Basics of Solid Mechanics 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

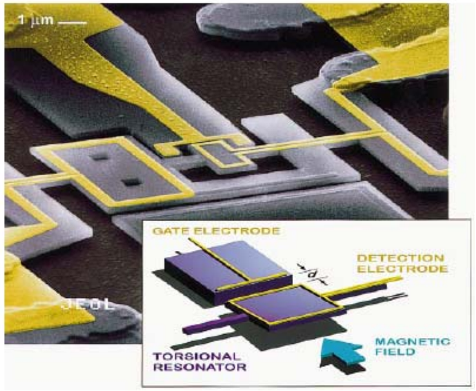
Mechanics at Nanoscale

- Why?
  - **Promising material behaviors** (reduced defects and faster recovery)

E.G. artists' view of space elevators using CNTs

  - **Coupling and quantum effect on mechanical response** (this lecture)

    (E.G. mechanical thermometer)



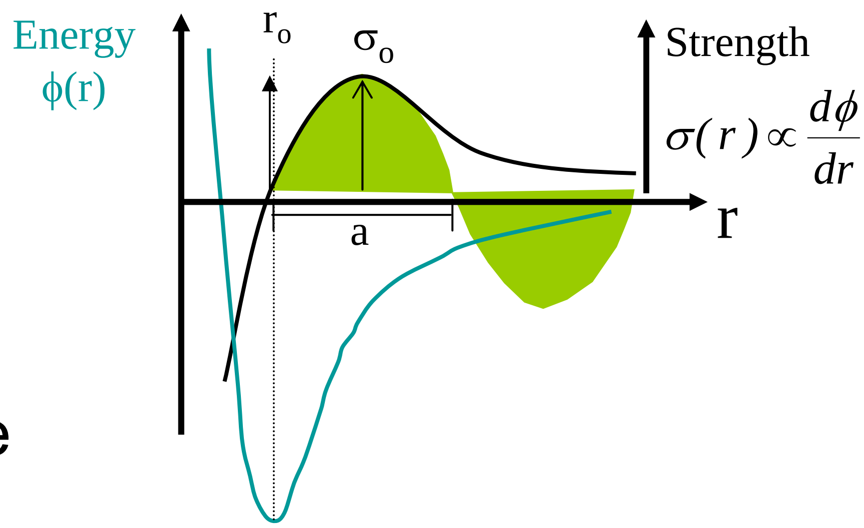
Cleland and Roukes, Nature, 1998

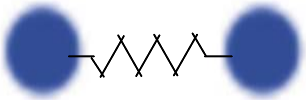
Theoretical Cohesive Strength

- Look back at the potential function for two atoms.
- Derivative is related to strength.
- Approximate strength curve with a sinusoid:

$$\sigma = \sigma_o \sin\frac{\pi r}{a}$$

  – σ_o = theoretical cohesive strength





How Close is Theory?

- Theory states: $$\sigma_o = \frac{E}{\pi}$$ OR $$\sigma_o \sim \frac{E}{8}$$
- Way too high for common materials (100-1000x too high)
- Look at "whiskers"
  - Small, "defect-free" fibers
  - Agreement is a little better.

	σ_f		E		
Material	**GPa**	**(psi × 10^6)**	**GPa**	**(psi × 10^6)**	E/σ_f
Silica fibers	24.1	(3.5)	97.1	(14.1)	4
Iron whisker	13.1	(1.91)	295.2	(42.9)	23
Silicon whisker	6.47	(0.94)	165.7	(24.1)	26
Alumina whisker	15.2	(2.21)	496.2	(72.2)	33
Ausformed steel	3.14	(0.46)	200.1	(29.1)	64
Piano wire	2.75	(0.40)	200.1	(29.1)	73

From: Hertzberg, p.76.

Defects in Solids

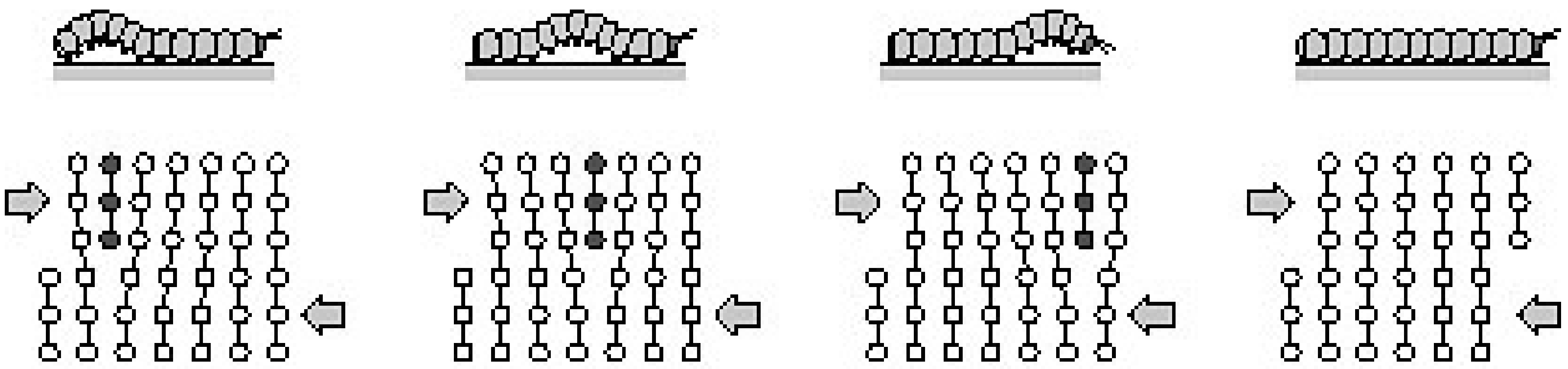
- To this point we have assumed perfect order in crystals
  - Defects always exist in real materials
  - Sometimes we add “defects” - alloying

- Classifications of defects
  - Usually referring to geometry or dimension of defect
  - ***Point*** : 1-2 atomic positions (10^{-10} m)- e.g. vacancies, interstitials
  - ***Line***: 1-Dimensional (10^{-9} to 10^{-5} m)- e.g. dislocations
  - ***Interfacial***: 2-Dimensional (10^{-8} – 10^{-2} m) - e.g. grain boundaries
  - ***Volume***: 3-Dimensional (10^{-4} – 10^{-2} m) - e.g. pores, cracks

Bulk Dislocation Movement

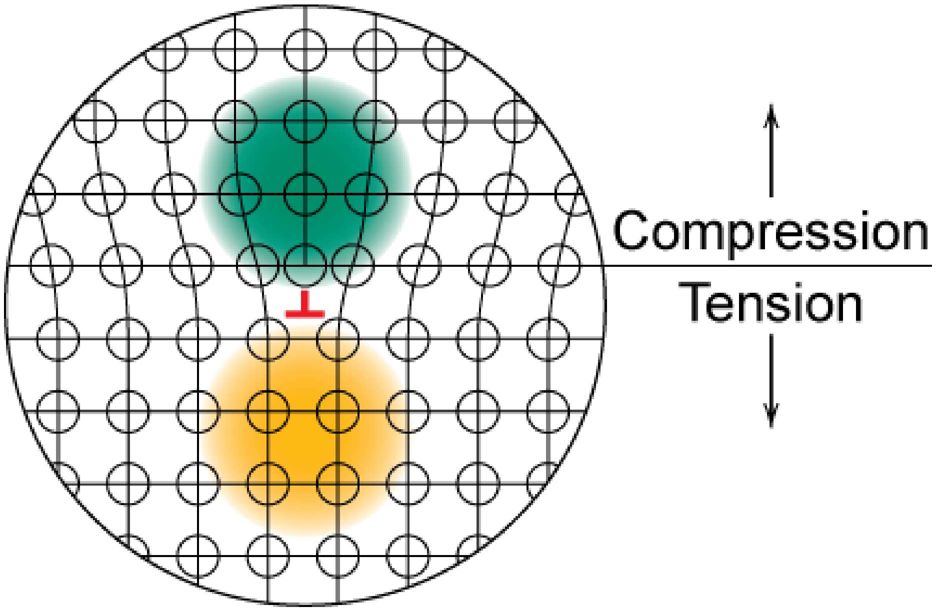
- Shear must act in direction of **Burgers vector** $\vec{b}$

- Edge
  - Positive & negative
- Screw
  - Right-hand & left-hand
- Analogies for motion
  - Caterpillar crawling



From: Callister, p.156

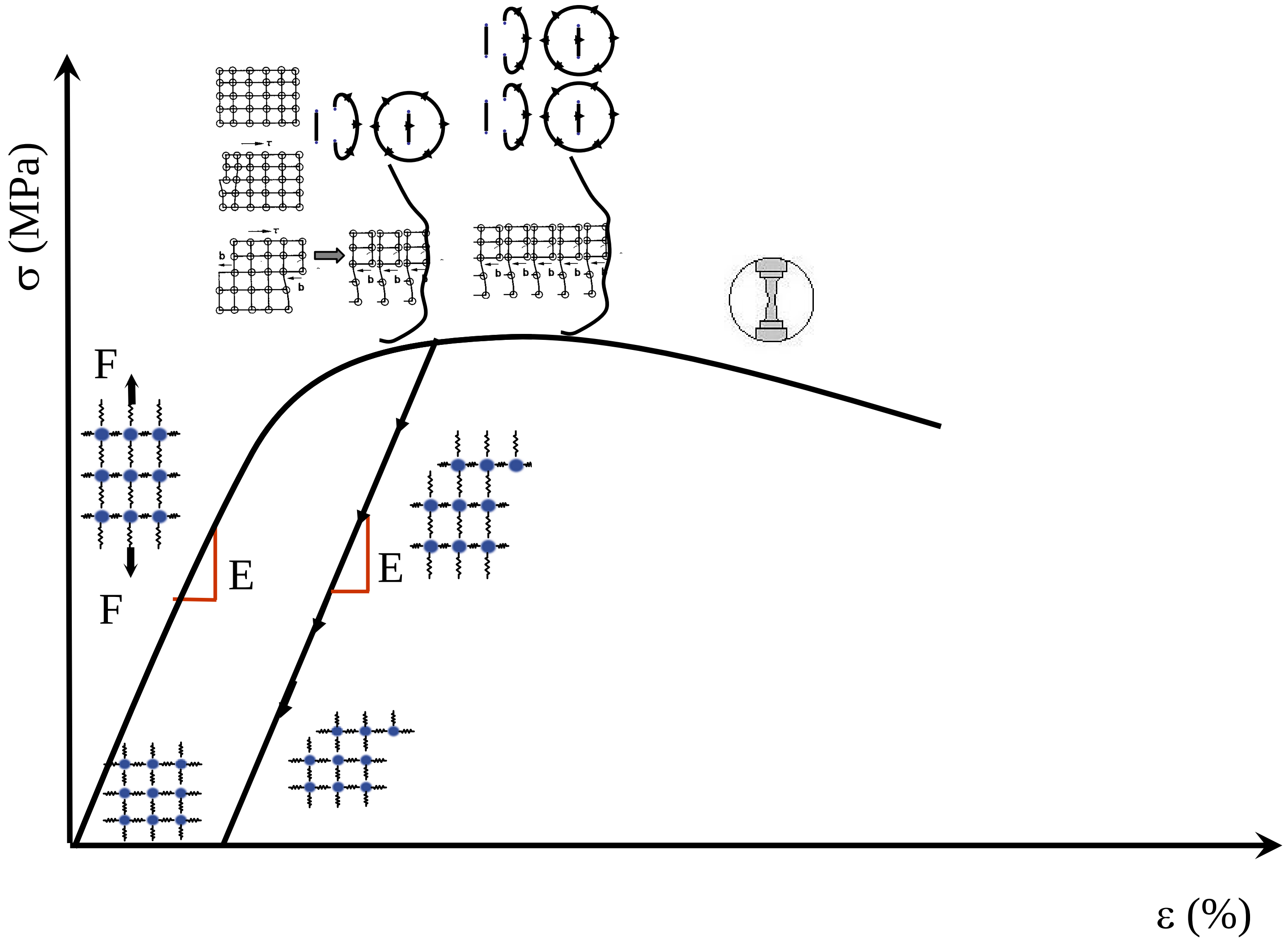
Stress Fields



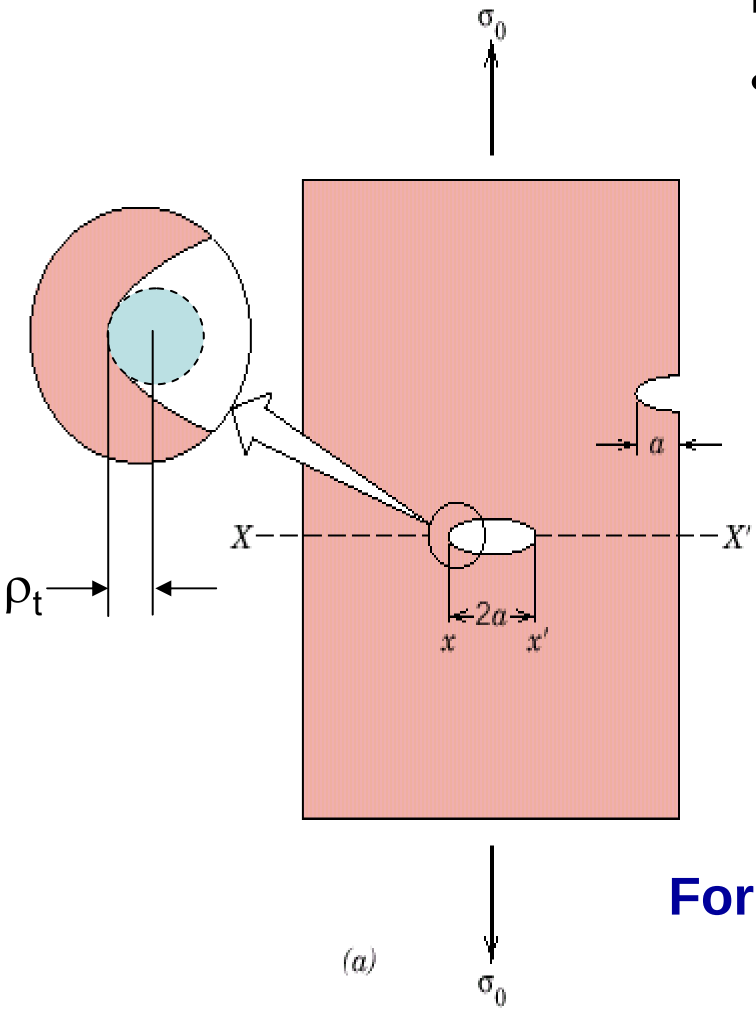
Adapted from Fig. 7.4, *Callister 7e.*

- Extra half plane of atoms cause lattice distortions
- Result in *tensile*, *compressive*, and *shear* strains in neighboring atoms
  - Magnitude decreases with distance
  - Pure compression and tension directly above and below slip line
  - Over most of the effected region combination of stresses
- Screw dislocation
  - Pure shear

Microscopic View of Strain-Stress



Flaws are Stress Concentrators!



Results from crack propagation

- Griffith Crack

$$\sigma_m = 2\sigma_o \left(\frac{a}{\rho_t}\right)^{1/2} = K_t \sigma_o$$

a stress concentration factor

where

ρ_t = radius of curvature

σ_o = applied stress

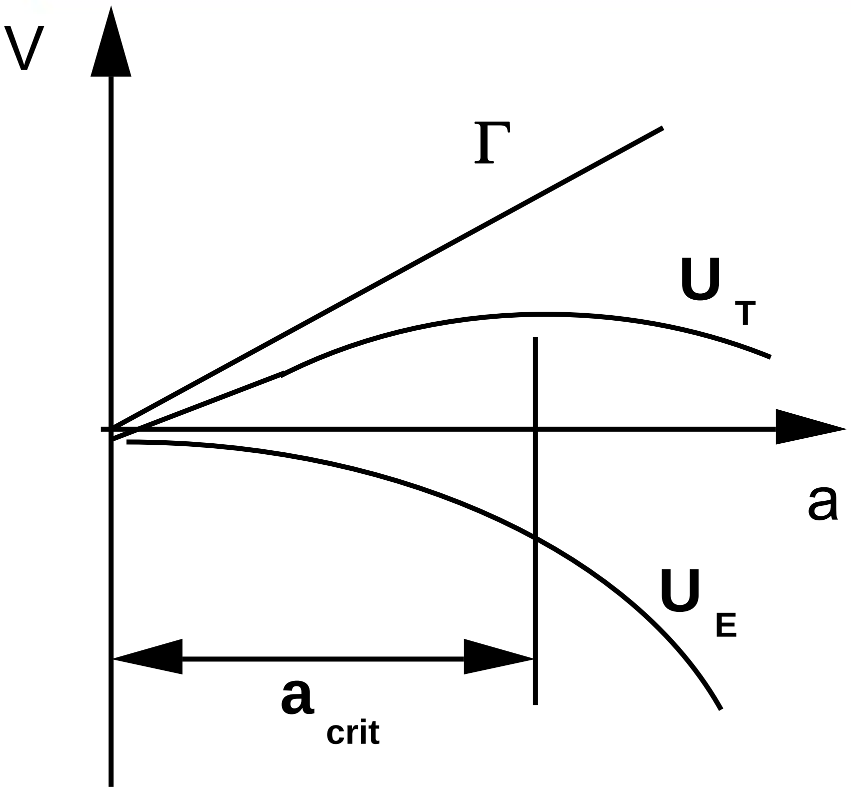
σ_m = stress at crack tip

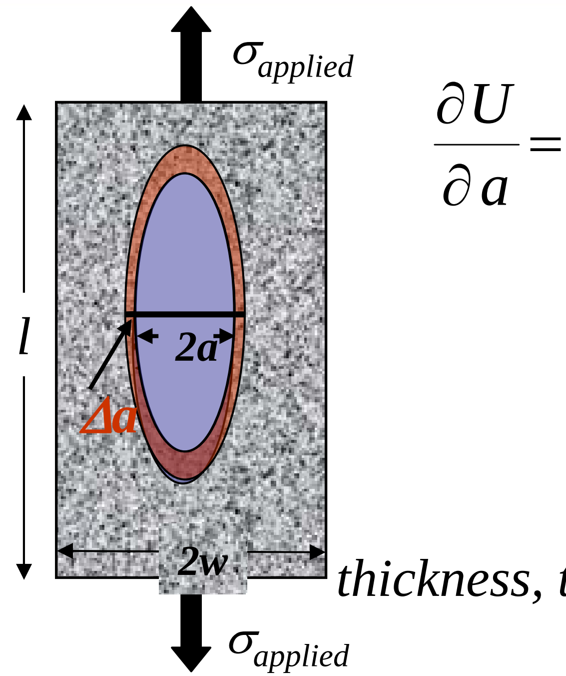
For a crack, typically have

a = 10^{-3}m

ρ = 10^{-9}m $\sigma_{local} = 2000 * \sigma_{applied}$

Griffith Approach





$$\frac{\partial U}{\partial a} = \frac{\partial \Gamma}{\partial a}$$

Minimum criterion for stable crack growth:

$$\frac{\partial}{\partial a}\left(\frac{\sigma^2}{2E}\pi 2a^2 t\right) = \frac{\partial}{\partial a}(\gamma_s 4 a t)$$

Strain energy goes into surface energy

$$\sigma = \sqrt{\frac{2 E \gamma_s}{\pi a}}$$

So When Does Crack Propagate?

Crack propagates rapidly if above critical stress

i.e., $\sigma_m > \sigma_c$

$$\sigma_c = \left(\frac{E G_c}{\pi a} \right)^{1/2}$$

$$\sigma_c \sqrt{\pi a} = \sqrt{E G_c}$$ = constant!!

Measurable (fixed) materials properties

Fracture Toughness, K_c

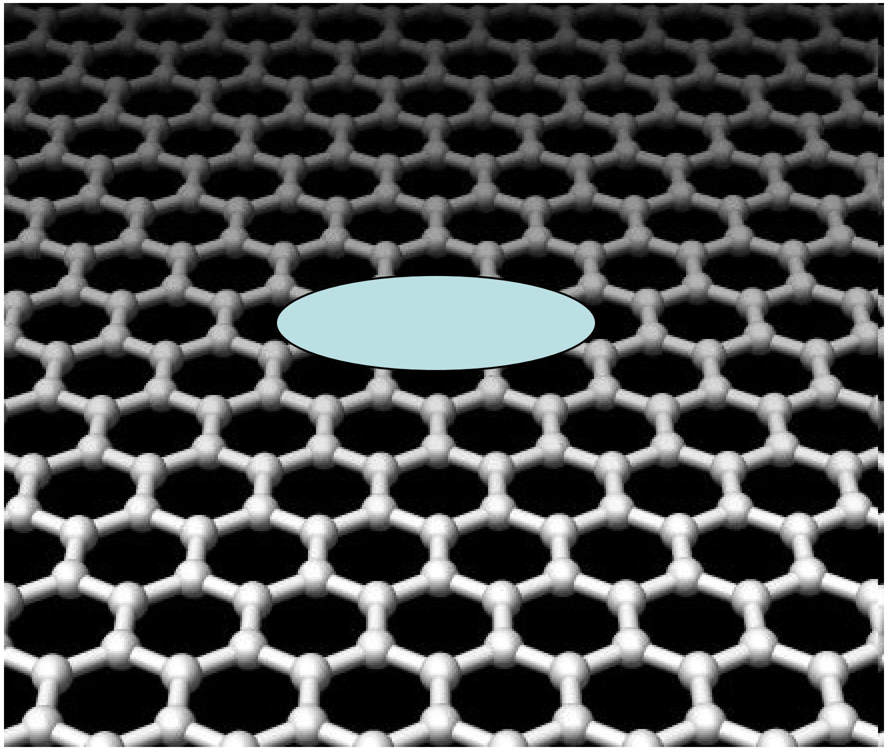
where

- ***E* = modulus of elasticity**
- **Gc = specific energy release rate**
- ***a* = one half length of internal crack**

Brittle: $G_C = 2\gamma_s$

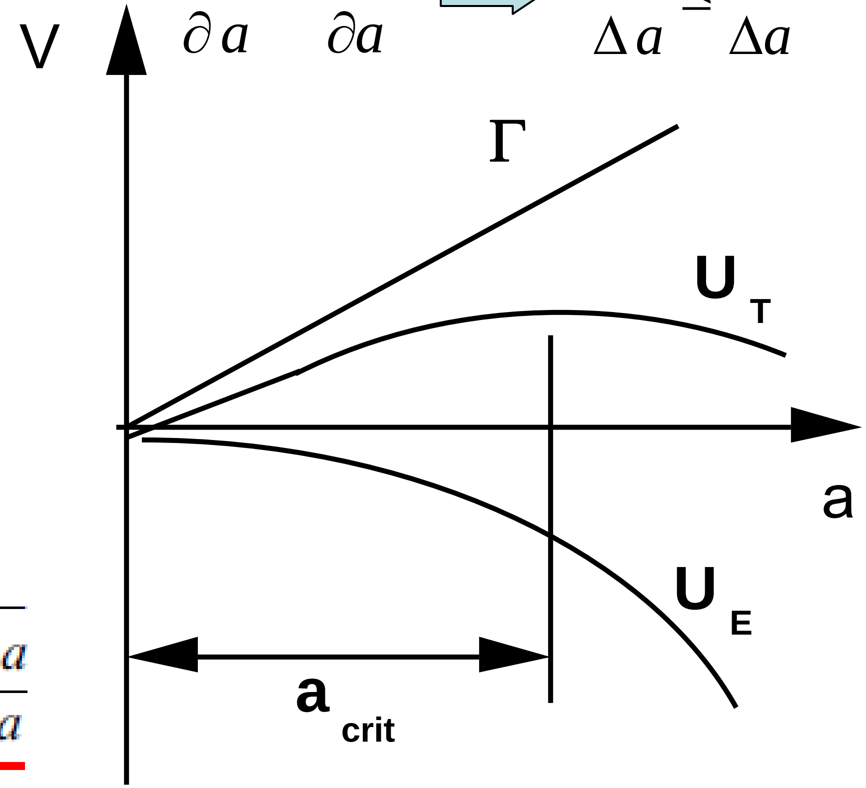
Ductile: $G_C = 2\left(\gamma_s + \gamma_p\right)$

Quantum Fracture Mechanics



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

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

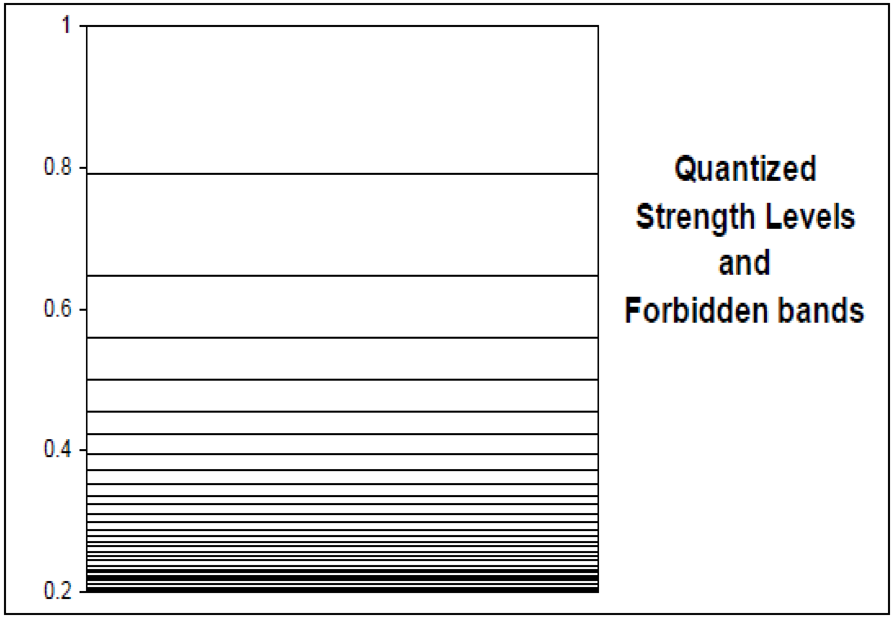


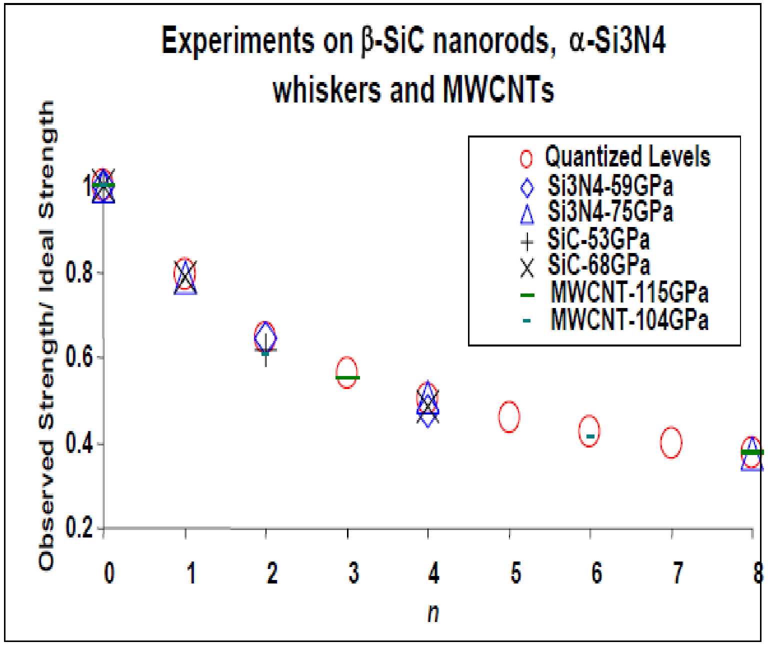
$$\sigma_f(l,\rho) = K_{IC}\sqrt{\frac{1+\rho/2a}{\pi(l+a/2)}} = \sigma_C\sqrt{\frac{1+\rho/2a}{1+2l/a}}$$

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

"Quantized" Critical Strength!

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

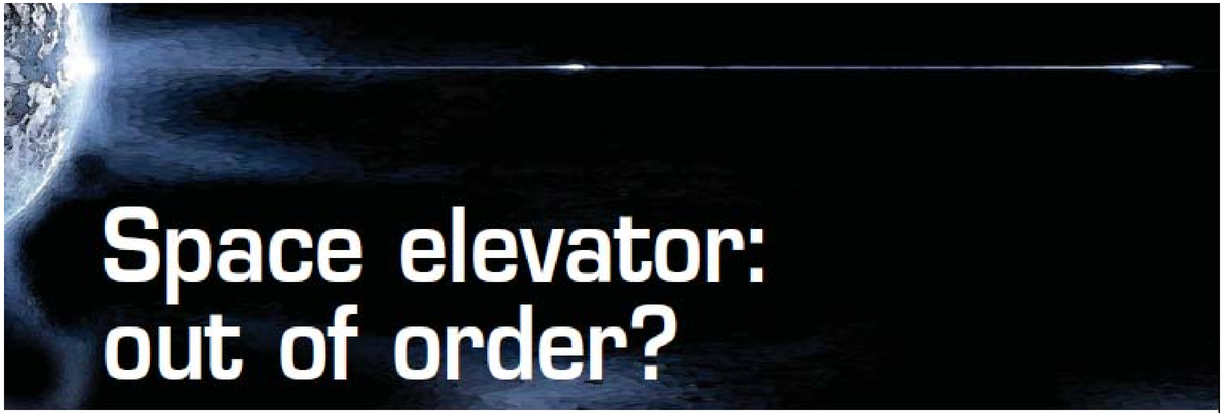




Quantized strength levels: experiments on β-SiC nanorods, α-Si_3N_4 whiskers and MWCNTs, and QFM predicted values.

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

Space Elevator: Out of Order?

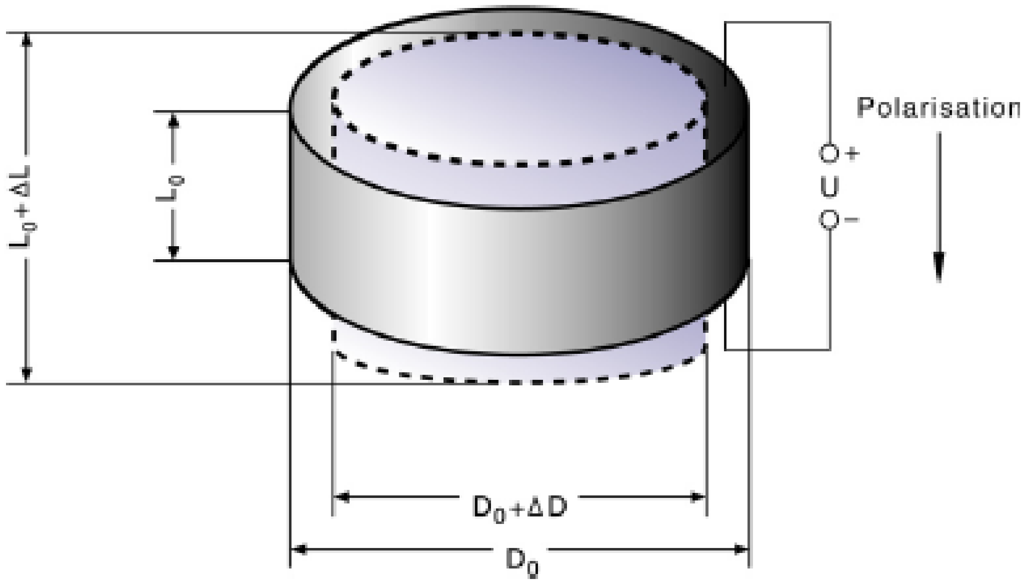


Classical theories of the strength of solids, such as fracture mechanics or those based on the maximum stress, assume a continuum. Even if such a continuum hypothesis can be shown to work at the nanoscale for elastic calculations, it has to be revised for computing the strength of nanostructures or nanostructured materials. Accordingly, quantized strength theories have recently been developed and validated by atomistic and quantum-mechanical calculations or nanotensile tests. As an example, the implications for the predicted strength, today erroneously formulated, of a carbon-nanotube-based space elevator megacable are discussed. In particular, the first *ab initio* statistical prediction for megacable strength is derived here. Our findings suggest that a megacable would have a strength lower than ~45 GPa.

Nicola Pugno, Nano Today, 2007(2)44-47

Mechanical coupling at Nanoscale

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

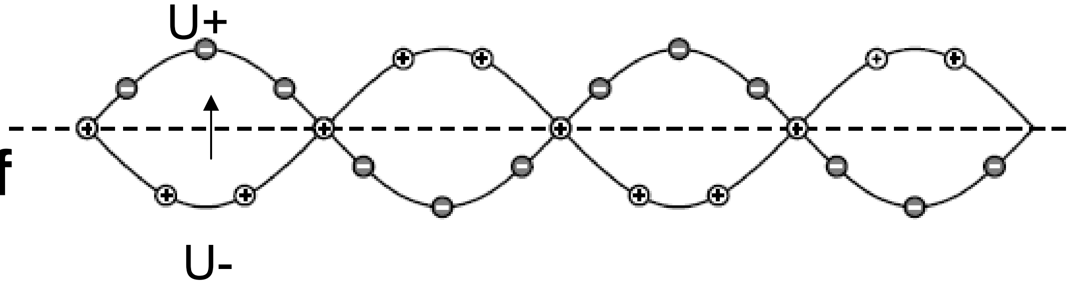


$$\Delta L = S \cdot L_0 \approx E \cdot d_{ij} \cdot L_0$$

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

Principle of Piezo-electric Effect

Asymmetry in crystal leads to separation of charges under stress



$$D_i = \varepsilon_{ij} E_j + d_{ji} \sigma_j$$

Electric polarization | Strain effect

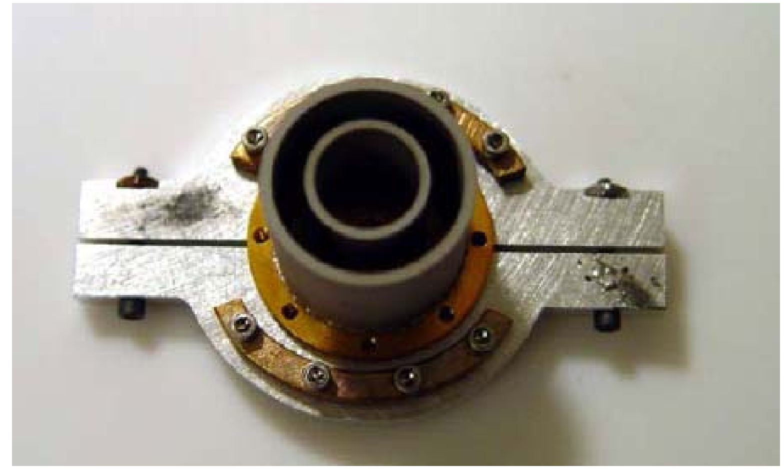
Inversely, polarization in crystal induces stress

$$\sigma_i = C_{ij} e_j + d_{ij} E_j$$

Hooke's law | piezo effect

Piezoelectric Sensing/Actuation

Quartz Tuning Forks,
typically f=32KHz



Stack of piezo-tubes

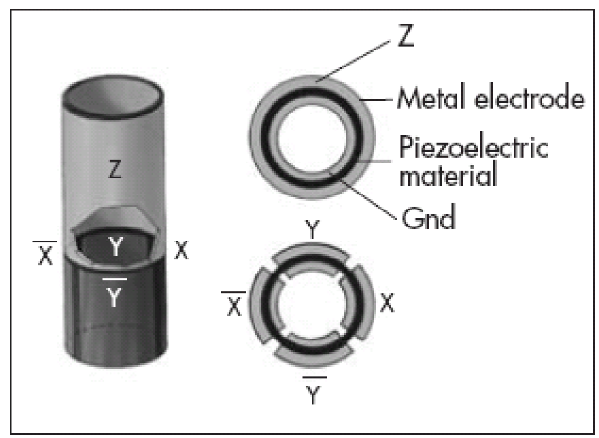
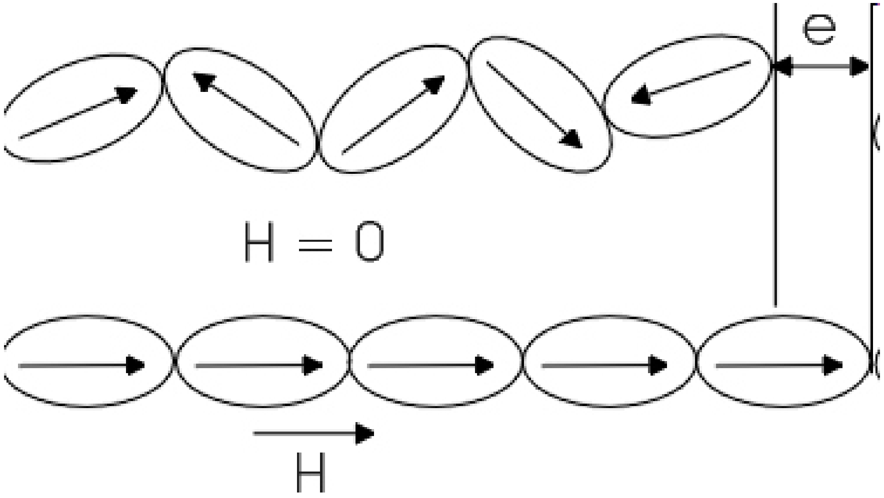


Figure 7-3. Typical scanner piezo tube and X-Y-Z configurations. AC signals applied to conductive areas of the tube create piezo movement along the three major axes.

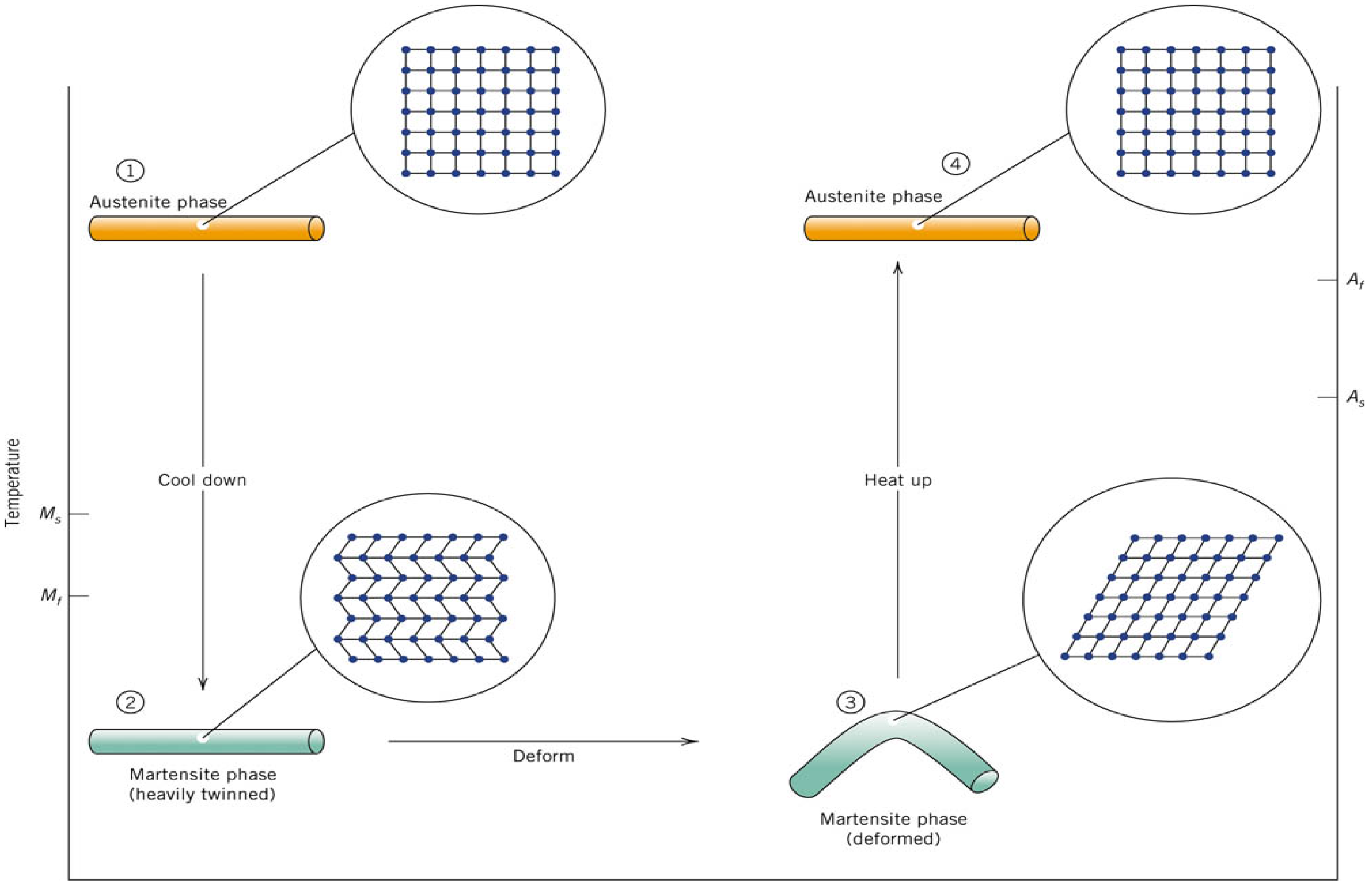
Magnetostriction is the strain of a material in response to change of magnetization.



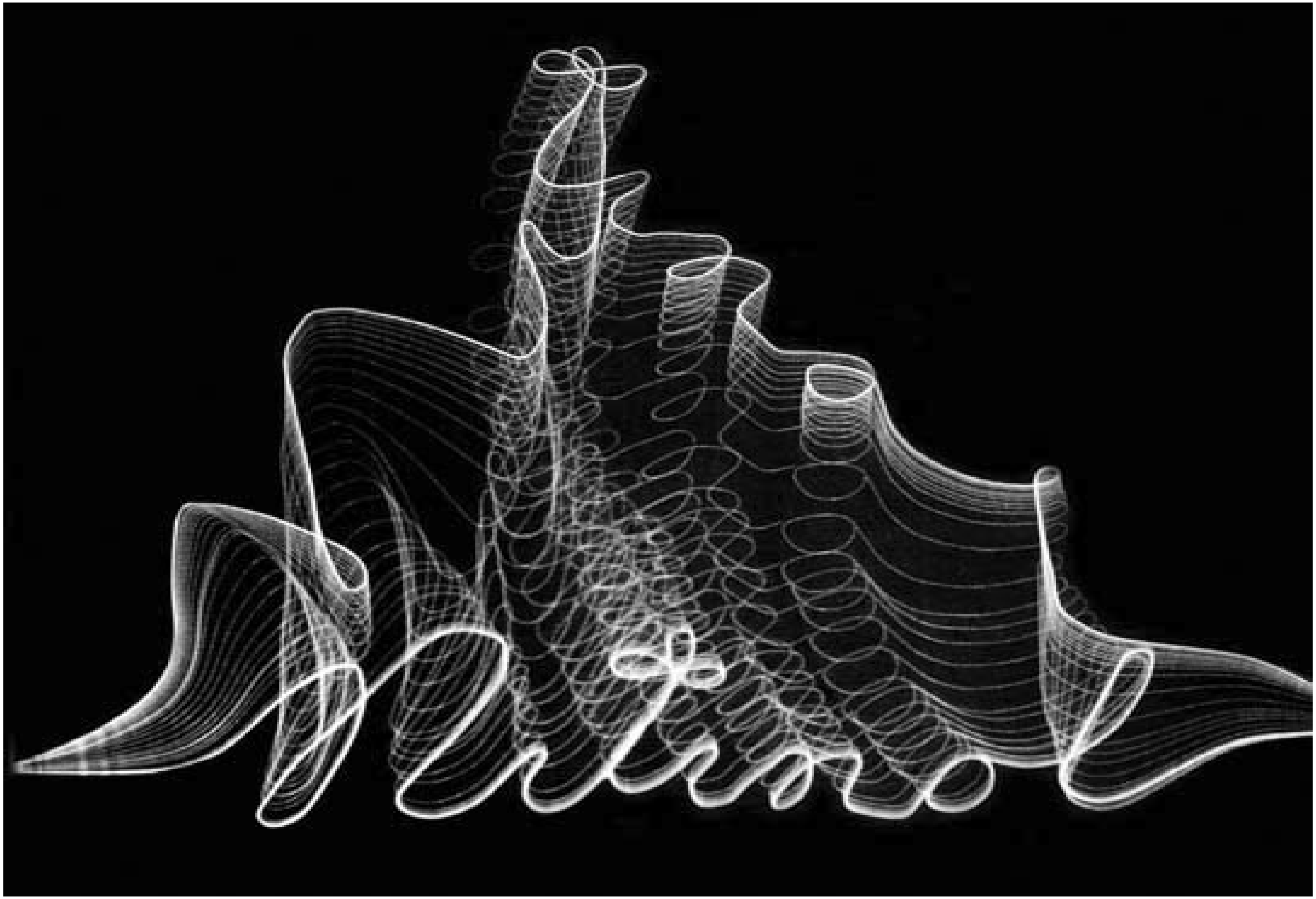
“giant” magnetorestriction found in nanostructured materials

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

Shape Memory Effect

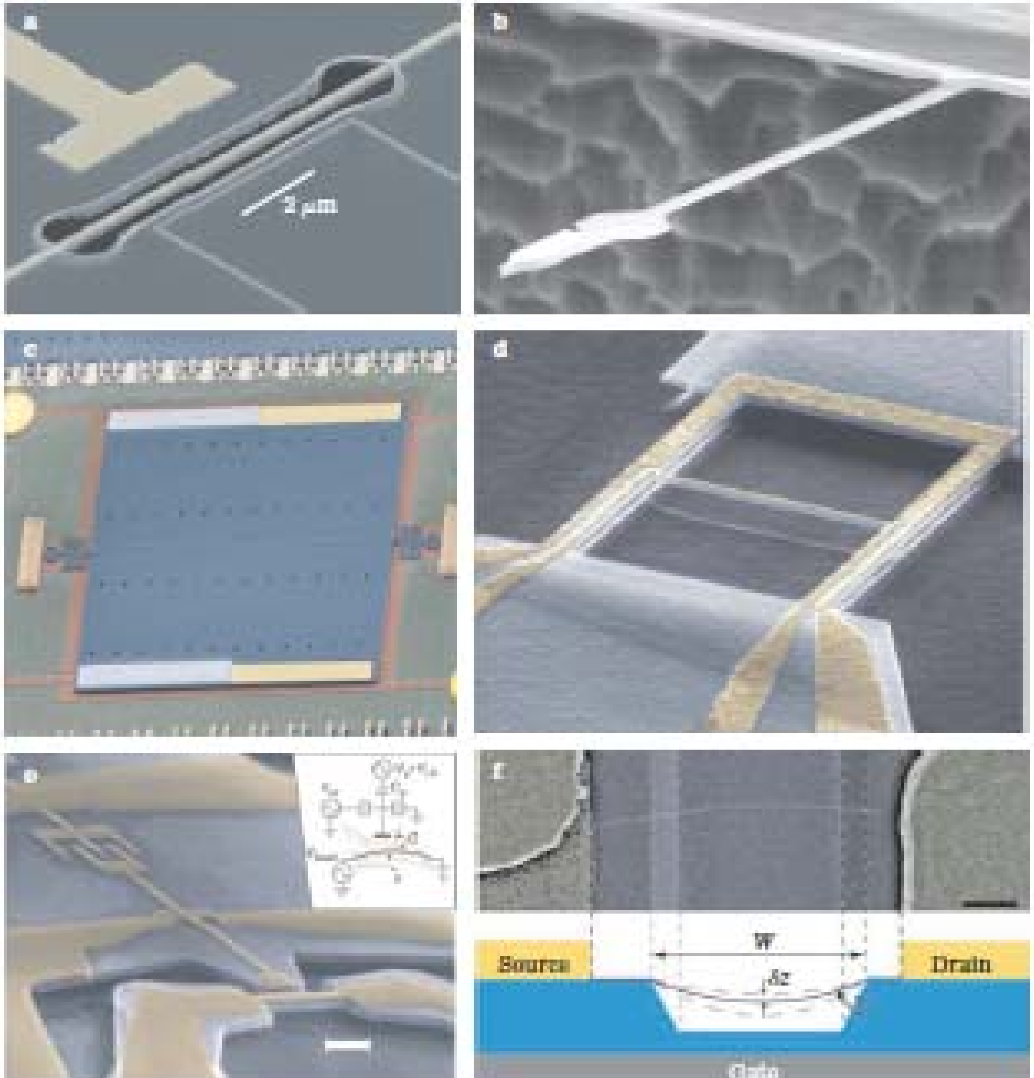


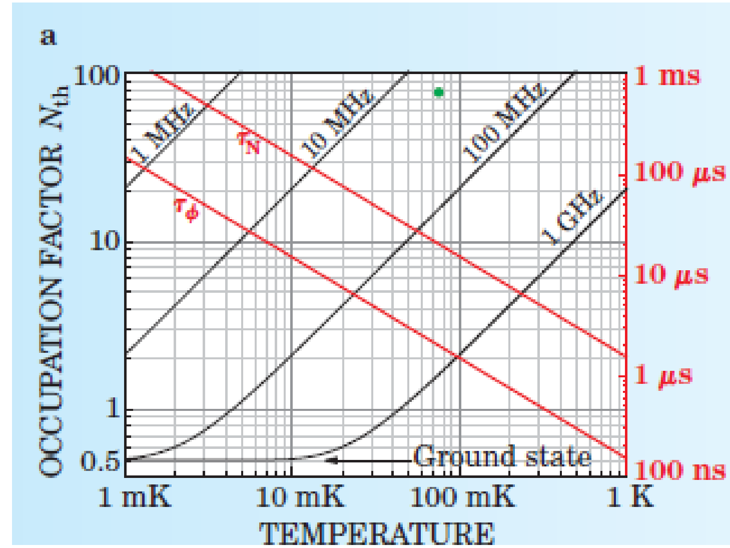
Memory Alloys Example



A nitinol wire reverts back to its original shape upon heating

Mechanical Nanoresonators





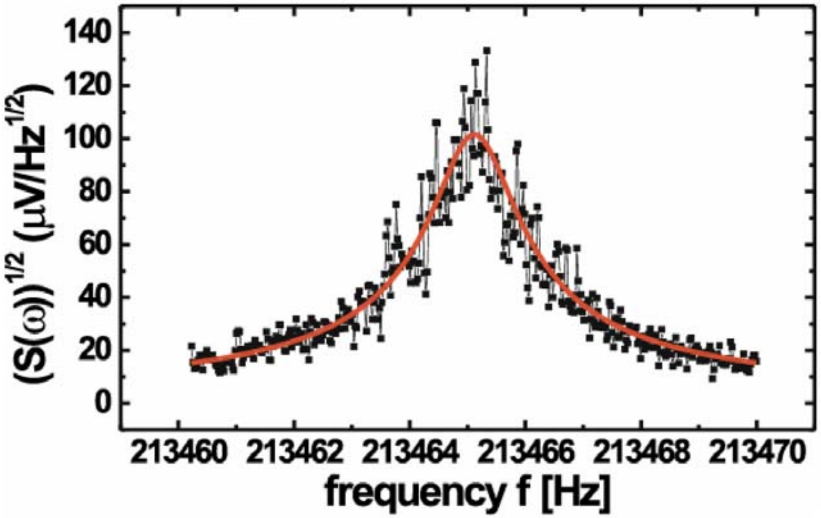
Putting Mechanics into Quantum Mechanics, Keith C. Schwab and Michael L. Roukes, Physics Today, 2005, 36-42)

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

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

Additional Reading

- **Callister, Chapter 7&8, in *Materials Science and Engineering***, 7th Edition, John Wiley, 2007
- NanoHUB resource: “Synthesis & Mechanics of Nanostructures & Nanocomposites” by Rod Ruoff
- Cleland and Roukes, “Noise processes in nanomechanical resonators”, JAP, 92(2002)2758