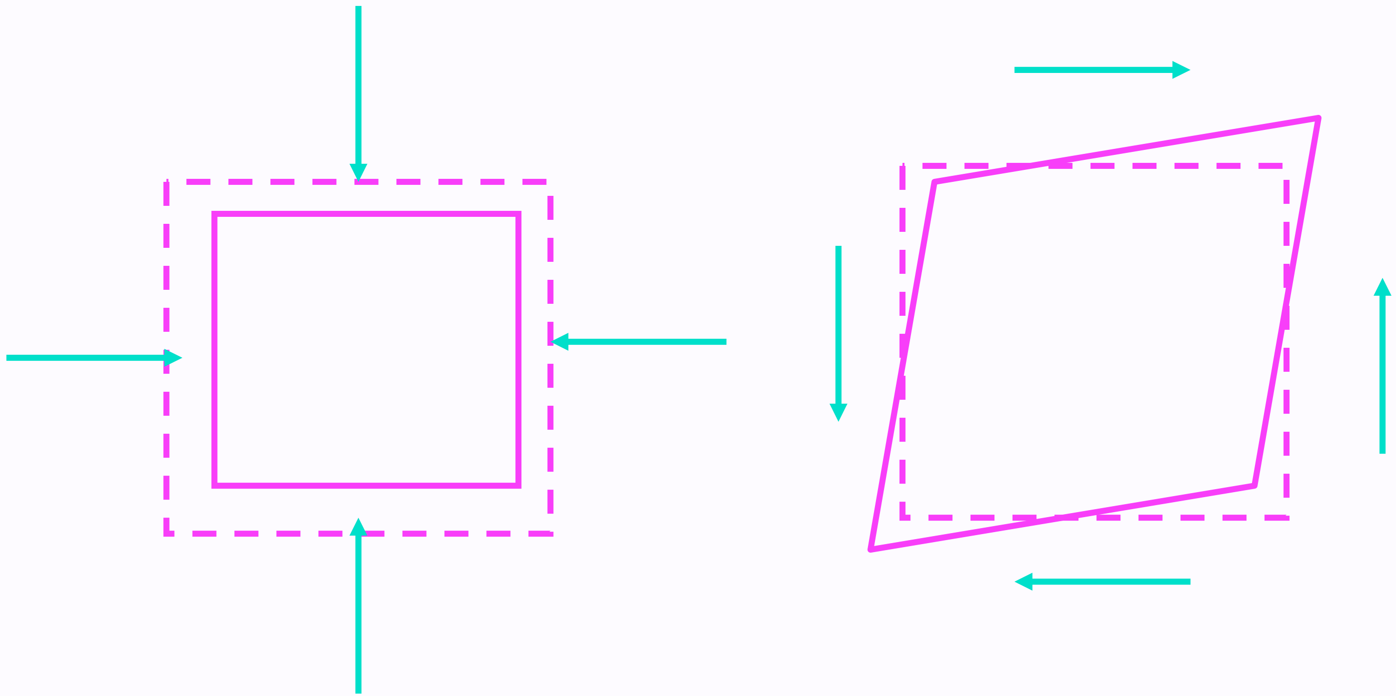
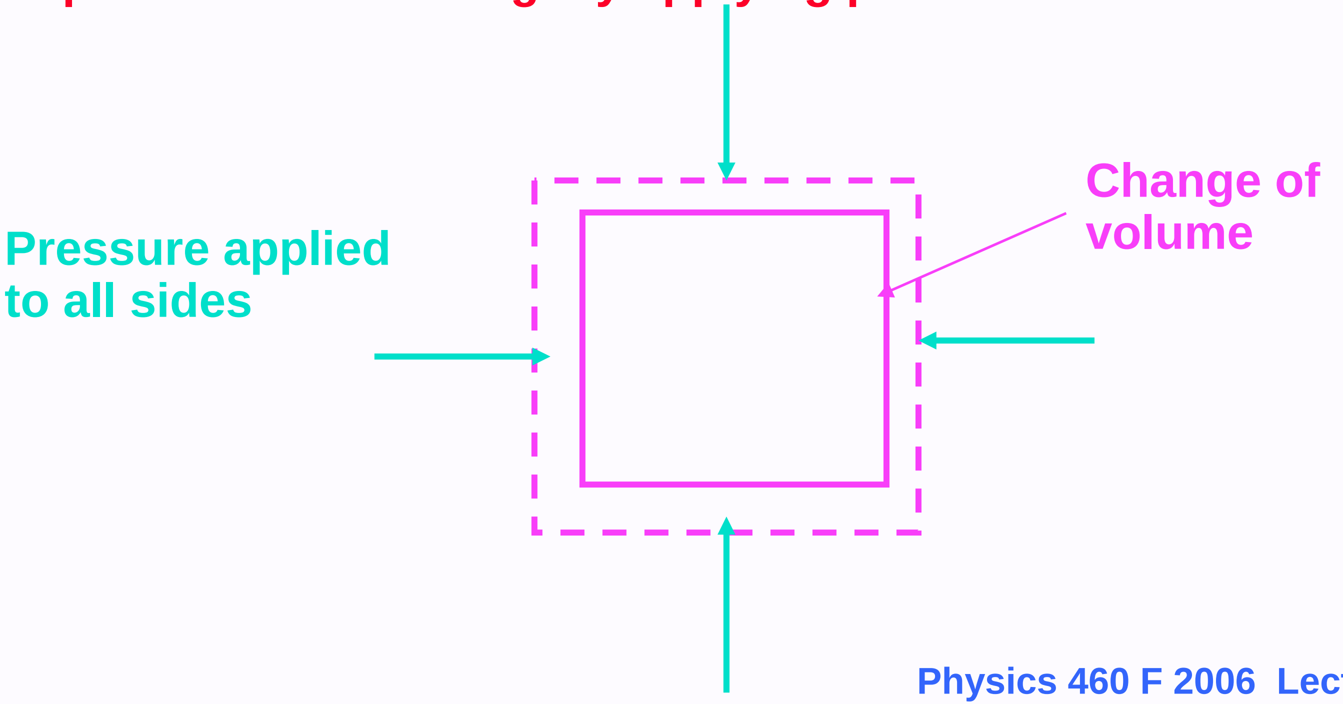
Elasticity
Stress and Strain in Crystals
Kittel – Ch 3



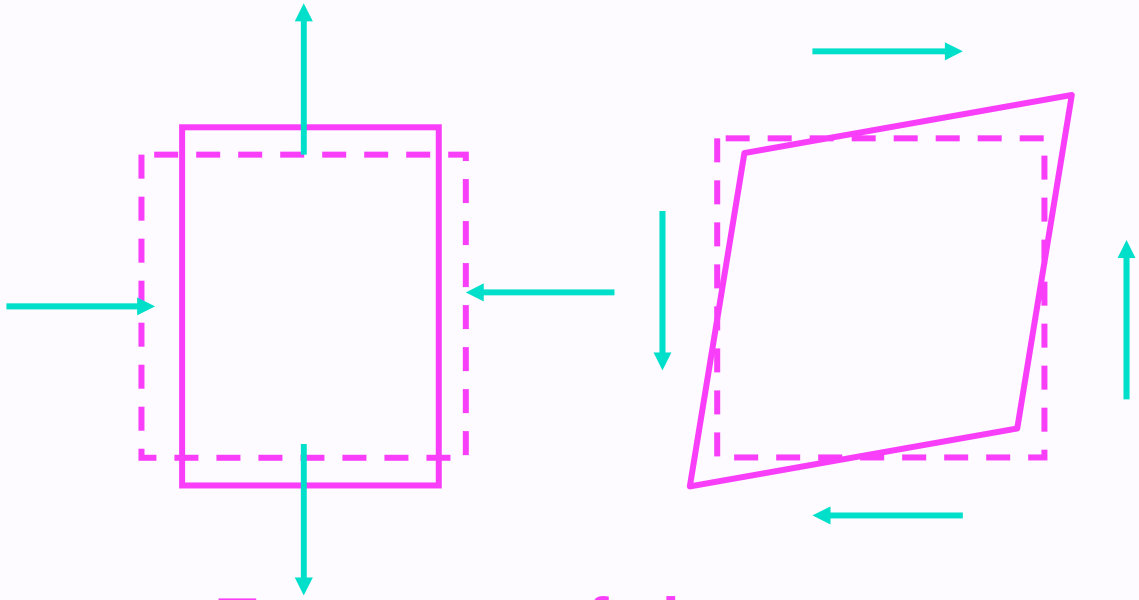
Elastic Behavior is the fundamental distinction between solids and liquids

- Similartity: both are “condensed matter”
- A solid or liquid in equilibrium has a definite density (mass per unit volume measured at a given temperature)
- The energy increases if the density (volume) is changed from the equilibrium value - e.g. by applying pressure



Elastic Behavior is the fundamental distinction between solids and liquids

- Difference:
- A solid maintains its shape
  - The energy increases if the shape is changed – “shear”
- A liquid has no preferred shape
  - It has no resistance to forces that do not change the volume

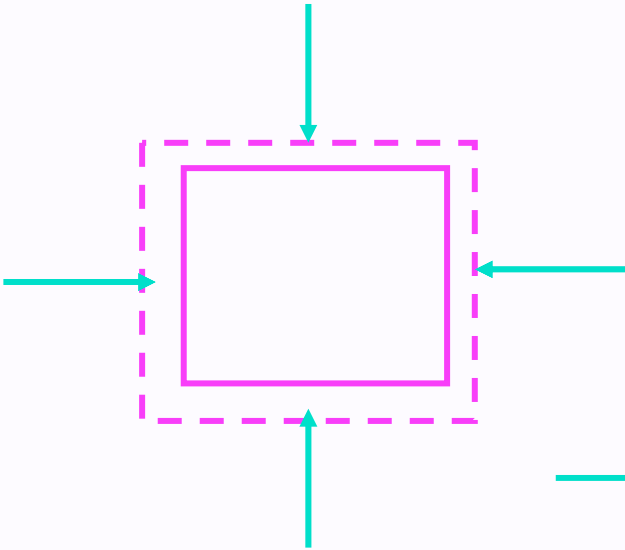


Two types of shear

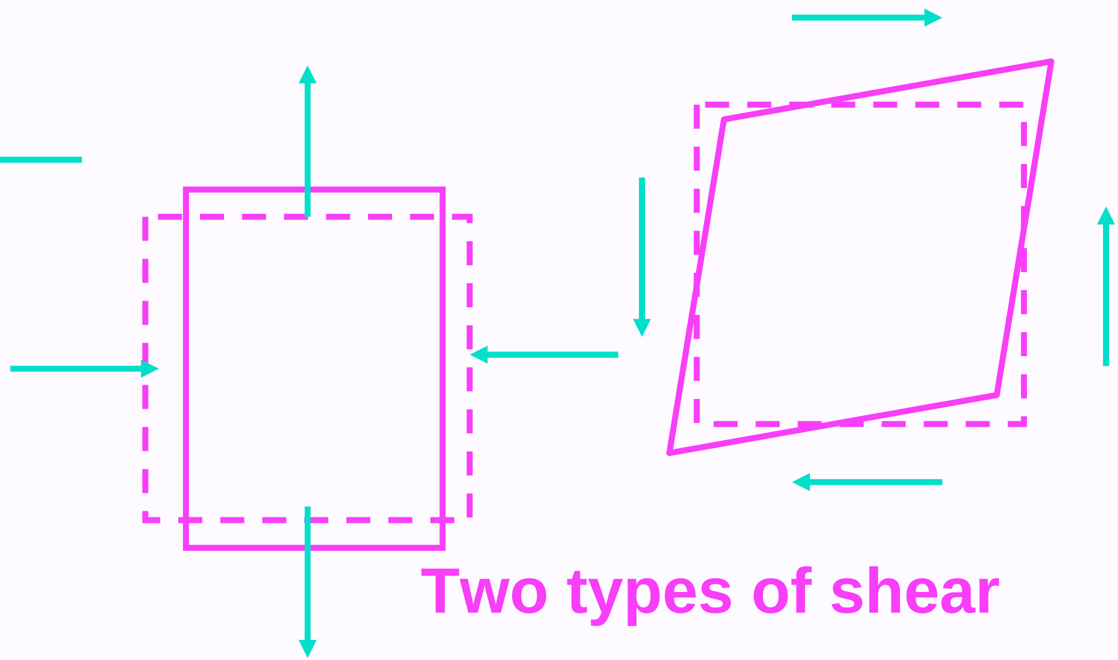
Strain and Stress

Strain is a change of relative positions of the parts of the material

Stress is a force /area applied to the material to cause the strain



Volume dilation



Two types of shear

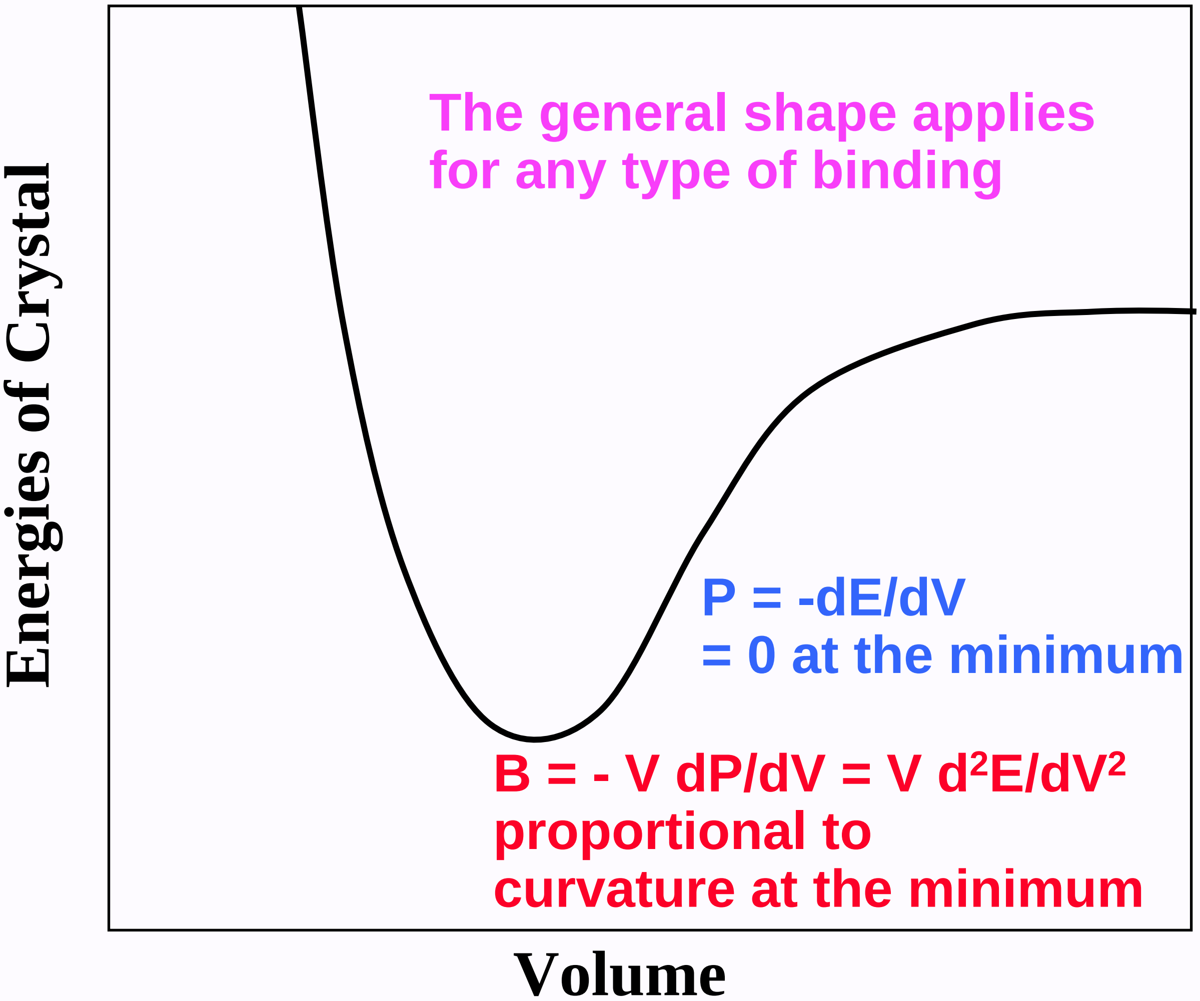
Pressure and Bulk Modulus

- **Consider first changes in the volume – applies to liquids and any crystal**
- **General approach:**
  E(V) where V is volume

  Can use ether $E_{crystal}(V_{crystal})$ or $E_{cell}(V_{cell})$ since $E_{crystal} = N\ E_{cell}$ and $V_{crystal} = N\ V_{cell}$

- **Pressure = $P = -\ dE/dV$ (units of Force/Area)**
- **Bulk modulus $B = -\ V\ dP/dV = V\ d^2E/dV^2$ (same units as pressure)**
- Compressibility $K = 1/B$

Total Energy of Crystal



Elasticity

- Up to now in the course we considered only perfect crystals with no external forces

- Elasticity describes:
  - Change in the volume and shape of the crystal when external stresses (force / area) are applied
  - Sound waves

- Some aspects of the elastic properties are determined by the symmetry of the crystal

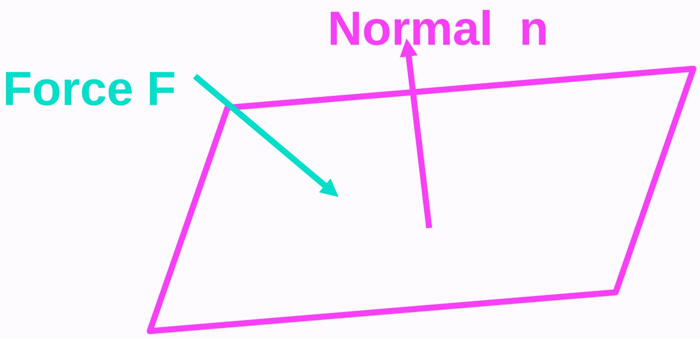
- Quantitative values are determined by strength and type of binding of the crystal?

Elastic Equations

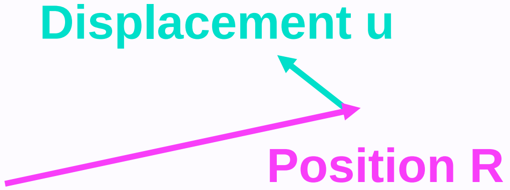
- The elastic equations describe the relation of stress and strain
- Linear relations for small stress/strain
  Stress = (elastic constants) x Strain
- Large elastic constants $\Rightarrow$ the material is stiff - a given strain requires a large applied stress
- We will give the general relations - but we will consider only cubic crystals
  - The same relations apply for isotropic materials like a glass
  - More discussion of general case in Kittel

Elastic relations in general crystals

- Strain and stress are tensors
- Stress e_{ij} is force per unit area on a surface
  - Force is a vector F_x, F_y, F_z
  - A surface is defined by the normal vector n_x, n_y, n_z
  - 3 x 3 = 9 quantities



- Strain σ_{ij} is displacement per unit distance in a particular direction
  - Displacement is a vector u_x, u_y, u_z
  - A position is a vector R_x, R_y, R_z
  - 3 x 3 = 9 quantities



Elastic Properties of Crystals

- **Definition of strain**

  Six independent variables:

  $e_1 \equiv e_{xx}$, $e_2 \equiv e_{yy}$, $e_3 \equiv e_{zz}$,
  $e_4 \equiv e_{yz}$, $e_5 \equiv e_{xz}$, $e_6 \equiv e_{xy}$

Using the relation
$e_{xy} = e_{yx}$ etc.

- **Stress**

  $\sigma_1 \equiv \sigma_{xx} = X_x$, $\sigma_2 \equiv Y_y$, $\sigma_3 \equiv Z_z$
  $\sigma_4 \equiv Y_z$, $\sigma_5 \equiv X_z$, $\sigma_6 \equiv X_y$

Here X_y denotes force in x direction applied to surface normal to y.

$\sigma_{xy} = \sigma_{yx}$ etc.

- **Linear relation of stress and strain**

  Elastic Constants C_{ij}

  $\sigma_i = \Sigma_j C_{ij} e_j$, (i,j = 1,6)

(Also compliances $S_{ij} = (C^{-1})_{ij}$)

Strain energy

- **For linear elastic behavior, the energy is quadratic in the strain (or stress)**
  Like Hooke's law for a spring

- Therefore, the energy is given by:

  $E = (1/2)\ \Sigma_i\ e_i\ \sigma_i\ = (1/2)\ \Sigma_{ij}\ e_i\ C_{ij}\ e_j$, (i,j = 1,6)

- Valid for all crystals

- Note 21 independent values in general
  (since $C_{ij} = C_{ji}$)

Symmetry Requirements Cubic Crystals

- **Simplification in cubic crystals due to symmetry** since x, y, and z are equivalent in cubic crystals

- For cubic crystals all the possible linear elastic information is in 3 quantities:
  $C_{11} = C_{11} = C_{22} = C_{33}$
  $C_{12} = C_{13} = C_{23}$
  $C_{44} = C_{55} = C_{66}$

- Note that by symmetry
  $C_{14} = 0$, etc
- Why is this true for cubic crystals?

Elasticity in Cubic Crystals

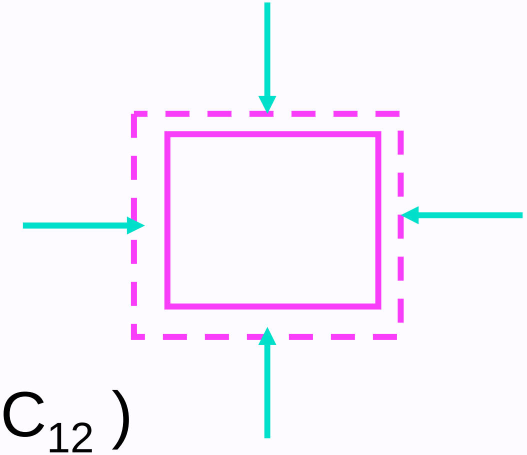
- **Elastic Constants** C_{ij} are completely specified by 3 values C_{11} , C_{12} , C_{44}

$$\sigma_1 = C_{11}\, e_1 + C_{12}\, (e_2 + e_3) \text{ , etc.}$$
$$\sigma_4 = C_{44}\, e_4 \text{ , etc.}$$

**Pure change in volume –
compress equally in x, y, z**

•For pure dilation $\delta = \Delta V / V$

$e_1 = e_2 = e_3 = \delta / 3$



•Define $\Delta E / V = 1/2\, B\, \delta^2$

•Bulk modulus $B = (1/3)\,(C_{11} + 2\, C_{12})$

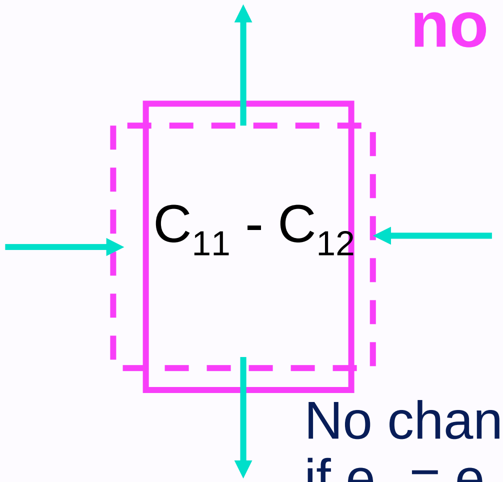
Elasticity in Cubic Crystals

- **Elastic Constants** C_{ij} are completely specified by 3 values C_{11} , C_{12} , C_{44}

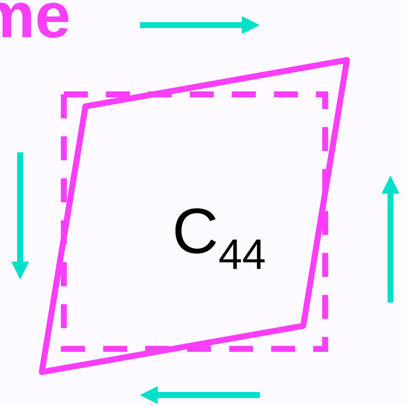
$$\sigma_1 = C_{11}\, e_1 + C_{12}\,(e_2 + e_3)\ , \text{etc.}$$

$$\sigma_4 = C_{44}\, e_4\ , \text{etc.}$$

Two types of shear –
no change in volume

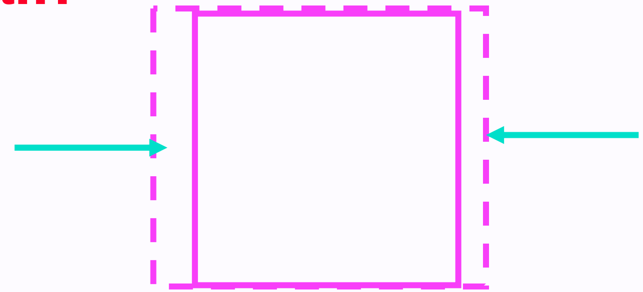


No change in volume
if $e_2 = e_3 = -\frac{1}{2}\, e_1$



Elasticity in Cubic Crystals

- **Pure uniaxial stress and strain**



- $\sigma_1 = C_{11} e_1$ with $e_2 = e_3 = 0$
- $\Delta E = (1/2)\, C_{11} (\delta x/x)^2$

- Occurs for waves where there is no motion in the y or z directions

  Also for a crystal under
  $\sigma_1 \equiv X_x$ stress
  if there are also stresses
  $\sigma_2 \equiv Y_y$, $\sigma_3 \equiv Z_z$ of just the right
  magnitude so that $e_2 = e_3 = 0$

Elastic Waves

- The general form of a displacement pattern is
  $\Delta\mathbf{\underline{r}}\,(\mathbf{\underline{r}}) = u(\mathbf{\underline{r}})\,\mathbf{\underline{x}} + v(\mathbf{\underline{r}})\,\mathbf{\underline{y}} + w(\mathbf{\underline{r}})\,\mathbf{\underline{z}}$

- A traveling wave is described by
  $\Delta\mathbf{\underline{r}}\,(\mathbf{\underline{r}},t) = \Delta\mathbf{\underline{r}}\,\exp(i\mathbf{\underline{k}}\cdot\mathbf{\underline{r}}\; - i\omega t)$

- For simplicity consider waves along the x direction in a cubic crystal

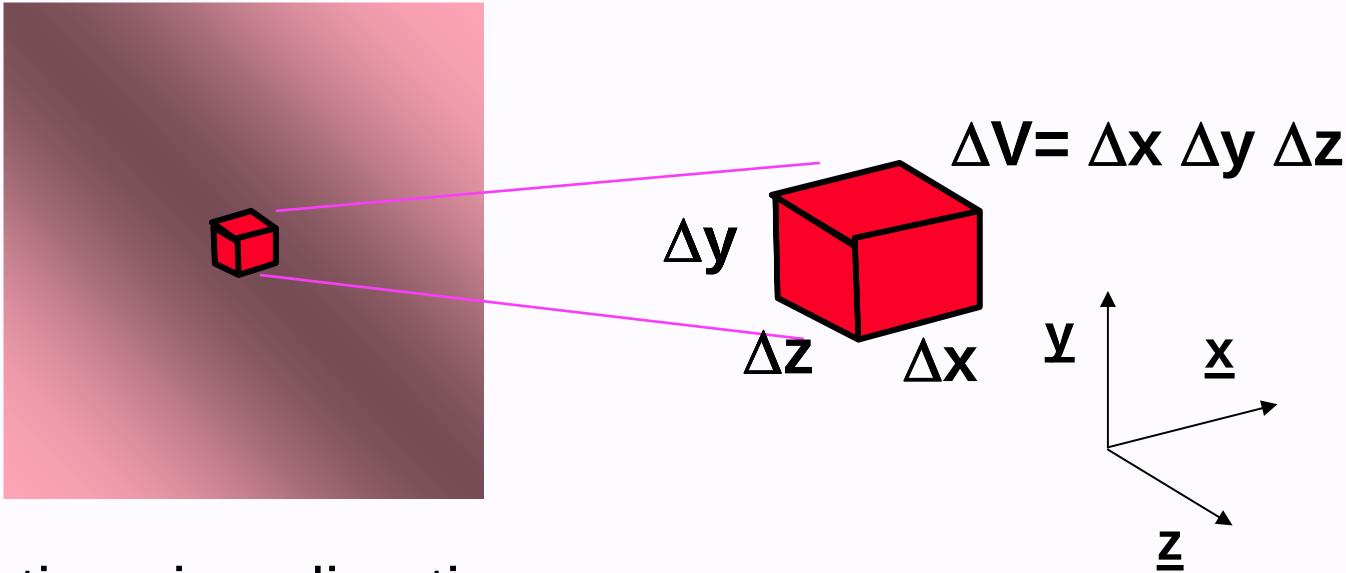
  Longitudinal waves (motion in x direction) are given by
  $u(x) = u\,\exp(ikx - i\omega t)$

  Transverse waves (motion in y direction) are given by
  $v(x) = v\,\exp(ikx - i\omega t)$

Waves in Cubic Crystals

- Propagation follows from Newton's Eq. on each volume element
- Longitudinal waves:
  $\rho \, \Delta V \, d^2 u / dt^2 = \Delta x \, dX_x / dx = \Delta x \, C_{11} \, d^2 u / dx^2$
  (note that strain is $e_1 = d u / dx$)
- Since $\Delta V / \Delta x$ = area and ρ area = mass/length = ρ_L, this leads to
  $\rho_L \, u / dt^2 = C_{11} \, du/ dx$
  or
  $\omega^2 = (C_{11} / \rho_L) \, k^2$
- Transverse waves (motion in the y direction) are given by
  $\omega^2 = (C_{44} / \rho_L) \, k^2$

Elastic Waves



- Variations in x direction
- Newton's Eq: ma = F
- Longitudinal: displacement u along x,

  $$\rho \, \Delta V \, d^2 u / dt^2 = \underbrace{\Delta x \, dX_x / dx} = \Delta x \, C_{11} \, d^2 u / dx^2$$

  Net force in x direction

- Transverse: displacement v along y,

  $$\rho \, \Delta V \, d^2 v / dt^2 = \underbrace{\Delta x \, dY_x / dx} = \Delta x \, C_{44} \, d^2 v / dx^2$$

  Net force in y direction

Sound velocities

- The relations before give (valid for any elastic wave):

$\omega^2 = (C / \rho_L)\, k^2$ or $\omega = s\, k$

- where s = sound velocity

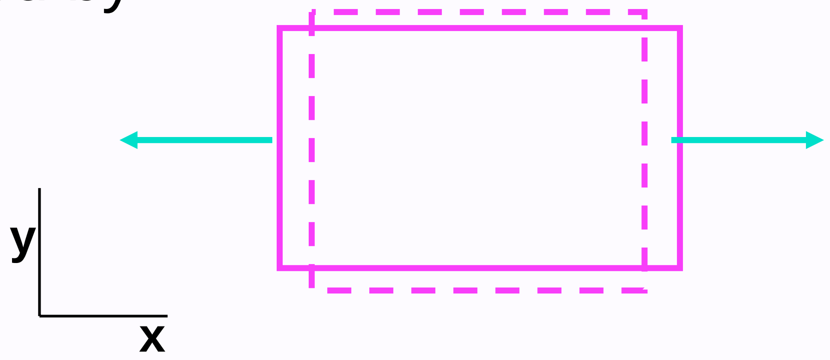
- Different for longitudinal and transverse waves
- Longitudinal sound waves can happen in a liquid, gas, or solid
- Transverse sound waves exist only in solids

- More in next chapter on waves

Young's Modulus & Poisson Ratio

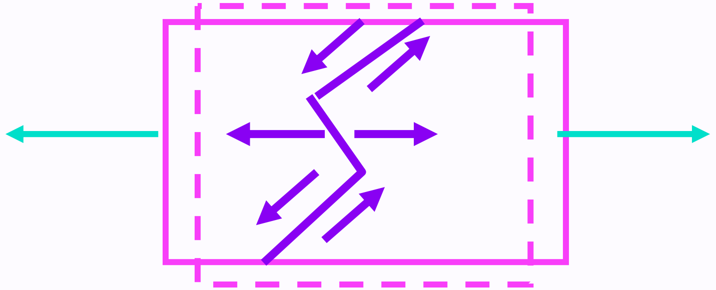
- Consider crystal under tension (or compression) in x direction
- If there are no stresses $\sigma_2 \equiv Y_y$, $\sigma_3 \equiv Z_z$ then the crystal will also strain in the y and z directions

- Poisson ratio defined by (dy/y) / (dx/x)
- Young's modulus defined by
  Y = tension/ (dx/x)
  Homework problem
  to work this out
  for a cubic crystal



When does a crystal break?

- Consider crystal under tension (or compression) in x direction
- For large strains, when does it break?
- Crystal planes break apart – or slip relative to one another
- Governed by “dislocations”
- See Kittel – Chapter 20



Next Time

- **Vibrations of atoms in crystals**
- **Normal modes of harmonic crystal**
- **Role of Brillouin Zone**
- **Quantization and Phonons**
- **Read Kittel Ch 4**