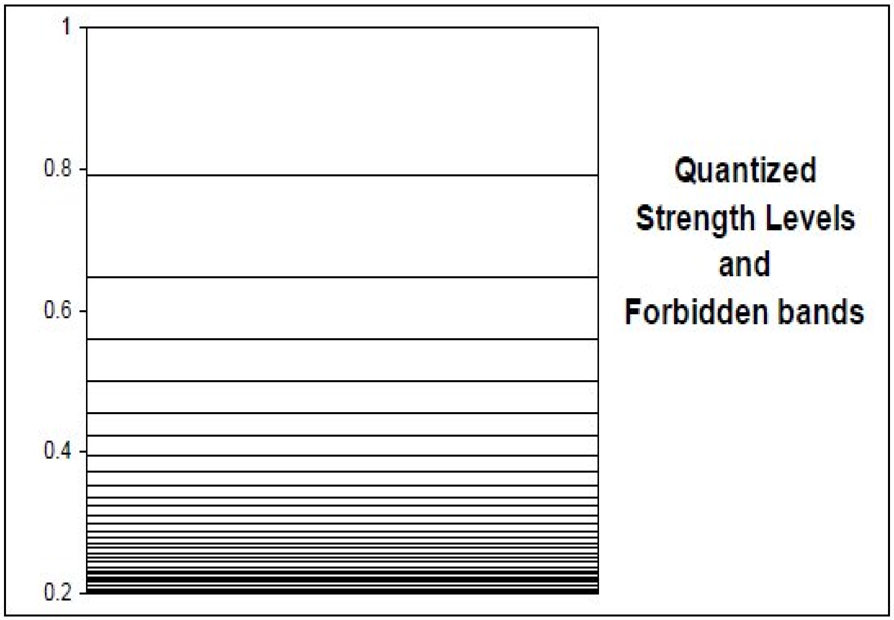


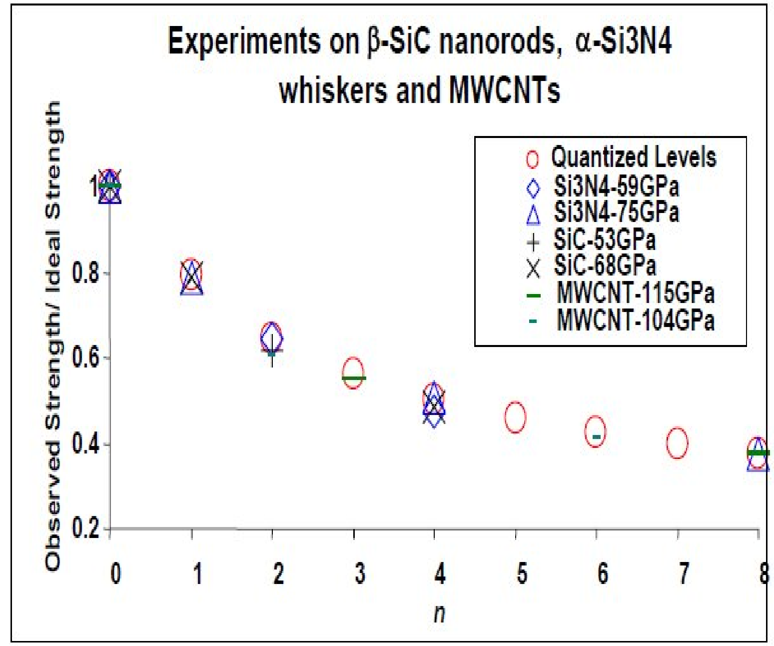
$$\sigma_f(l,\rho) = K_{IC}\sqrt{\frac{1+\rho/2a}{\pi(l+a/2)}} = \sigma_C\sqrt{\frac{1+\rho/2a}{1+2l/a}}$$

From N. Pugno and R. S. Ruoff, Quantized fracture mechanics, Philosophical Magazine 84 (2004), 2829-2845

“Quantized” Critical Strength!

$$\sigma_f(n) \approx \sigma_{ideal}\sqrt{1+\frac{\rho}{2a}(1+n)^{-1/2}}, \quad n>0$$



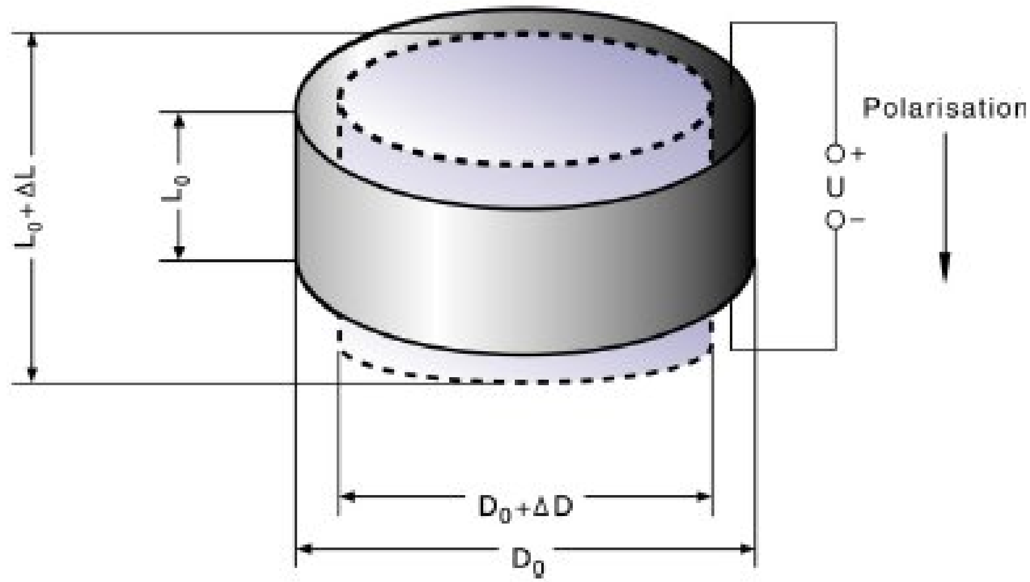


Quantized strength levels: experiments on β-SiC nanorods, α-Si_3N_4 whiskers and MWCNTs, and QFM predicted values.

From N. Pugno and R. S. Ruoff, Quantized fracture mechanics, Philosophical Magazine 84 (2004), 2829-2845

Mechanical coupling at Nanoscale

- E.G. Piezo-electricity (i.e. electric potential in response to applied stress)



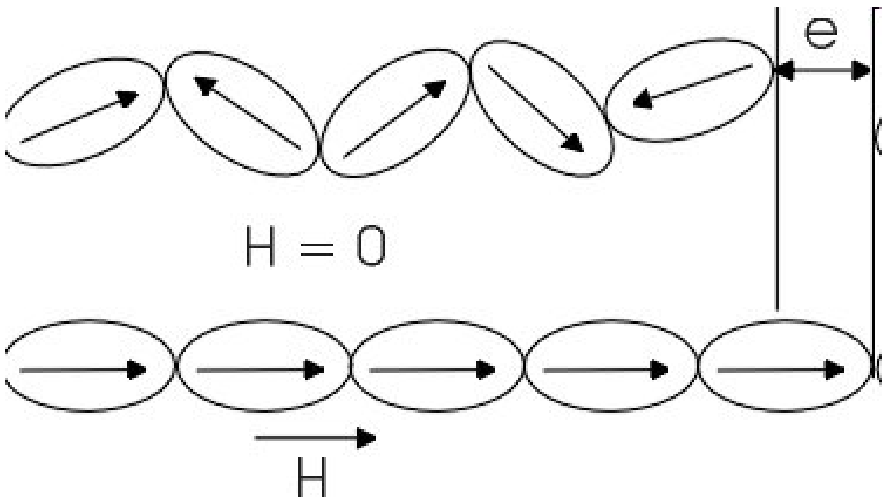
$$\Delta L = S \cdot L_0 \approx E \cdot d_{ij} \cdot L_0$$

S = strain (relative length change ΔL/L, dimensionless)
L0= ceramic length [m]
E = electric field strength [V/m]
dij= piezoelectric coefficient of the material [m/V]

See: www.physikinstrument.com

Magneto-restrictive Effect

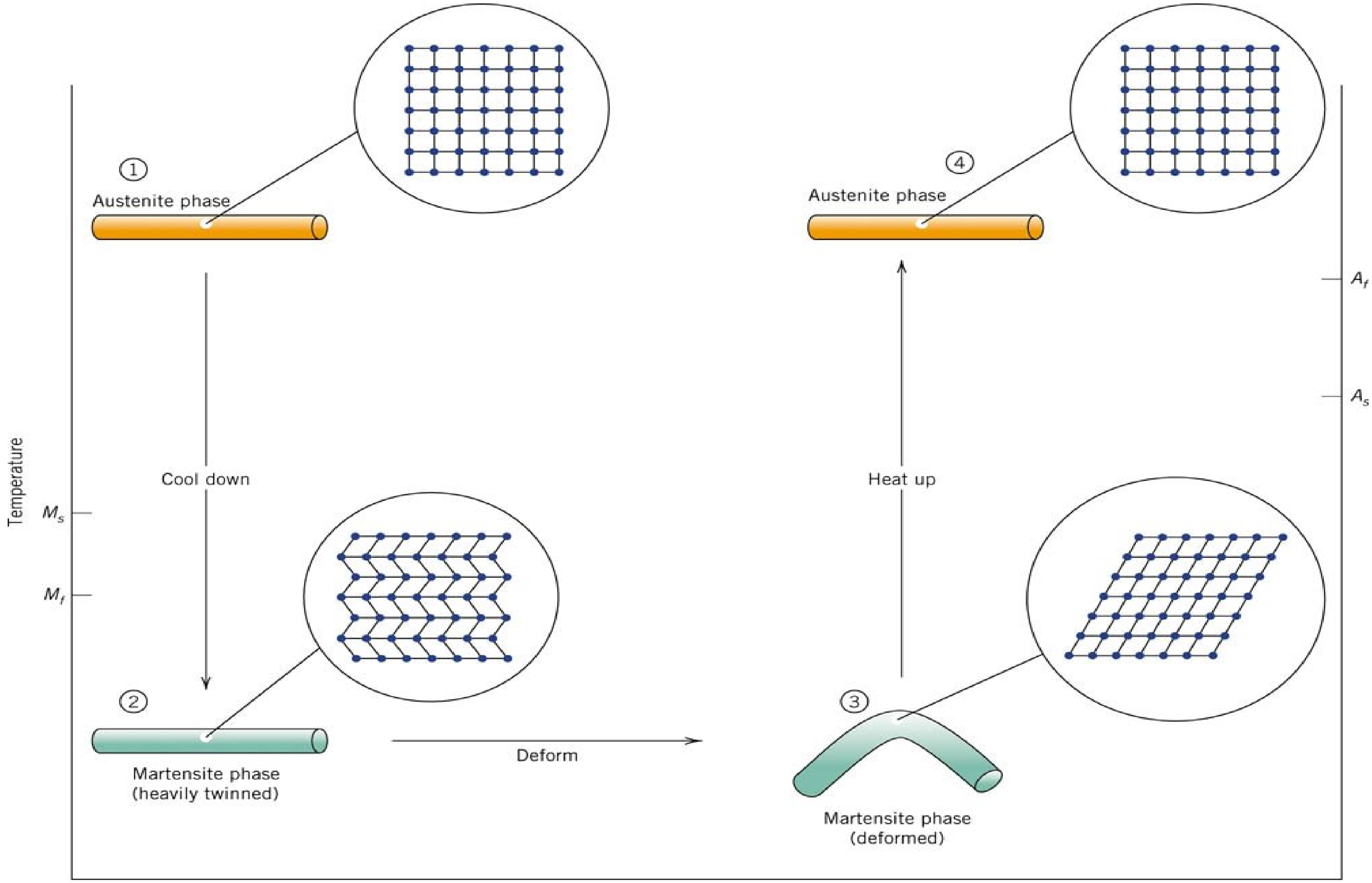
Magnetostriction is the strain of a material in response to change of magnetization.



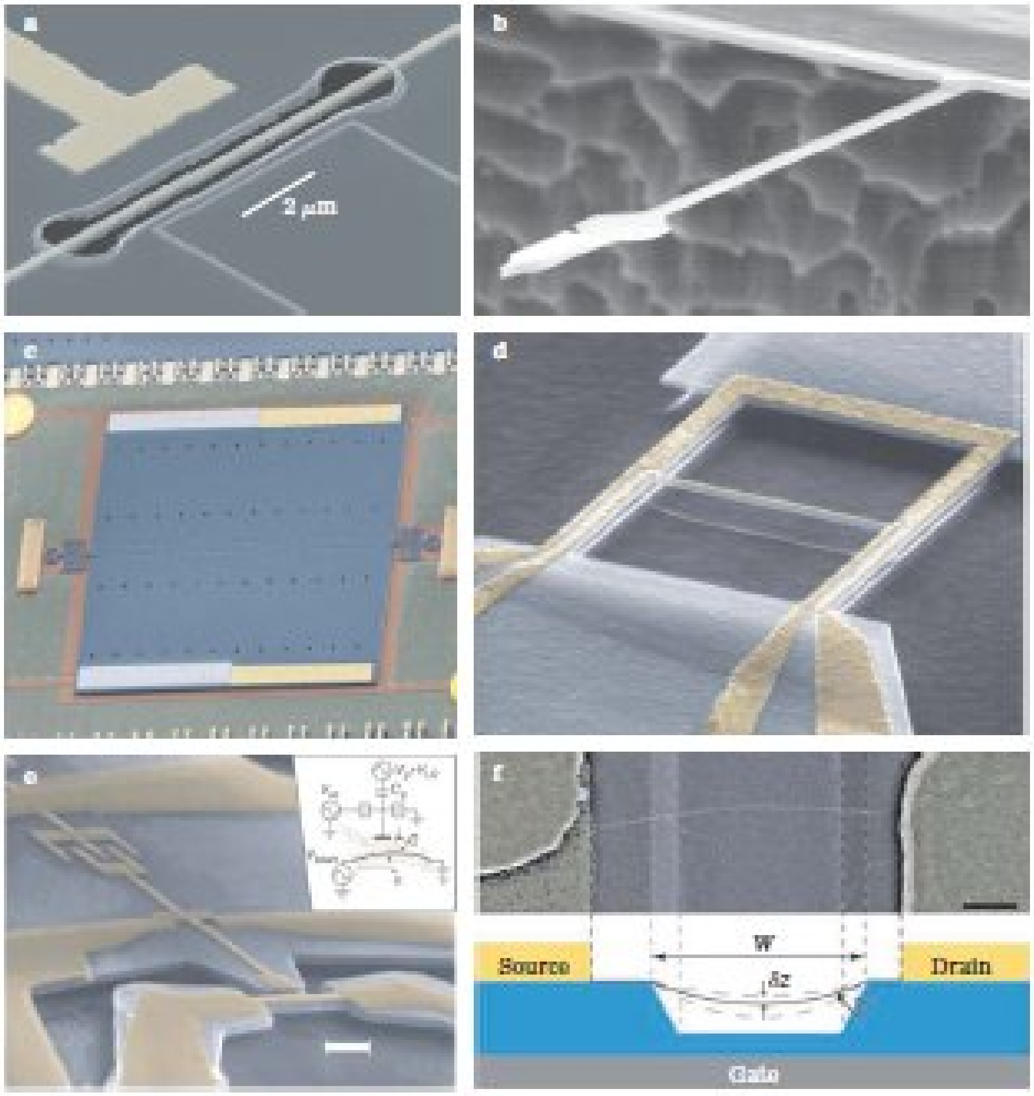
"giant" magnetorestriction found in nanostructured materials

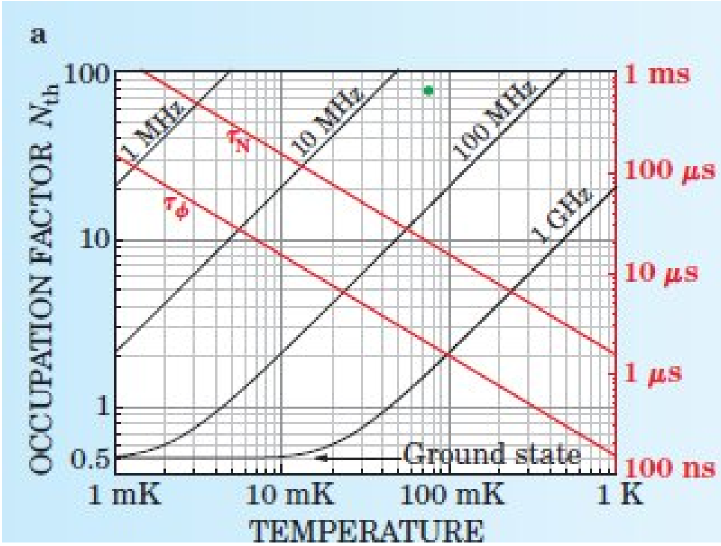
Application: Flat panel speakers (e.g. sound bugs) http://www.feonic.com/#commInfo

Shape Memory Effect



Mechanical Nanoresonators





Putting Mechanics into Quantum Mechanics, Keith C. Schwab and Michael L. Roukes, Physics Today, 2005, 36-42)

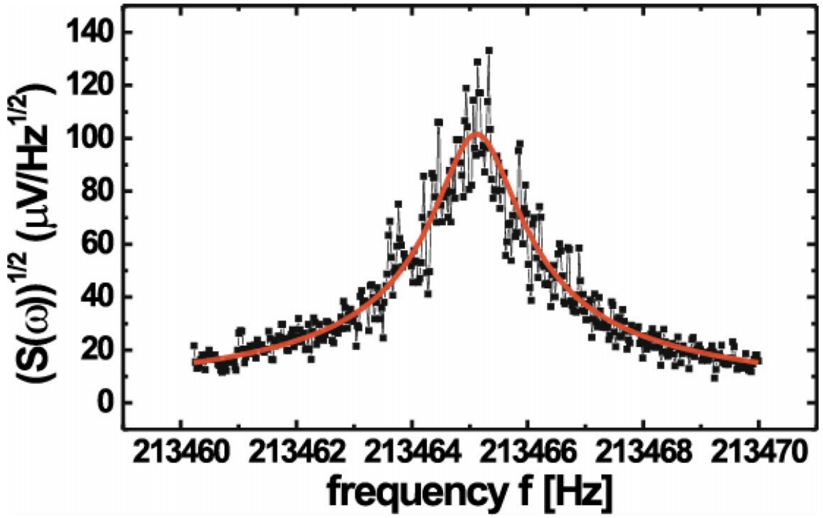
Thermal Noise in Resonators

Cantilever total energy:

$$W = \frac{1}{2} m \left(\frac{\partial z}{\partial t}\right)^2 + \frac{1}{2} m\omega_0^2 z^2$$

Each are subject to thermal noise 1/2kT

$$W_p(\omega) = \frac{2\gamma KT}{m^2(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2}$$



where $\gamma = m\omega_0/Q$ and $\omega_0^2 = k/m$

$$\Rightarrow \quad 2B\, W_p(\omega) = \frac{4KTBQ}{k\omega_0} \frac{1}{Q^2(1 - \omega^2/\omega_0^2)^2 + \omega^2/\omega_0^2}$$

From

$$\langle \delta z^2 \rangle^{1/2} = \sqrt{2BW_p(\omega)}$$

We get

$$\langle \delta z^2 \rangle^{1/2} = \frac{4kTB}{k\omega_0} \frac{Q}{\sqrt{Q^2(1 - \omega^2/\omega_0^2)^2 + \omega^2/\omega_0^2}}$$

Back to Constitutive Equations

- Hooke's Law $\sigma = E\varepsilon$
- Fourier's Law $\mathbf{q} = -k\nabla T$
- Fick's Law of Diffusion $\mathbf{J} = -D\nabla C$
- Newton's law on shear stress $\tau = -\mu\,(du/dy)$
- Ohm's Law $J = \sigma E$

How are they correlated in the nanoscale?

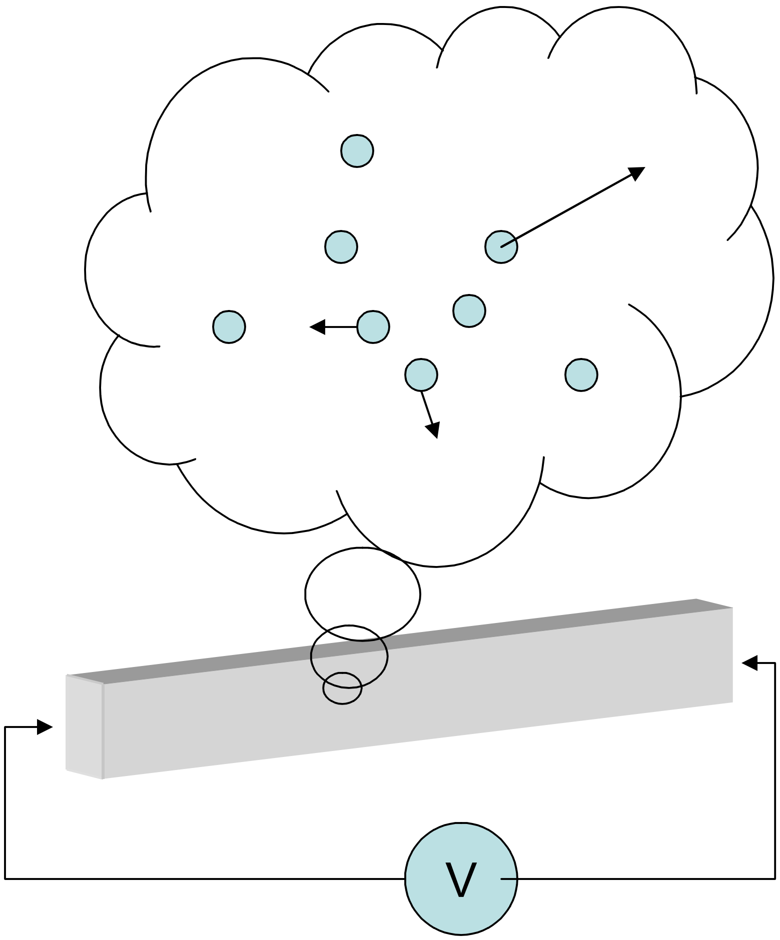
Look Into the Conducting Nanowires

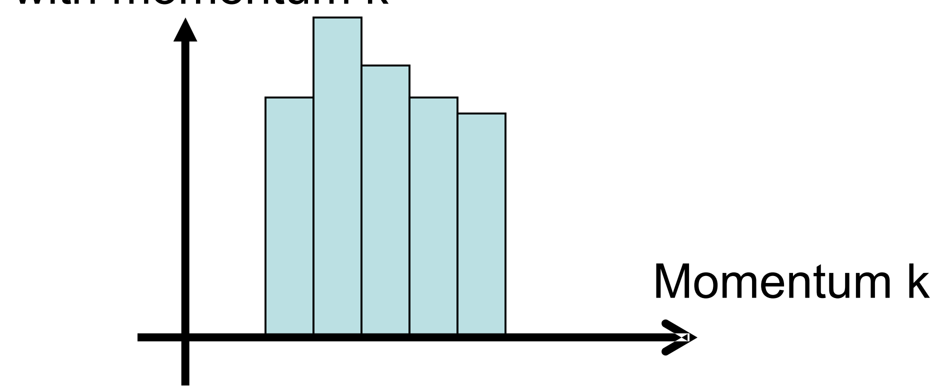
A Cloud of moving carriers

- Some are slow

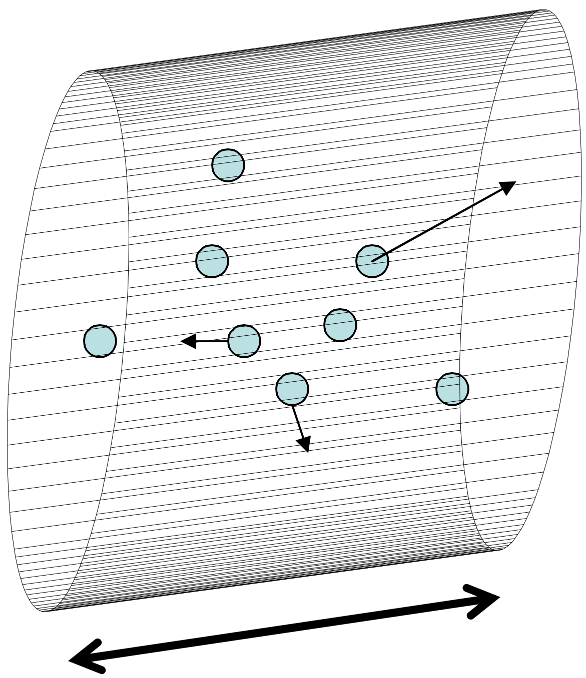
- Some are fast

- Some move against the mainstream





Calculating Current Density



Current = # electrons through A per second

$$I = e \times \underline{n(r,k)} \times A \underline{dr/dt}$$

Average number of electrons (n(r,k))

Average velocity (dr/dt)

Current density:

$$J = e \times n(r,k) \times v(r,k)$$

Power density:

$$Q = E(r,k) \times n(r,k) \times v(r,k)$$

Net Charge/Energy Flux

In order to find the net charge/energy flux (net current/power density), we need to consider all possible states at thermal equilibrium

$$J = \int_k e \times n(r,k) \times v(r,k)\,dk$$

$$Q = \int_k E(r,k) \times n(r,k) \times v(r,k)\,dk$$

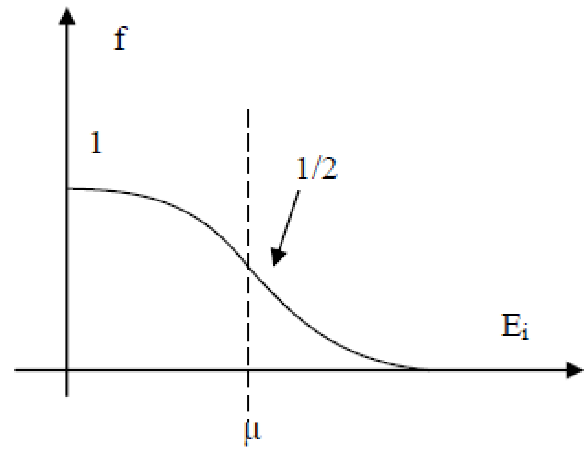
Note: $n(r,k)dk = DOS(r,k)\,p(r,k)\,dk$

- $DOS(r,k)$: Density of States
- $p(r,k)$: Boltzmann Distributions

Recall: For Quantum Particles

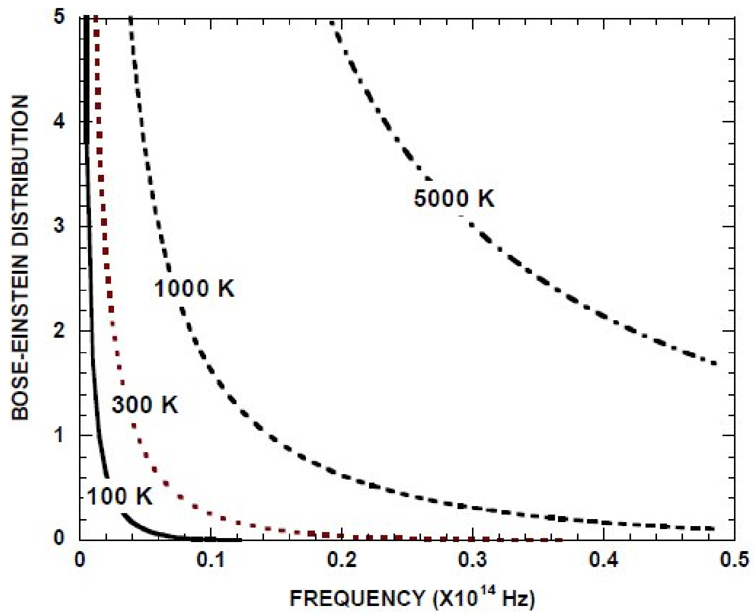
- Electrons: only two states possible (conduction, valence)

$$p(E_i) = \frac{\exp((E_F - E_i)/k_B T)}{1 + \exp((E_F - E_i)/k_B T)}$$



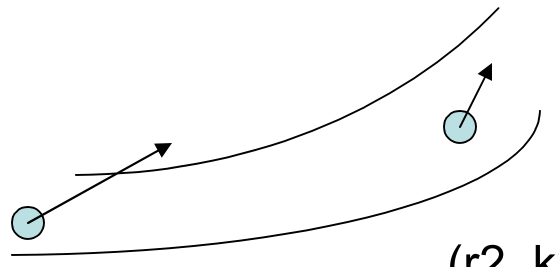
- Photons and Phonons: all possible states of energy $n\hbar\omega$

$$p(\omega) = \frac{1}{\exp(\hbar\omega / k_B T) - 1}$$



Time Evolution in f(r, k)

We Learned from fluidic mechanics:



$$\frac{D}{Dt}F = \frac{\partial}{\partial t}F + \boxed{\frac{\partial \vec{r}}{\partial t}\cdot\nabla F}$$

(Corrected for particle motion)

Since *k* is also changing over time, we add:

(Since total number of states is unchanged over time)

$$\frac{D}{Dt}p(r,k) = \underbrace{\frac{\partial}{\partial t}p}_{\text{Reaction}} + \underbrace{\frac{\partial \vec{r}}{\partial t}\cdot\nabla_r p}_{\text{Convection}} + \underbrace{\frac{\partial \vec{k}}{\partial t}\cdot\nabla_k p}_{\text{Acceleration}} = 0$$

"Reaction" "Convection" "Acceleration"

Boltzmann Transport Equation

$$\frac{\partial}{\partial t} p = -\vec{v} \cdot \nabla_r p - \frac{\vec{F}}{\hbar} \cdot \nabla_k p$$

"**Convection**" "**Acceleration**"

So how to estimate reaction?

Locally, the system that is away from thermal equilibrium has a tendency to relax toward equilibrium state:

$$\frac{\partial}{\partial t} p = -\frac{p - p_0}{\tau}$$

Equilibrium Distribution

Steady State Boltzmann TE

$$\frac{p-p_0}{\tau} = \vec{v}\cdot\nabla_r p + \frac{\vec{F}}{\hbar}\cdot\nabla_k p$$

In order to write *p(r, k)* explicitly, we further assume

$$p = p_0 + \delta p(r,k) \qquad \delta p(r,k) << p_0$$

Further, we learned the trick from DOS: $\nabla_k p = \nabla_k E \dfrac{\partial p}{\partial E}$

Velocity!

$$p \approx p_0 + \tau\vec{v}\cdot(\nabla_r p_0 + \frac{\vec{F}}{\hbar}\frac{\partial p_0}{\partial E})$$

Current Density and Mobility

$$J = \int_k e \times n(r,k) \times v(r,k) dk$$

$$J = \int_E e \times D(r,E) \times v(r,E) \times (\tau \vec{v} \cdot (\nabla_r p_0 + \frac{\vec{F}}{\hbar}\frac{\partial p_0}{\partial E}))dE$$

Assume F along z direction, we find:

$$J = \frac{\partial}{\partial z}(e\frac{k_B T n_e \langle \tau \rangle}{m}) + F_z \frac{e n_e \langle \tau \rangle}{m}$$

Electron diffusion

Migration under external field