Chapter #3:
Crystal Binding

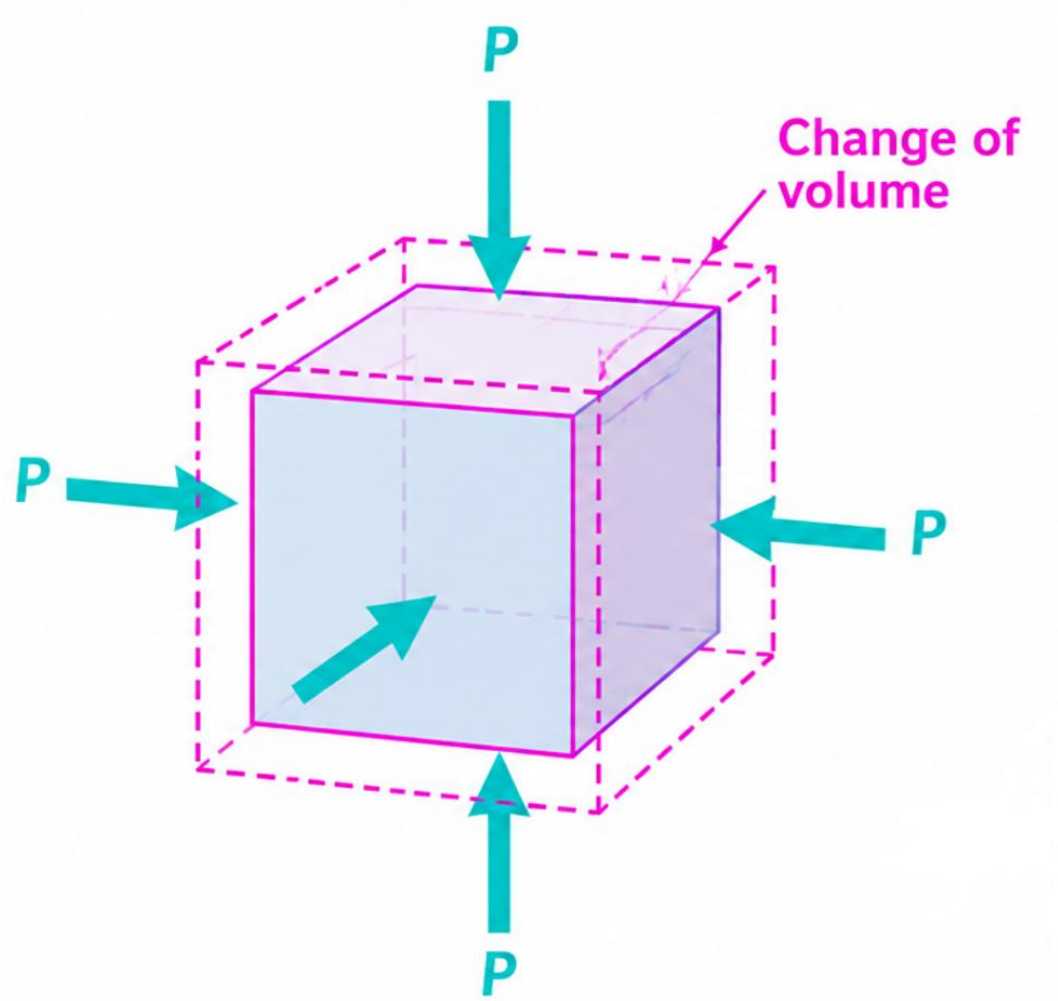
Lecture 4: Introduction to Elasticity, Stress, and Strain

1. What is elasticity?

Elasticity is the ability of a material to deform under an applied force and recover its original shape and size when the force is removed, provided the deformation remains within the elastic range. Deformation is a change in the shape or dimensions of a body. In elastic deformation, the change is reversible. If the applied stress is large enough to cause permanent deformation, the material has entered the plastic regime; that behavior is outside the main scope of this lecture.

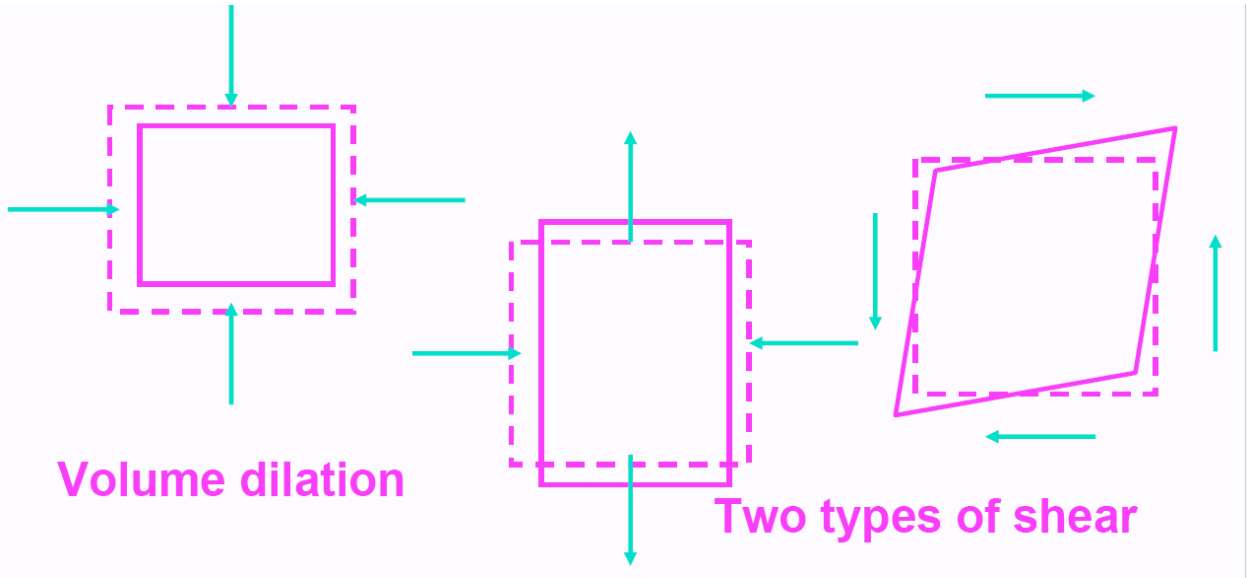
2. Solids and liquids: volume change versus shape change

Both solids and liquids can change volume when pressure is applied. A liquid is not perfectly incompressible; its volume generally changes, although often only slightly, under pressure.
The key distinction is the response to shear. A solid at rest can sustain a static shear stress and maintain a deformed shape. A liquid cannot sustain a static shear stress: under shear stress it flows and continually changes shape. Therefore, avoid saying that a liquid has no resistance to every force that leaves its volume unchanged; the more precise statement concerns static shear.



Two common types of deformation

Volume deformation (dilation or compression): the volume changes. For example, uniform external pressure compresses a crystal.
Shear deformation: the shape changes as layers or parts of the material move sideways relative to one another. For small shear, the angular distortion is small.



2. Strain and Stress

Strain is a change of relative positions of the parts of the material. It compares a change in length, angle, or volume with the original dimension. Unlike displacement, strain does not simply measure how far an object moves; **it measures how its shape or size changes.**

➢ Normal strain

For a small change in length, the normal strain along x is

$$\varepsilon_{xx} \approx \frac{\Delta L_x}{L_x}$$

It is positive for extension and negative for compression.

➢ Shear strain

Shear strain measures angular distortion. For small deformation in the xy plane, the tensorial shear strain is:

$$\varepsilon_{xy} = \frac{1}{2}\left(\frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y}\right)$$

➢ Volume strain (dilation)

For small deformation, the fractional change in volume is approximately the sum of the three normal strains:

$$\delta \equiv \frac{\Delta V}{V} \approx \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$$

A positive δ means expansion; a negative δ means compression. This approximation is for small strains.

Stress is a force per unit area (F/A) applied to the material to cause the strain.

- Normal stress acts perpendicular to a surface and tends to stretch or compress the material.
- Shear stress acts parallel to a surface and tends to slide adjacent parts relative to each other.

Stress is generally represented by the second-rank tensor σ_{ij}. The first index identifies the force direction; the second identifies the normal direction of the surface. In ordinary classical elasticity without couple stresses, $\sigma_{ij} = \sigma_{ji}$, so the stress tensor has six independent components.

Quantity	Meaning	Units
Stress, σ	Force transmitted per unit area; describes loading/internal force	Pa (N m^{-2})
Strain, ε	Relative change in length, angle, or volume; describes deformation	Dimensionless

➢ Young's Modulus:

Young's modulus, (Y), is a measure of a material's resistance to stretching or compression along a particular direction. It is defined as the ratio of normal stress to normal strain, provided the material is within its linear elastic regime.

According to Hooke's law, force and displacement and also stress and strain are linearly related:

Normal Stress (σ) = Young's modulus (Y) * Normal Strain (ε) (remember that: F=-kx)

$$Y = \frac{\sigma}{\varepsilon}$$

For more information regarding the elastic modulus, see the following page, video, and associated simulation:

https://dewesoft.com/blog/understanding-elastic-moduli

https://openstax.org/books/college-physics-ap-courses/pages/5-3-elasticity-stress-and-strain

3. Pressure and bulk modulus

Pressure is an isotropic normal stress: it acts equally in all directions in a fluid at rest. Positive pressure is conventionally compressive. In a crystal, a hydrostatic pressure applies equal compressive stress along all three axes.

Bulk modulus

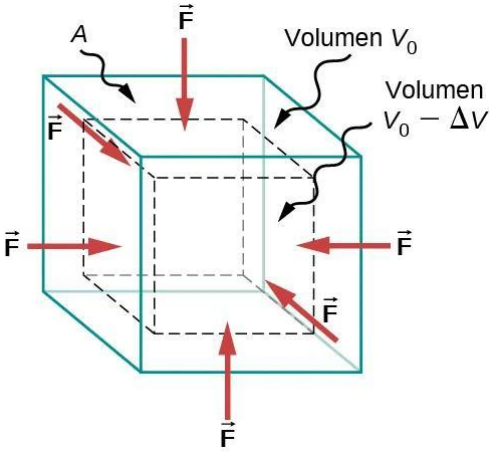
The bulk modulus B measures resistance to uniform compression. A large bulk modulus means that a relatively large pressure change is needed to produce a given fractional volume change. Basically,

$$\Delta P = -B\,\frac{\Delta V}{V_0}$$

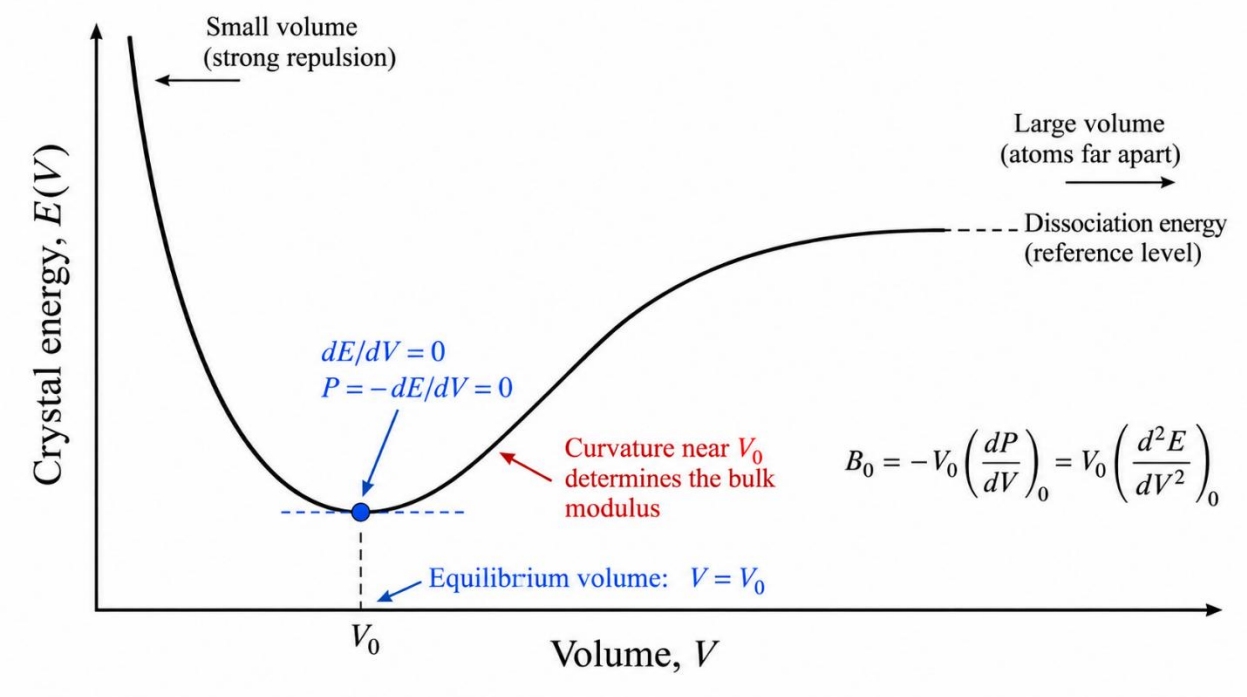
$$B = -V_0\left(\frac{dP}{dV}\right) = -\frac{dP}{d(\frac{\Delta V}{V_0})}$$

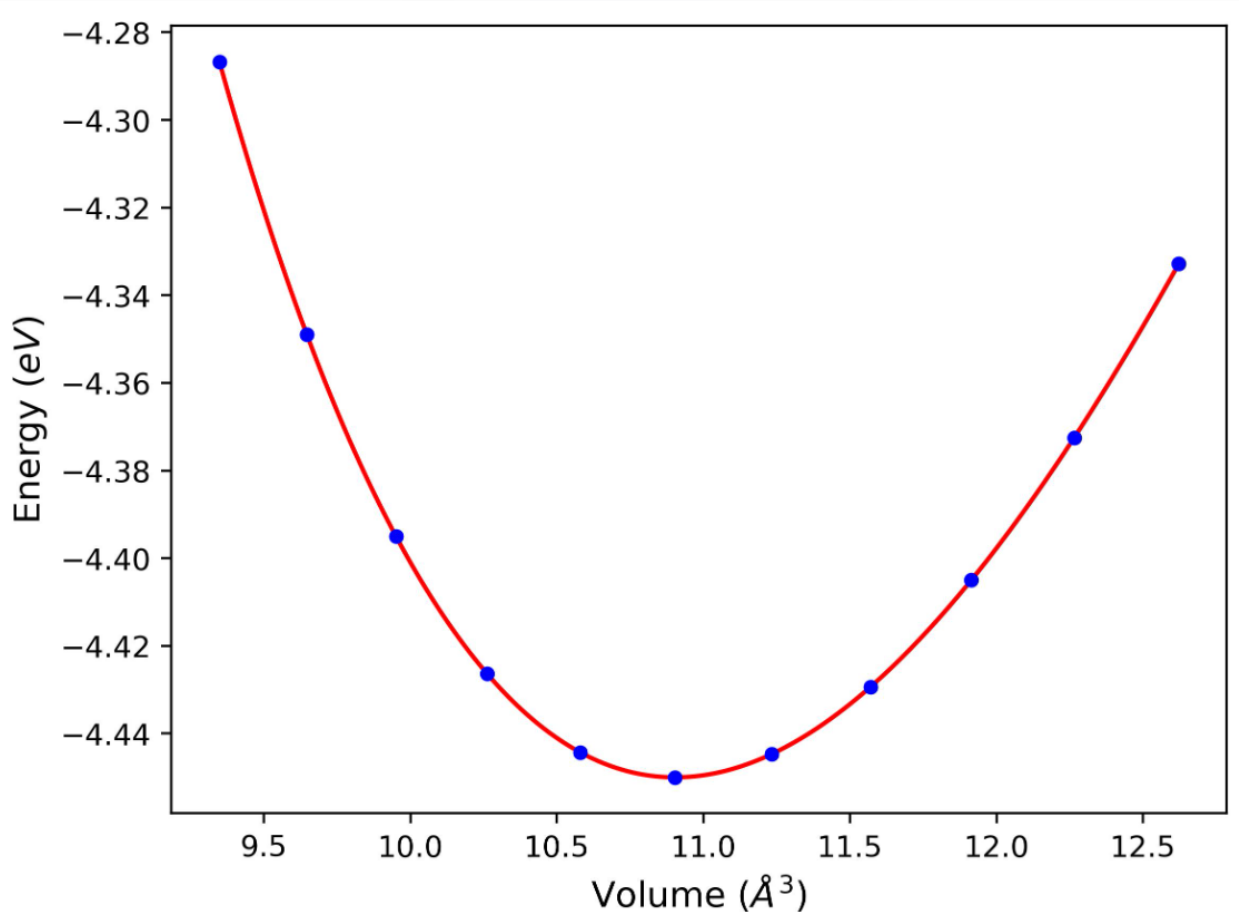
For small changes around equilibrium, B is often written as $B = -V_0(dP/dV)$. The negative sign ensures B is positive for a stable material: increasing pressure normally decreases volume.

In the figure, an inward force on all surfaces compresses this cube. Its change in volume is proportional to the force per unit area and its original volume, and is related to the compressibility of the substance.



6. Energy versus volume and equilibrium





The crystal's energy depends on its volume because changing the volume changes the interatomic separations and therefore the balance of attractive and repulsive interactions.

At zero external pressure, the equilibrium volume V_0 is a minimum of E(V).

At equilibrium: dE/dV = 0; stable minimum: $\frac{d^2E}{dV^2} > 0$

The curvature of the energy curve near the minimum indicates how strongly the energy rises when the volume is changed. **A sharper minimum corresponds to a larger bulk modulus.**

- For a system described by its energy E(V), pressure is P = −dE/dV, and at zero external pressure the equilibrium condition gives dE/dV = 0.
- At nonzero external pressure, equilibrium is found by minimizing the appropriate thermodynamic potential (at fixed temperature, commonly the enthalpy-like quantity $E + P_{ext} V$ at zero temperature), rather than E(V) alone.

At zero-pressure equilibrium: $B = V_0 (d^2E/dV^2)$

This relation assumes the energy description and derivatives are evaluated consistently. If using finite-temperature thermodynamics, specify the appropriate free energy and held-fixed variables.

Exercise: Lennard–Jones Potential in an FCC Crystal

For a face-centered cubic lattice of inert gas, such as Argon turned solid at low temperature, the potential energy is indicated by:

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Where the distance between the nearest neighbors is indicated by r = 3.6 Å, and the constants of the crystal are σ = 3.2 Å and ε = 0.95 kJ/mol.
(a) Find the equilibrium distance (r_0) for the lattice.
(b) Determine the minimum value of the potential energy ($V(r_0)$).
(c) Calculate the bulk modulus B in this case.
(d) Calculate the pressure of the system.

Solution: