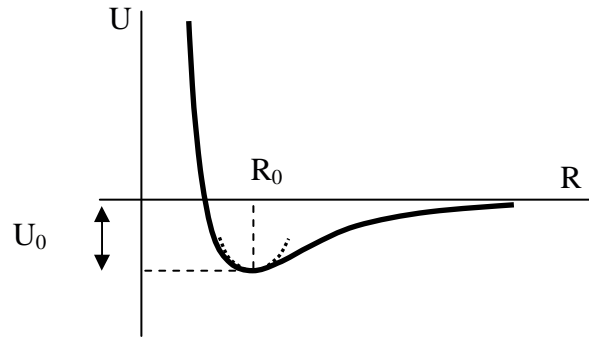


Section 4: Elastic Properties

Elastic constants

Elastic properties of solids are determined by interatomic forces acting on atoms when they are displaced from the equilibrium positions. At small deformations these forces are proportional to the displacements of atoms. As an example, consider a 1D solid. A typical binding curve has a minimum at the equilibrium interatomic distance R_0 :



Expanding the energy at the minimum in the Taylor series we find:

$$U(R) = U_0 + \left. \frac{\partial U}{\partial R} \right|_{R_0} (R - R_0) + \left. \frac{\partial^2 U}{\partial R^2} \right|_{R_0} (R - R_0)^2 + \dots \quad (4.1)$$

At equilibrium $\left. \frac{\partial U}{\partial R} \right|_{R_0} = 0$, so that

$$U(R) = U_0 + \frac{1}{2} k u^2, \quad (4.2)$$

where we defined $\frac{1}{2} k = \left. \frac{\partial^2 U}{\partial R^2} \right|_{R_0}$ and $u = R - R_0$ is the displacement of an atom from equilibrium

position R_0 . Differentiating Eq.(4.2), $F = -\frac{\partial U}{\partial R}$, we obtain force F acting on an atom :

$$F = -k u. \quad (4.3)$$

The constant k is an interatomic force constant. Eq.(4.3) represents the simplest expression for the *Hooke's law* showing that the force acting on an atom, F , is proportional to the displacement u . This law is valid only for small displacements and characterizes a *linear region* in which the restoring force is linear with respect to the displacement of atoms.

The elastic properties are described by considering a crystal as a homogeneous continuum medium rather than a periodic array of atoms. In a general case the problem is formulated as follows:

- (i) Apply forces, which are described in terms of *stress* σ , and determine displacements of atoms which are described in terms of *strain* ε .
- (ii) Define elastic constants C relating stress σ and strain ε , so that $\sigma = C\varepsilon$.

Example: In 1D case, $F = -ku$, where u is a change in the crystal length under applied force F . We can therefore write

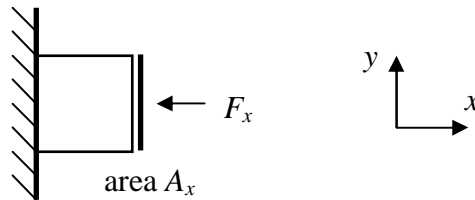
$$\sigma = \frac{F}{A} = \left(\frac{-kL}{A} \right) \left(\frac{u}{L} \right) = C\varepsilon, \quad (4.4)$$

where A is the area of the cross section, and L is the equilibrium length of the 1D crystal. The stress σ is defined as the force per unit area and the strain ε is the dimensionless constant which describes the relative displacement (deformation).

In a general case of a 3D crystal the stress and the strain are tensors which are defined as follows.

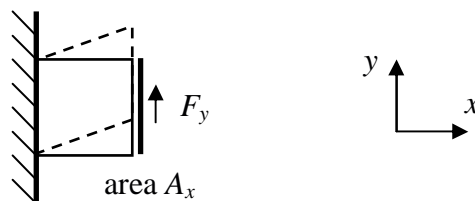
Stress has the meaning of local applied “pressure”. It has components σ_{ij} , showing that the force can be applied along 3 directions “ i ” and 3 faces “ j ”. The stress is defined locally, so that $\sigma_{ij} = \sigma_{ij}(\mathbf{r})$.

Compression stress (σ_{xx} σ_{yy} σ_{zz}):

$$\sigma_{xx} = \frac{F_x}{A_x},$$


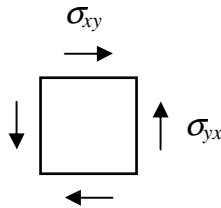
$$(4.5)$$

Shear stress (σ_{xy} σ_{yx} σ_{xz} σ_{zx} σ_{yz} σ_{zy}):

$$\sigma_{yx} = \frac{F_y}{A_x},$$


$$(4.6)$$

Shear forces must come in pairs to conserve angular acceleration inside the crystal:



That makes the stress tensor diagonal, i.e.

$$\sigma_{ij} = \sigma_{ji}. \quad (4.7)$$

Strain determines relative atomic displacement:

$$\varepsilon_{ij}(\mathbf{r}) = \frac{du_i}{dx_j}, \quad (4.8)$$

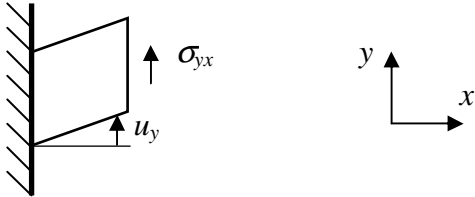
where u_i is displacement in “ i ” direction and x_j is the direction along which u_i may vary.

Compression strain (ϵ_{xx} ϵ_{yy} ϵ_{zz}):

$$\epsilon_{xx} = \frac{du_x}{dx}, \quad (4.9)$$

In a homogeneous crystal ϵ_{xx} is a constant $\epsilon_{xx} = \frac{u}{L}$, where u is the change in the crystal length L .

Shear strain (ϵ_{xy} ϵ_{yx} ϵ_{xz} ϵ_{zx} ϵ_{yz} ϵ_{zy}):

$$\epsilon_{yx} = \frac{du_y}{dx}, \quad (4.10)$$


Since σ_{ij} and σ_{ji} must always be applied together, we can define shear strains symmetrically:

$$\epsilon_{ij} = \epsilon_{ji} = \frac{1}{2} \left(\frac{du_i}{dx_j} + \frac{du_j}{dx_i} \right). \quad (4.11)$$

Elastic constants C relate the strain and the stress in a linear fashion:

$$\sigma_{ij} = \sum_{kl} C_{ijkl} \epsilon_{kl}. \quad (4.12)$$

Eq.(4.12) is a general form of the Hooke's law. The matrix C in a most general form has $3 \times 3 \times 3 \times 3 = 81$ components. However, due to the symmetrical form of σ_{ij} and ϵ_{ij} - each of them have 6 independent components, we need only 36 elastic constants. There is a convention to denote these constants by C_{mn} , where indices m and n are defined as 1= xx , 2= yy , 3= zz for the compression components and as 4= yz , 5= zx , 6= xy for the shear components. For example, $C_{11} = C_{xxxx}$, $C_{12} = C_{xxyy}$, $C_{44} = C_{zyyz}$.

Therefore, the general form of the Hooke's law is given by

$$\begin{array}{c} \left(\begin{array}{c} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{array} \right) = \begin{array}{cc} \begin{array}{ccc} \text{compression} & & \text{mixed} \\ \left(\begin{array}{ccc|ccc} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ \hline C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{array} \right) & \begin{array}{c} \left(\begin{array}{c} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{yz} \\ \epsilon_{zx} \\ \epsilon_{xy} \end{array} \right) \\ \text{compression} \\ \text{shear} \end{array} \end{array} \end{array} \quad (4.13)$$

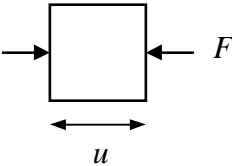
stress mixed shear strain

All 36 elastic constants are independent. However in crystals many of them are the same due to symmetry. In particular, in cubic crystals $C_{11} = C_{22} = C_{33}$, $C_{12} = C_{21} = C_{23} = C_{32} = C_{13} = C_{31}$, $C_{44} = C_{55} = C_{66}$ due the fact that x , y , and z axes are identical by symmetry. Also the off diagonal shear components are zero, i.e. $C_{45} = C_{54} = C_{56} = C_{65} = C_{46} = C_{64} = 0$, and mixed compression/shear coupling does not occur, i.e. $C_{14} = C_{41} = \dots = 0$. Therefore, the cubic elasticity matrix has the form

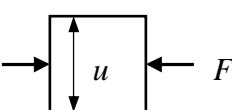
$$\begin{pmatrix} C_{11} & C_{12} & C_{12} & & & \\ C_{12} & C_{11} & C_{12} & & & \\ C_{12} & C_{12} & C_{11} & & & \\ & & & C_{44} & 0 & 0 \\ & & & 0 & C_{44} & 0 \\ & & & 0 & 0 & C_{44} \end{pmatrix}. \quad (4.14)$$

We have only 3 independent constants.

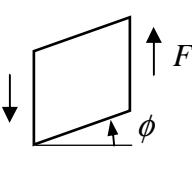
Longitudinal compression (Young's modulus):

$$C_{11} = \frac{\sigma_{xx}}{\epsilon_{xx}} = \frac{F/A}{u/L} \quad (4.15)$$


Transverse expansion:

$$C_{12} = \frac{\sigma_{xx}}{\epsilon_{yy}} \quad (4.16)$$


Shear modulus:

$$C_{44} = \frac{\sigma_{xy}}{\epsilon_{xy}} = \frac{F/A}{\phi} \quad (4.17)$$


Elastic waves

So far, we have assumed that atoms were at rest at their lattice sites. Atoms, however, are not quite stationary, but can oscillate around their equilibrium positions (e.g., as a result of thermal energy). This leads to lattice vibrations.

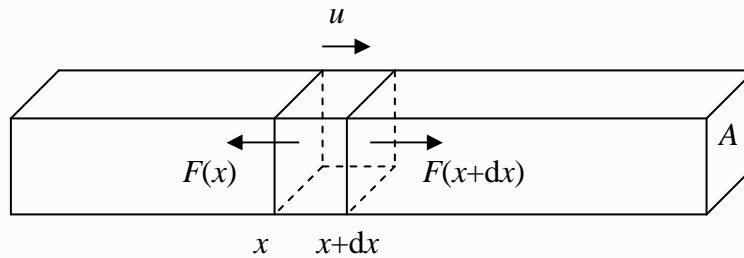
When considering lattice vibrations three major approximations are made:

- (i) It is assumed that displacements of atoms are small, i.e. $u \ll a$, where a is a lattice parameter.
- (ii) Forces acting on atoms are assumed to be *harmonic*, i.e. proportional to the displacements: $F = -Cu$. This is the same approximation which is used to describe a harmonic oscillator.
- (iii) It is assumed that the adiabatic approximation is valid – electrons follow atoms, so that the nature of bond is not affected by vibrations.

The discreteness of the lattice must be taken into account in the discussion of lattice vibrations. However, when the wavelength is very long, i.e. $\lambda \gg a$, one may disregard the atomic nature and treat the solid as a continuous medium. Such vibrations are referred to as *elastic waves*.

We consider an elastic wave in a long bar of cross-sectional area A and mass density $\rho = M/V$.

- (1) First, we consider a *longitudinal wave* of compression/expansion.



We look at a segment of width dx at the point x and denote the elastic displacement by u . According to the Newton's second law

$$m \frac{d^2 u}{dt^2} = \sum F, \quad (4.18)$$

which implies that

$$(\rho A dx) \frac{d^2 u}{dt^2} = F(x+dx) - F(x), \quad (4.19)$$

$$\rho \frac{d^2 u}{dt^2} = \frac{1}{A} \frac{dF}{dx} = \frac{d\sigma_{xx}}{dx}, \quad (4.20)$$

where we introduced the compression stress σ_{xx} . Assuming that the wave propagates along the [100] direction, we can write the Hooke's law in the form

$$\sigma_{xx} = C_{11} \epsilon_{xx}, \quad (4.21)$$

where C_{11} is Young's modulus. Since $\epsilon_{xx} = \frac{du}{dx}$, this leads to the *wave equation*

$$\frac{d^2u}{dt^2} = \left(\frac{C_{11}}{\rho} \right) \frac{d^2u}{dx^2}. \quad (4.22)$$

A solution if the wave equation has the form of a propagating *longitudinal plane wave*

$$\mathbf{u}(x,t) = A e^{i(qx-\omega t)} \hat{\mathbf{x}}, \quad (4.23)$$

where q is the wave vector,

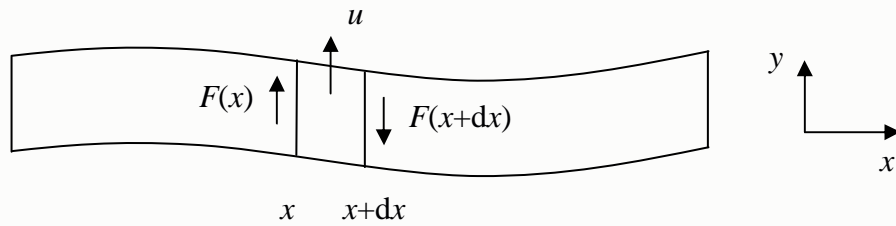
$$\omega = v_L q,$$

is the frequency, and (4.24)

$$v_L = \sqrt{\frac{C_{11}}{\rho}} \quad (4.25)$$

is the *longitudinal velocity of sound*.

(2) Now we consider a *transverse wave* which is controlled by shear stress and strain.



In this case

$$\rho \frac{d^2u}{dt^2} = \frac{d\sigma_{xy}}{dx}, \quad (4.26)$$

where the shear stress σ_{xy} is determined by the shear modulus C_{44} and shear strain $\epsilon_{xy} = \frac{du}{dx}$:

$$\sigma_{xy} = C_{44} \epsilon_{xy}. \quad (4.27)$$

Therefore Eq.(4.26) takes the form

$$\rho \frac{d^2u}{dt^2} = C_{44} \frac{d\epsilon_{xy}}{dx} = C_{44} \frac{d^2u}{dx^2}, \quad (4.28)$$

resulting in the wave equation

$$\frac{d^2u}{dt^2} = \left(\frac{C_{44}}{\rho} \right) \frac{d^2u}{dx^2}. \quad (4.29)$$

This is the equation for the transverse plane wave, which has displacements in the y direction but propagates in the x direction:

$$\mathbf{u}(x,t) = A e^{i(qx-\omega t)} \hat{\mathbf{y}}, \quad (4.30)$$

where q is the wave vector,

$$\omega = v_T q,$$

in the frequency, and

$$(4.31)$$

$$v_T = \sqrt{\frac{C_{44}}{\rho}}$$

$$(4.32)$$

is the *transverse velocity of sound*. Note that there are two linear independent transverse modes characterized by the displacements in y and in z directions. For the [100] direction, by symmetry the velocities of these modes are the same and given by Eq.(4.32).

Normally $C_{11} > C_{44}$ and therefore $v_L > v_T$.

Waves we have considered are in [100] direction, i.e. $\mathbf{q} \parallel [100]$. In other directions, the sound velocity depends on combinations of elastic constants:

$$v = \sqrt{\frac{C_{eff}}{\rho}}, \quad (4.33)$$

where C_{eff} is an effective elastic constant which is given for cubic crystals in the table:

Mode	$\mathbf{q} \parallel [100]$	$\mathbf{q} \parallel [110]$.	$\mathbf{q} \parallel [111]$
L	C_{11}	$\frac{1}{2}(C_{11}+C_{12}+2C_{44})$	$\frac{1}{3}(C_{11}+2 C_{12}+4C_{44})$
T ₁	C_{44}	C_{44}	$\frac{1}{3} (C_{11}-C_{12}+C_{44})$
T ₂	C_{44}	$\frac{1}{2}(C_{11}-C_{12})$	$\frac{1}{3} (C_{11}-C_{12}+C_{44})$

The relation connecting the frequency ω and the wave vector q is known as the *dispersion relation*. For elastic waves, ω is proportional to q , and the ratio ω/q gives a constant velocity. The figure below shows the dispersion relation for elastic waves. There are three modes – one longitudinal and two transverse, which represent straight lines whose slopes are equal to the respective velocities of sound. For the [100] and [111] directions the two transverse modes are degenerate, i.e. have the same v_T .

