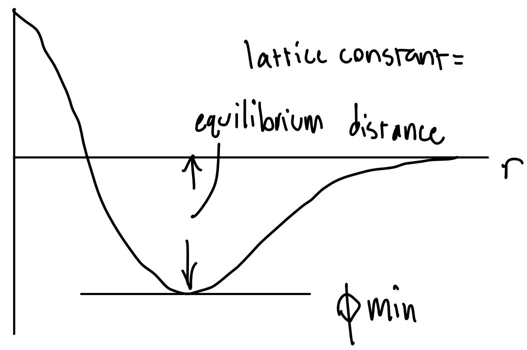
Phys 425
Lecture 6

Last time

General interatomic potential

$$\underset{\text{interatomic distance}}{\phi(r)} = \underbrace{\frac{A}{r^n}}_{\text{repulsive}} - \underbrace{\frac{B}{r^m}}_{\text{attractive}} \qquad n > m$$

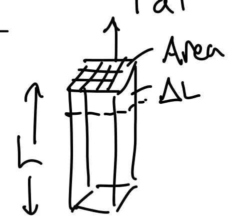


we'll focus on measurable macroscopic properties determined by this potential
↳ • mechanical properties
• thermal properties

Mechanical Properties

How does system respond to external forces?

Stress σ



Tensile stress

$$\sigma = \frac{F_{ext}}{A}$$

$$[\sigma] = Pa$$

Strain ϵ $\quad \epsilon = \frac{\Delta L}{L} \quad [\epsilon] = 1$

→ mechanical response to stress.

Simplest possible case:
stress and strain are linearly related.

Generalized Hooke's Law:

$$\vec{F}_{spring} = -k\Delta x$$

$$\sigma = YE$$

↳ Young's modulus

$$Y = \underbrace{\frac{F}{\Delta L}}_{\text{"k"}} \frac{L}{A}$$

Thermal Properties:

coefficient of thermal expansion: α

$$\underbrace{\frac{\Delta L}{L}}_{\text{thermal strain}} = \alpha \underbrace{\Delta T}_{\text{change in temp}}$$

We can guess that mechanical/thermal properties will be aggregates of interatomic bond strength

↳ Let's think back to $\phi(r)$

- expand $\phi(r)$ about equilibrium

$$\phi(r) = \underbrace{\phi(a)}_{1} + \underbrace{\phi'(a)(r-a)}_{2} + \underbrace{\frac{1}{2}\phi''(a)(r-a)^2}_{3} + \underbrace{\frac{1}{3!}\phi''' 6(r-a)^3}_{4}$$

① Just defines the location of our energy min

② $r = a$ is equilibrium pos. $\Rightarrow \phi'(a) = 0$

③ notice that we have quadratic potential

$$\text{"}U = \frac{1}{2}kx^2\text{"} \quad \nwarrow (r-a)^2$$

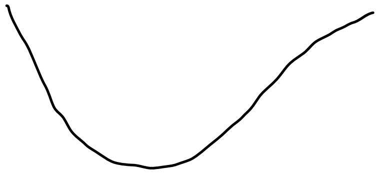
↳ $U(r) = \frac{1}{2}\gamma(r-a)^2$

where $\gamma = \left.\frac{d^2\phi}{dr^2}\right|_{r=a}$

this tells us the curvature of interatomic potential

$\Rightarrow$ elastic properties of solids

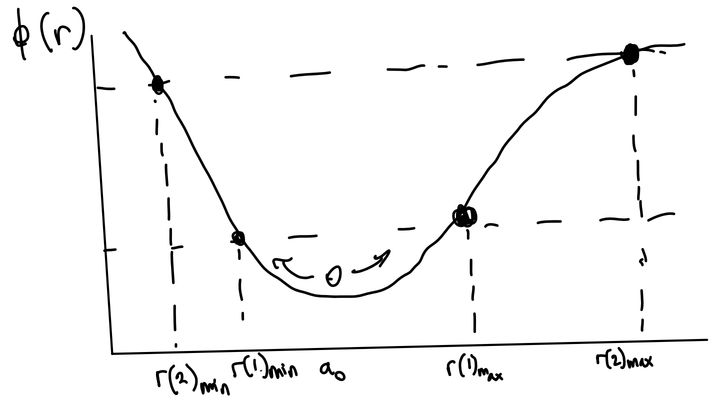
high γ



low γ

$$Y = \frac{\gamma}{a} = \frac{\phi''(a)}{a}$$

(4) This term tells us about anharmonicity of the potential.



↳ Due to the asymmetry of ϕ raising T changes the average bond length.

$$\alpha = \frac{1}{L}\frac{\Delta L}{\Delta T} \approx \frac{k_B \phi'''(a)}{2a(\phi''(a))^2}$$