Dr. Gregory W. Clark
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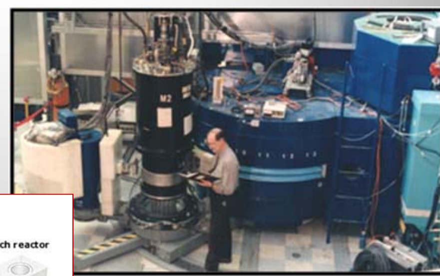
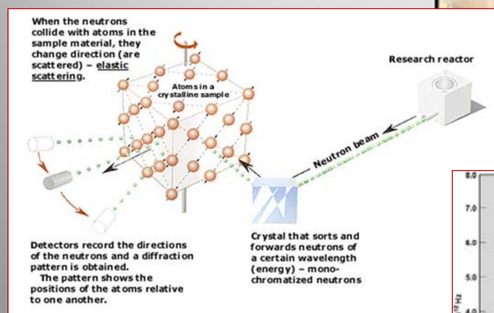
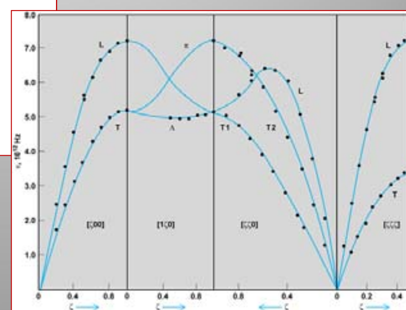




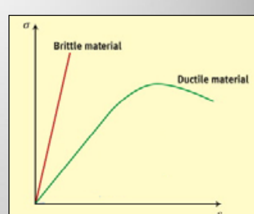


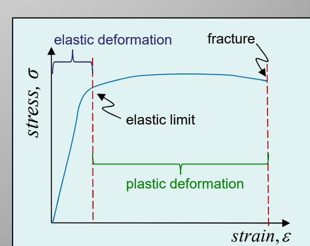
PHYS485
Materials Physics

Mechanical Properties

- Materials: Ductile vs. brittle

- Stress-strain for ductile material
  - Elastic regime: *Hooke's Law!*
  - Plastic regime: *deformation*
  - Fracture: *busted!*



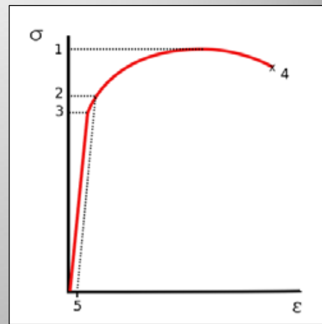


General relationship:

⟶ ***Stress = Strain x Modulus***

Mechanical Properties

- yield strength (yield stress, yield point, elastic limit) = stress at which material begins to deform plastically
- tensile strength (ultimate tensile stress, ultimate strength) = maximum stress material can handle
- compressive strengths not necessarily equal to tensile strengths
- brittle materials – no plastic deformation region; rupture occurs without elongation (*e.g.*, concrete, carbon fiber)
- ductile materials – beyond yield point, where linear elastic response ends

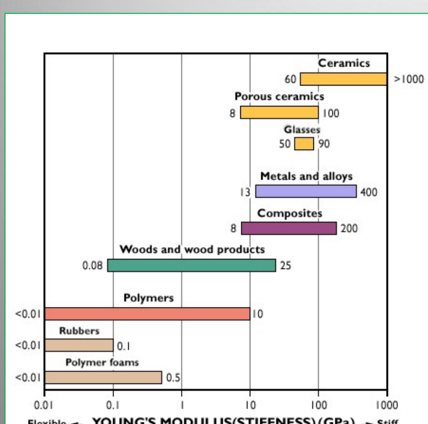


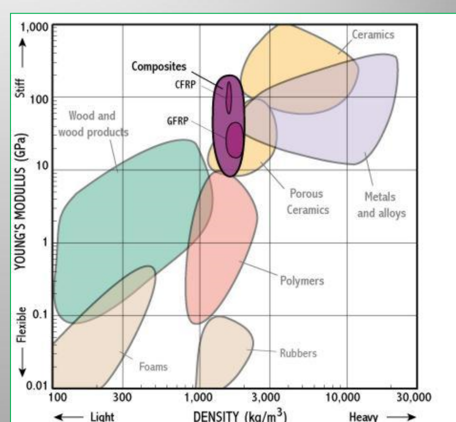
"engineering" stress-strain curve for Al

1. ultimate strength
2. yield strength
3. proportional limit stress
4. fracture
5. offset strain

Mechanical Properties

- The range of Young's modulus values





Source http://www-materials.eng.cam.ac.uk/mpsite/interactive_charts/stiffness-density/IEChart.html

Mechanical Properties

- Can show that …

$$G = \frac{Y}{2(1+\nu)}$$

$$K = \frac{Y}{3(1-2\nu)}$$

∴ can characterize **elastic regime** of a material with four quantities: ***Y*, *G*, *K*, and *α***

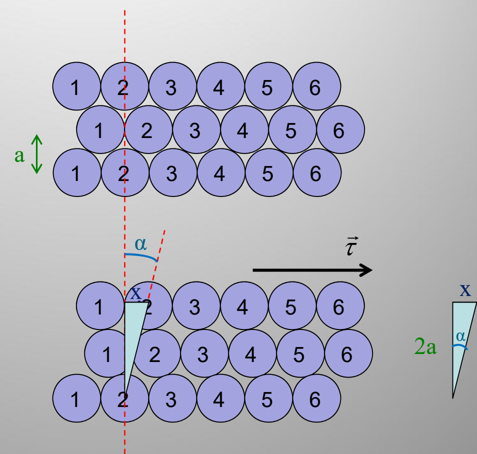
	B (GPa)	*G* (GPa)	*Y* (GPa)	ρ (kg/m^3)
Sc	27.2	17.0	42.1	1424
Ti	27.6	17.7	43.8	1491
V	27.7	19.1	46.5	1539
Cr	27.3	19.5	47.2	1565
Mn	27.3	20.2	48.6	1593
Fe	27.3	19.8	47.8	1607
Co	27.2	19.4	47.0	1627
Ni	27.8	19.9	48.2	1607
Cu	26.8	20.4	48.8	1936
Zn	26.7	20.3	48.7	1989
Na	23.3	15.0	37.0	1255
Al	27.4	20.7	49.7	1539
Si	27.7	20.9	50.1	1589
P	28.1	15.9	40.1	1462
S	27.1	12.7	32.9	1439
Cl	24.3	8.4	22.6	1384

Typical values of Young's modulus, *Y*, the modulus of rigidity, *G*, the bulk modulus, *K*, and Poisson's ratio, *v*, for a selection of solids.

	Y (10^9 N/m^2)	G (10^9 N/m^2)	K (10^9 N/m^2)	v
Diamond	950	390	540	0.21
Al	70	24	72	0.33
Cu	130	48	140	0.35
Fe	120	70	170	0.17
Pb	15	6	43	0.40
W	350	150	320	0.28
Brass	100	37	110	0.35
Glass	75	23	41	0.22
Steel	210	84	170	0.29

Mechanical Properties

- Shearing Stress
- Atoms in a close-packed plane
- Shearing stress, τ, applied parallel to surface

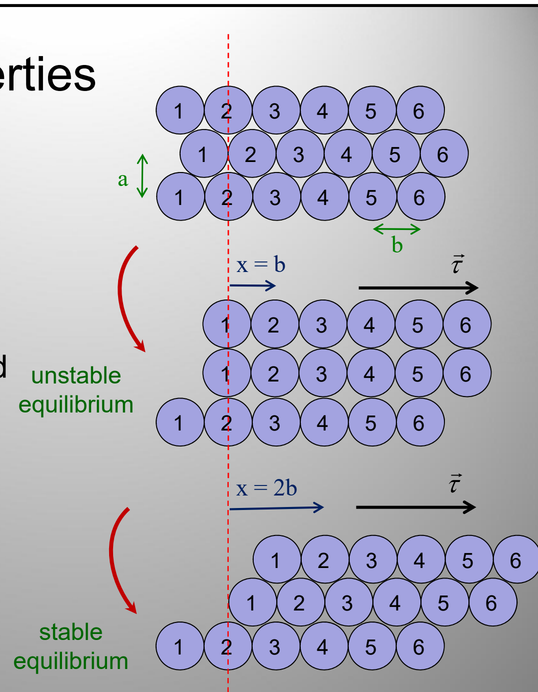


Mechanical Properties

- Elastic Limit (yield strength):

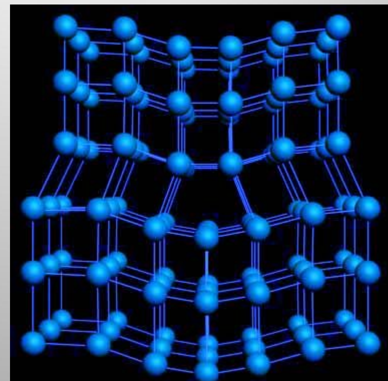
  a cheesy model!

- Atoms in a close-packed plane
- Shearing stress, τ, applied parallel to surface



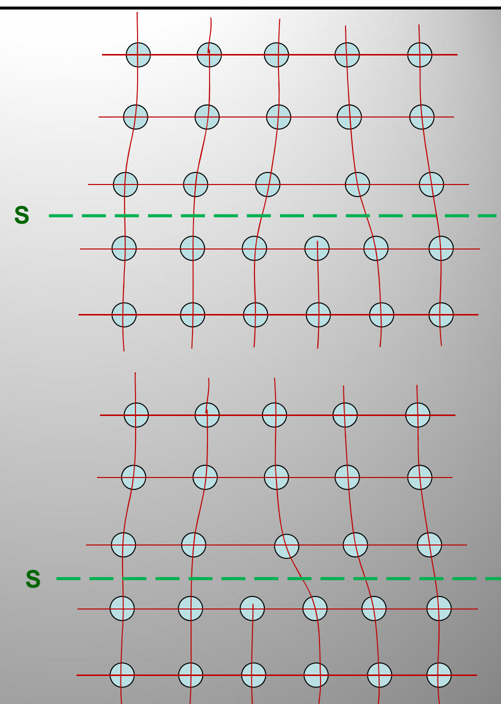
Mechanical Properties

- Role of dislocations
- Lower values of modulii



Mechanical Properties

- Microscopic scale: edge dislocation
- Propagates through material with applied shear stress
- small force required to move dislocation along **S**, the slip plane
- So, don't have to move entire plane above and below **S** to get deformation! Thus, yield stress is lowered.
- Helps explain *plastic deformation* regime



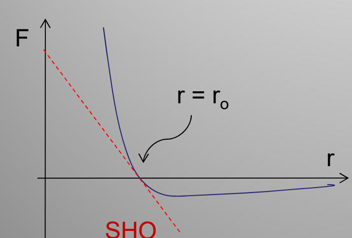
Modeling a Solid

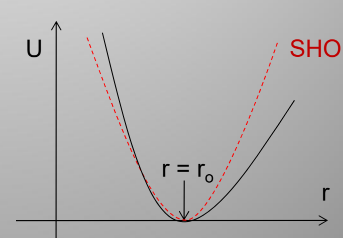
- There are many types of waves that can propagate through a lattice as elementary excitations
- We can model a solid in various ways, classically and quantum mechanically
- The lattice symmetry (periodicity) induces a symmetry (periodicity) in any wave propagating through the lattice.

Name	**Field**
Electron	--
Photon	Electromagnetic wave
Phonon	Elastic wave
Plasmon	Collective electron wave
Magnon	Magnetization wave
Polaron	Electron + elastic deformation
Exciton	Polarization wave

Modeling Interatomic Interactions

- Model interactions as harmonic, *i.e.,* governed by Hooke's law
- For example, $Na^{+}Cl^{-}$ pair … for small displacements from equilibrium, looks like a harmonic potential





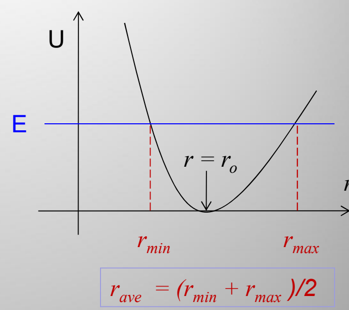
Modeling Interatomic Interactions: thermal expansion

- Asymmetry in potential energy curve can explain thermal expansion
- Thermal energy increases with temperature
- To a first approximation, the change in length ΔL measurement of an object is proportional to the temperature change ΔT by the coefficient of linear expansion:

$$\alpha_L = \frac{1}{L}\frac{dL}{dT}$$

$$\Rightarrow \frac{\Delta L}{L} = \alpha_L \Delta T$$

if α_L does not vary too much in the temperature range under consideration

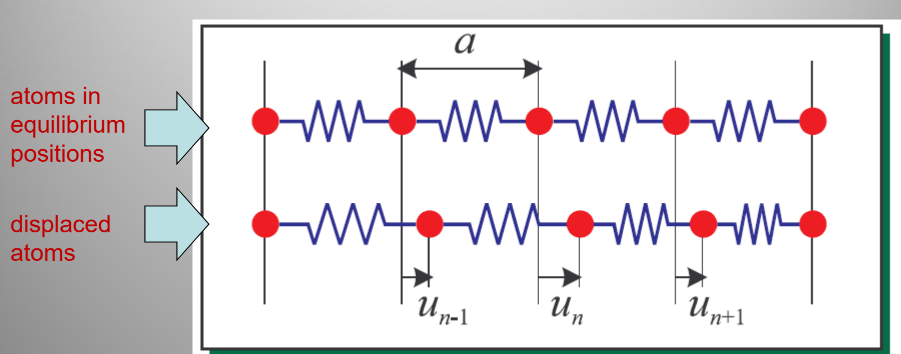


For *isotropic* materials, we can define the coefficient of volume expansion:

$$\alpha_V = \frac{1}{V}\frac{dV}{dT}, \quad \alpha_V = 3\alpha_L$$

Modeling Interatomic Interactions

- First Step: Monatomic lattice



Monatomic Lattice

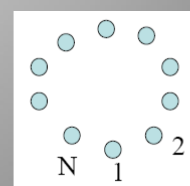
- Hooke's law: $x_n = n\,a = \text{equilibrium positions}$

$$F_n = -\alpha(2u_n - u_{n+1} - u_{n-1}) = \text{force on n}^{\text{th}} \text{ atom}$$

- Try harmonic solutions (longitudinal waves):

$$u_n = A\,e^{i k x_n - i\omega t}$$

- Boundary conditions = "Born von Karman" BC: assume ends of the chain are connected ("periodic BC") $u_{N+1} = u_1,\ u_0 = u_1$

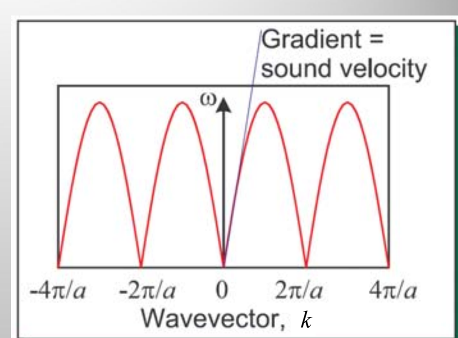


Monatomic Lattice

- Dispersion relation for acoustic phonons;

  relates ω to k:

$$\omega(k) = \sqrt{4\alpha / m}\,\left|\sin(k\,a/2)\right|$$



- Phase velocity

$$v = \omega / k$$

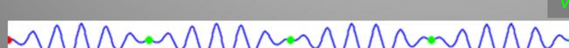
- Group velocity:

$$v_g = d\omega / dk$$

… or more generally:

$$\vec{v}_g = \vec{\nabla}_k \omega$$

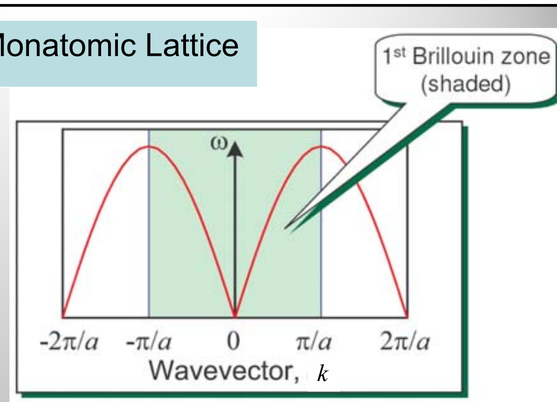
V_g = velocity at which energy travels



green = group, red = phase

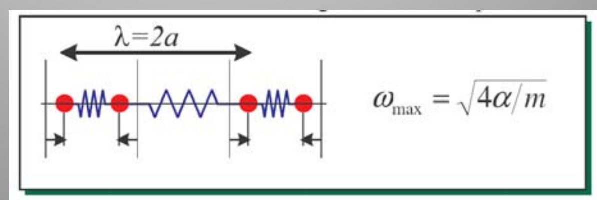
Monatomic Lattice

- There is redundancy by multiples of the reciprocal lattice vector



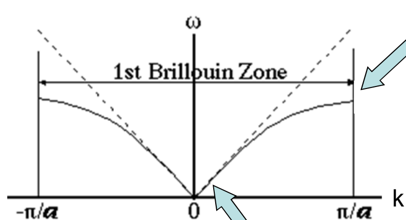
- Long wavelength limit: $v_g = v =$ indep of λ

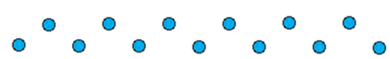
Stokes' models



Monatomic Lattice

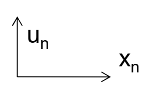
$$\omega = 2\sqrt{\frac{\alpha}{m}}\,|\sin(ka/2)|$$





$$\omega \approx 2\sqrt{\frac{\alpha}{m}}$$

Note: here pictures of transversal waves although calculation for the longitudinal case



$$\omega = \sqrt{\frac{\alpha}{m}}\,a\,k$$

Continuum limit of acoustic waves: $k = \frac{2\pi}{\lambda} \rightarrow 0$

$\sin ka/2 = ka/2 + \ldots$ ➡ $\omega = \sqrt{\frac{\alpha}{m}}\,a\,k$ ➡ $\boxed{\frac{\omega}{k} = v = \sqrt{\frac{\alpha}{m}}\,a}$

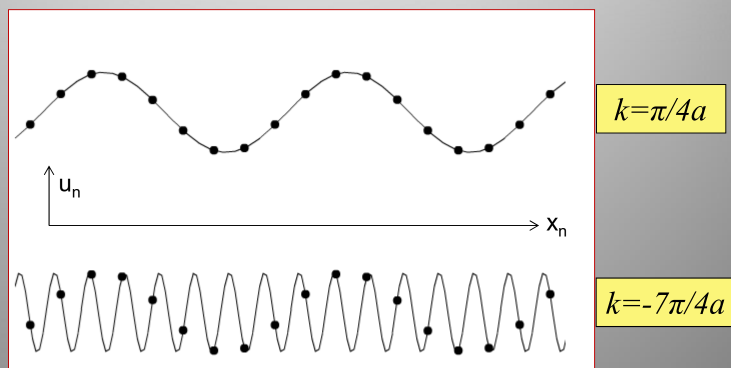
(large λ)

Monatomic Lattice

What if the wavevector is outside the first Brillouin zone?

We get the same atomic motions as if we were with in it!
But with different wavelengths.

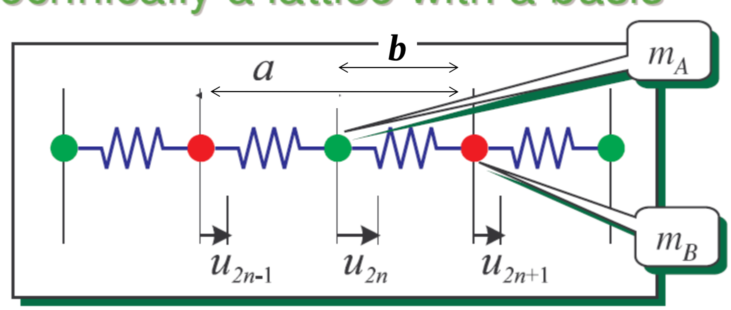
Stokes anim



Diatomic Lattice

- Now try two different masses connected by same strength "spring" bonds

Technically a lattice with a basis



Dispersion relation:

$$\omega^2 = \alpha\left(\frac{1}{m_A}+\frac{1}{m_B}\right) \pm \alpha\sqrt{\left(\frac{1}{m_A}+\frac{1}{m_B}\right)^2 - \frac{4\sin^2(ka/2)}{m_A m_B}}$$