UNIT 6 ELASTIC PROPERTIES

Structure

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6.1 INTRODUCTION

In the study of crystal structures and crystal bonding, we have assumed that atoms remain at rest at lattice sites. Actually, atoms oscillate around their equilibrium positions. Further, for simplicity, we assume that the crystal can be regarded as a continuous medium. That is, we ignore the fact that the crystalline solid is composed of discrete atoms. Waves generated by oscillating atoms in such a (continuous) medium are referred to as **elastic waves**. In this unit, you will study the elastic properties of solids and propagation of elastic waves in solids.

In general, solids are rigid but you may be aware that even the strongest block of steel can be stretched, compressed or twisted. Further, it is our common observation that strips of different materials, say iron and lead of same thickness behave differently under bending forces. When the bending force is removed, the strip of iron tries to come back to its original shape whereas the strip of lead retains its deformed shape. In your school physics, you must have learnt that most solids possess **elasticity**, which opposes the applied force and tends to restore the body to its original state once the applied force has been removed. The greater the resistance of a solid to deformation, the higher would be its elasticity. That is why steel is said to be highly elastic, though it is not easily stretchable. On the other hand, lead solder is not an elastic material because it can be permanently deformed by relatively small force. You are familiar with the detailed terminology of elasticity from your +2 physics. We would advise you to refresh your knowledge.

An exact and detailed knowledge of the elastic properties of the materials like steel and other metals used in the construction of buildings and bridges is very essential. These enable us to choose an appropriate design and type of material. In Sec. 6.2 you will learn to analyse stress-strain relations for crystalline solids. Section 6.3 is devoted to the discussion of elastic constants of cubic crystals. You will learn about elastic wave propagation through cubic crystals in Sec. 6.4. The elastic properties of non-cubic crystals are discussed in Sec. 6.5.

Objectives

After studying this unit, you should be able to:

- differentiate between different types of strains and stresses produced in a crystal:
- express stress-strain relation in terms of the elastic constants of a crystal;
- explain the role of energy density in deciding the number of independent elastic constants;
- list the various elastic constants for cubic crystals;
- describe propagation of elastic waves in cubic crystals; and
- explain elastic properties of non-cubic crystals.

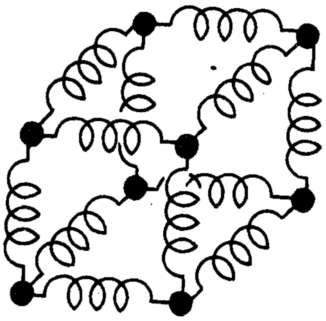


Fig.6.1: A mechanical model of a crystal. Each spring represents the bond between a pair of atoms

6.2 ELASTICITY OF CRYSTALS

You know that most solid materials are crystalline in nature and that crystals have a regular pattern. The atoms in a crystal have a definite spacing and they resist being pulled further apart or squeezed close together. If you want to get a mechanical picture of the structure of a crystal, you can imagine tiny springs joining each atom to its neighbours, as shown in Fig.6.1. We can think of each spring as a bond between a pair of atoms. In terms of this model, it is easy to visualize why even a small force can deform a crystal and how a crystal returns to its original size and shape when the applied force has been removed.

From Block 1 you may recall that we cannot see the structure of a crystal with unaided eye but it exhibits all the properties and characteristics of the solid. A one mm long copper or iron wire may contain 25 lakh atoms along its length with 4Å spacing. Does this mean that the crystal can be taken to be *homogeneous* and *continuous*? To seek answer to this question, we recall that ultrasonic wave of frequency 1000 MHz travels with a speed of 5000 ms^{-1} in most of the metallic, covalent and ionic crystals. This corresponds to a wavelength of 50,000 Å, which is much more than 4Å. In view of this, the crystals can indeed be considered as homogeneous and continuous media for elastic wave propagation.

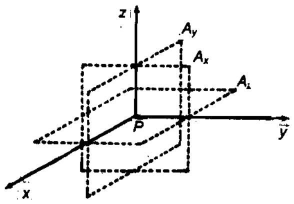


Fig.6.2: Three elements of area at a reference point *P*

6.2.1 Stress Analysis

When a force is applied on a body, it is opposed by a force arising due to elasticity, which tends to restore the body to its original condition. The force developed due to elasticity is called **restoring force**. Restoring force per unit area is known as **stress**. It has dimensions of pressure.

For analysis of stress, it is necessary to specify the stress at a given point in a crystal. To do so, refer to Fig. 6.2. Let P be a point in the crystal at which stress has to be specified. Note that there are three different elements of area, viz. A_x, A_y and A_z in the yz-, xz- and xy-planes, respectively, passing through the same point P. We know that a force can be resolved into three components along three mutually perpendicular axes. Let γ_{yy} denote the component of force acting per unit area in the y-direction on the element of area A_y (that is, on the element of area whose normal lie along the y-axis). Similarly, γ_{xy} and γ_{zy} define the components of the force per unit area on A_y in x- and z-directions, respectively (Fig. 6.3). Let γ_{xx}, γ_{yx} and γ_{zx} denote the components on A_x in x, y and z directions respectively and γ_{xz}, γ_{yz} and γ_{zz} be the components on A_z in x, y and z directions, respectively.

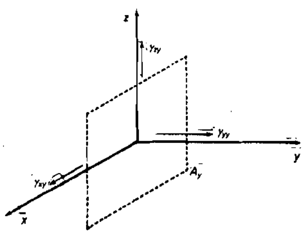


Fig.6.3: Stress components γ_{xy}, γ_{yy} and γ_{zy} on an element of area A_y

Note that out of nine components, γ_{xx}, γ_{yy} and γ_{zz} act normal to the element of area and are known as **normal stresses**, while the other six components (γ_{xy}, γ_{yx}, γ_{xz}, γ_{zx}, γ_{yz}, γ_{zy}) act along the plane of element and are known as **shear stresses**. Now, if the body is in static equilibrium, that is, it does not rotate, the total torque acting on the body about any point must be zero. This situation is depicted in Fig. 6.4. Under this condition, we can write

$$\gamma_{yz} = \gamma_{zy},$$

$$\gamma_{zx} = \gamma_{xz},$$

and

$$\gamma_{xy} = \gamma_{yx}. \qquad (6.1)$$

It means that the number of independent stress components is only six (γ_{xx}, γ_{yy}, γ_{zz}, γ_{yz}, γ_{zx} and γ_{xy}) and these are sufficient to describe the state of stress at any point in the crystal.

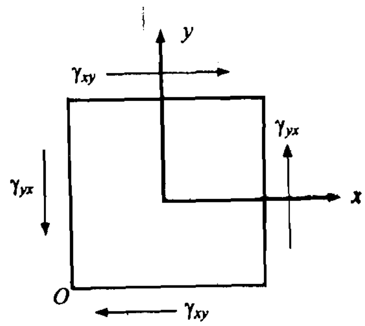


Fig.6.4: For a body in static equilibrium, $\gamma_{yx} = \gamma_{xy}$. The sum of forces in the *x*-direction as well as in *y*-direction is zero. The total torque about the origin (say *O*) is zero if $\gamma_{yx} = \gamma_{xy}$

6.2.2 Strain Analysis

In the above discussion, we analysed stress components. As you may be guessing, *corresponding to every stress component, there is a strain component.* It means that we shall have six strain components. Let us denote these by e_{xx}, e_{yy}, e_{zz}, e_{yz}, e_{zx}, e_{xy}. We now elaborate upon these. Depending on their magnitude, strain components result into uniform or non-uniform deformations. For simplicity, let us first consider uniform deformation.

Uniform Deformation

Uniform deformation means that each primitive cell of the crystal is deformed in the same way. Imagine three orthogonal unit vectors $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$ embedded in the unstrained solid, as shown in Fig. 6.5a. If a small uniform deformation of the solid takes place, the axes shall be distorted in their orientations as well as dimensions, as shown in Fig. 6.5b.

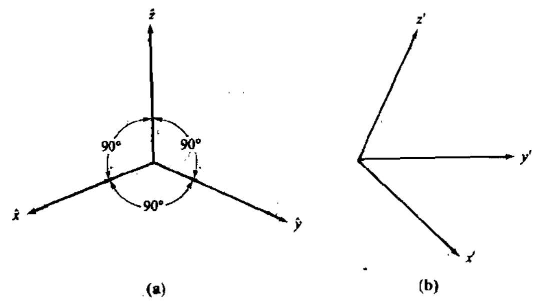


Fig.6.5: a) Orthogonal unit vectors in the unstrained state; and b) in the strained state

Can you express new axis vectors, $\mathbf{x}', \mathbf{y}', \mathbf{z}'$ in terms of $\hat{\mathbf{x}}, \hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$? If the strain is small, we can write

$$\mathbf{x}' = (1 + \varepsilon_{xx})\hat{\mathbf{x}} + \varepsilon_{xy}\,\hat{\mathbf{y}} + \varepsilon_{xz}\,\hat{\mathbf{z}},$$

$$\mathbf{y}' = \varepsilon_{yx}\,\hat{\mathbf{x}} + (1 + \varepsilon_{yy})\hat{\mathbf{y}} + \varepsilon_{yz}\,\hat{\mathbf{z}},$$

and

$$\mathbf{z}' = \varepsilon_{zx}\,\hat{\mathbf{x}} + \varepsilon_{zy}\,\hat{\mathbf{y}} + (1 + \varepsilon_{zz})\,\hat{\mathbf{z}}. \qquad (6.2)$$

The coefficients $\varepsilon_{\alpha\beta}(\alpha, \beta = x, y, z)$ are **measure of deformation**; they are dimensionless and have values much less than one for small strain. The value of deformation coefficient in the case of steel wire is of the order of 10^{-5}. Note that we have not put caps over $\mathbf{x}', \mathbf{y}'$ and $\mathbf{z}'$. This is because $\hat{\mathbf{x}}, \hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ *were of unit length and the new axes may not necessarily be of unit length.* To convince yourself, answer SAQ 1.

Spend 2 min.

SAQ 1

Calculate the self dot product of strained vectors.

Having answered SAQ 1, you must have noted that the strained vectors ($\mathbf{x}', \mathbf{y}'$ and $\mathbf{z}'$) are not of unit length and fractional change in lengths of $\hat{\mathbf{x}}, \hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$, to the first order approximation, is $\varepsilon_{xx}, \varepsilon_{yy}$ and ε_{zz}, respectively. The positive fractional change correspond to *expansion*, whereas negative change would refer to *contraction*. We now define **linear strain components** as

$$e_{xx} \equiv \varepsilon_{xx},$$

$$e_{yy} \equiv \varepsilon_{yy},$$

and

$$e_{zz} \equiv \varepsilon_{zz}. \qquad (6.3)$$

You must have noted that the unit vectors $\hat{\mathbf{x}}, \hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ were defined along mutually orthogonal axes. You may now ask the question: Does the same hold for new configuration? The new axes after deformation may not necessarily be so. To see this, calculate the dot product of vector $\mathbf{x}'$ with vector $\mathbf{y}'$ and even if you retain only the first power of deformation coefficients, the result is non-zero.

Spend 2 min.

SAQ 2

Show that deformed coordinate axes are not orthogonal.

Having solved SAQ 2, you have noted that $\mathbf{x}'$ and $\mathbf{y}'$ are not orthogonal to each other. Further, since the dot product of $\hat{\mathbf{x}}$ with $\hat{\mathbf{y}}$ is zero, $\mathbf{x}'.\mathbf{y}'$ as such gives a measure of the change in orientation between initial unit vectors due to deformation. Thus, if we define e_{xy} in terms of the change in angles between the axes, we can write

$$e_{xy} \equiv \mathbf{x}'.\mathbf{y}' \approx \left(\varepsilon_{xy} + \varepsilon_{yx}\right).$$

Similarly, you can easily convince yourself that

$$e_{yz} \equiv \mathbf{y}'.\mathbf{z}' \cong \varepsilon_{yz} + \varepsilon_{zy},$$

and

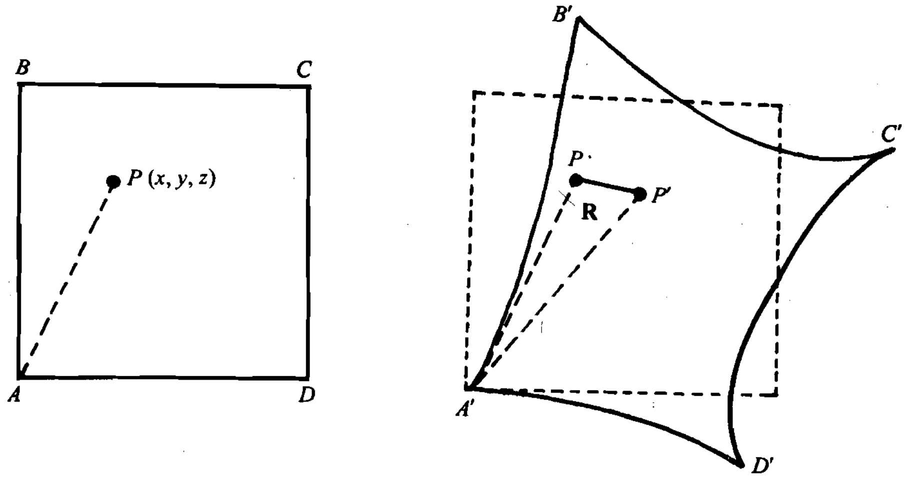
$$e_{zx} \equiv \mathbf{z}'.\mathbf{x}' \cong \varepsilon_{zx} + \varepsilon_{xz}. \qquad (6.4)$$

The coefficients e_{xy}, e_{yz} and e_{zx} are known as **shear strain components** and characterise the change in inclination between the axes.

So far we have considered uniform deformation. But quite often in practice, the deformation is non-uniform in all three dimensions and the analysis made in preceding paragraphs does not hold. The question then arises: Can we express the effect of non-uniform distortion in terms of strain components? If so, how? Let us discover answers to all such questions now.

Non-uniform Deformation

Refer to Fig. 6.6a which shows the cross-sectional view of a three dimensional unstrained specimen. The deformed section is shown in Fig. 6.6b. To examine the effect of deformation at any point, we express the result in terms of local strain. Suppose that the point $P\,(x, y, z)$ moves to a new position $P'\,(x', y', z')$. If u_1, u_2 and u_3 are components of the displacement vector $\mathbf{R}$, the linear strain components e_{xx}, e_{yy} and e_{zz} (which are a measure of stretching in the x, y and z directions) can be written as



(a) (b)

Fig.6.6: a) ***ABCD*** **is cross-sectional view of a three dimensional body before deformation; and b)** ***A'B'C'D'*** **is deformed section**

$$e_{xx} \equiv \varepsilon_{xx} = \frac{\partial u_1}{\partial x},$$

$$e_{yy} \equiv \varepsilon_{yy} = \frac{\partial u_2}{\partial y},$$

and

$$e_{zz} \equiv \varepsilon_{zz} = \frac{\partial u_3}{\partial z}. \qquad (6.5)$$

Similarly, the shear strain components e_{xy}, e_{yz} and e_{zx} corresponding to non-uniform deformation can be written as

$$e_{xy} \cong \varepsilon_{xy} + \varepsilon_{yx} = \frac{\partial u_1}{\partial y} + \frac{\partial u_2}{\partial x},$$

$$e_{yz} \cong \varepsilon_{zy} + \varepsilon_{yz} = \frac{\partial u_3}{\partial y} + \frac{\partial u_2}{\partial z},$$

and

$$e_{zx} \cong \varepsilon_{zx} + \varepsilon_{xz} = \frac{\partial u_3}{\partial x} + \frac{\partial u_1}{\partial z}. \qquad (6.6)$$

The strain components $e_{\alpha\beta}$ ($= e_{\beta\alpha}$) given by Eqs. (6.5) and (6.6) completely define the strain.

Note that *linear strain components give a measure of change in the volume of crystal*; the shape of the crystal is not influenced in anyway. On the other hand, *shear strain components refers to the change in the shape of the crystal and do not affect its volume.*

6.2.3 Stress-Strain Relations and Elastic Constants

So far we have separately analysed the stress and strain components related with elastic deformation. But knowledge of these components is not sufficient for obtaining information about physical properties of a body under the action of external forces. What we need to know is the physical law connecting them. To this end, we make use of **Hookes' law**, which states that for small deformations, *strain is directly proportional to stress*. You may think that strain components are linear functions of stress components. This is only logical and relation may be written as

$$e_{ik} = S_{ikmn}\, \gamma_{mn}, \tag{6.7}$$

where i, k, m, n run over x, y, z. For practical purposes, two suffixes i, k or m, n are replaced by a single digit according to the following scheme:

ik	*xx*	*yy*	*zz*	*yz, zy*	*zx, xz*	*xy, yx*
i	1	2	3	4	5	6

Before you make these substitutions in Eq. (6.7), we would advise you to familiarise yourself with indicial notation and summation convention given in Appendix A. Once you are convinced, you can easily see that expansion in Eq. (6.7) can be expressed by

$$e_{xx} = S_{11}\gamma_{xx} + S_{12}\gamma_{yy} + S_{13}\gamma_{zz} + S_{14}\gamma_{yz} + S_{15}\gamma_{zx} + S_{16}\gamma_{xy},$$

$$e_{yy} = S_{21}\gamma_{xx} + S_{22}\gamma_{yy} + S_{23}\gamma_{zz} + S_{24}\gamma_{yz} + S_{25}\gamma_{zx} + S_{26}\gamma_{xy},$$

$$e_{zz} = S_{31}\gamma_{xx} + S_{32}\gamma_{yy} + S_{33}\gamma_{zz} + S_{34}\gamma_{yz} + S_{35}\gamma_{zx} + S_{36}\gamma_{xy},$$

$$e_{yz} = S_{41}\gamma_{xx} + S_{42}\gamma_{yy} + S_{43}\gamma_{zz} + S_{44}\gamma_{yz} + S_{45}\gamma_{zx} + S_{46}\gamma_{xy},$$

$$e_{zx} = S_{51}\gamma_{xx} + S_{52}\gamma_{yy} + S_{53}\gamma_{zz} + S_{54}\gamma_{yz} + S_{55}\gamma_{zx} + S_{56}\gamma_{xy},$$

and

$$e_{xy} = S_{61}\gamma_{xx} + S_{62}\gamma_{yy} + S_{63}\gamma_{zz} + S_{64}\gamma_{yz} + S_{65}\gamma_{zx} + S_{66}\gamma_{xy}. \tag{6.8}$$

In matrix notation, we can express Eq. (6.8) as

$$[e] = [S]\,[\gamma]$$

where $[e]$ is (6×1) column matrix, $[S]$ is (6×6) matrix of S coefficients and $[\gamma]$ is (6×1) column matrix.

Similarly Eq. (6.9) can be expressed as

$$[\gamma] = [C]\,[e]$$

Conversely, the stress components are linear function of the strain components and we can write

$$\gamma_{xx} = C_{11}e_{xx} + C_{12}e_{yy} + C_{13}e_{zz} + C_{14}e_{yz} + C_{15}e_{zx} + C_{16}e_{xy},$$

$$\gamma_{yy} = C_{21}e_{xx} + C_{22}e_{yy} + C_{23}e_{zz} + C_{24}e_{yz} + C_{25}e_{zx} + C_{26}e_{xy},$$

$$\gamma_{zz} = C_{31}e_{xx} + C_{32}e_{yy} + C_{33}e_{zz} + C_{34}e_{yz} + C_{35}e_{zx} + C_{36}e_{xy},$$

$$\gamma_{yz} = C_{41}e_{xx} + C_{42}e_{yy} + C_{43}e_{zz} + C_{44}e_{yz} + C_{45}e_{zx} + C_{46}e_{xy},$$

$$\gamma_{zx} = C_{51}e_{xx} + C_{52}e_{yy} + C_{53}e_{zz} + C_{54}e_{yz} + C_{55}e_{zx} + C_{56}e_{xy},$$

and

$$\gamma_{xy} = C_{61}e_{xx} + C_{62}e_{yy} + C_{63}e_{zz} + C_{64}e_{yz} + C_{65}e_{zx} + C_{66}e_{xy}. \tag{6.9}$$

The coefficients S_{11}, S_{12},..... are called **elastic compliance constants** or the **elastic constants** and the coefficients C_{11}, C_{12},..... are called the **elastic stiffness constants** or **moduli of elasticity**. The *S*'s have the dimension of [area]/[force] or [volume]/[energy]. The *C*'s have the dimension of [force]/[area] or [energy]/[volume]. The linear form of relationship explains experimental results for many materials under simple tension or compression. Note that Eq. (6.8) as well as Eq. (6.9) contains 36 constant coefficients. They characterize elastic properties of a body. The number of elastic constants is, in general, very large. However, their number can be reduced by invoking several physical considerations. We illustrate it by considering elastic energy density.

6.2.4 Elastic Energy Density

We know that to deform a solid, work has to be done on it. This work is stored in the solid as potential energy. The *elastic energy density is defined as the potential energy stored in a body per unit volume.*

To calculate the work done per unit volume or increment in elastic energy per unit volume δU, we recall that the product of stress and corresponding strain has the dimensions of work done per unit volume. Therefore, when an external force is applied, we can write

$$\delta U = \gamma_{xx}\ \delta e_{xx} + \gamma_{yy}\ \delta e_{yy} + \gamma_{zz}\ \delta e_{zz} + \gamma_{yz}\ \delta e_{yz} + \gamma_{zx}\ \delta e_{zx} + \gamma_{xy}\ \delta e_{xy}\,. \tag{6.10}$$

$\gamma_{xx} = \dfrac{\text{force}}{\text{area}}$

$e_{xx} = \dfrac{\text{change in length}}{\text{length}}$

Therefore, $\gamma_{xx} \times e_{xx}$ will have the dimensions of

$$\frac{MLT^{-2}}{L^2}\cdot\frac{L}{L} = \frac{ML^2T^{-2}}{L^3} = \frac{\text{work done}}{\text{volume}}$$

The elastic energy density is therefore given by

$$U = \gamma_{xx}\, e_{xx} + \gamma_{yy}\, e_{yy} + \gamma_{zz}\, e_{zz} + \gamma_{yz}\ e_{yz} + \gamma_{zx}\, e_{zx} + \gamma_{xy}\, e_{xy}\,. \tag{6.11}$$

In terms of elastic energy density, the stress components can be expressed as

$$\frac{\partial U}{\partial e_{xx}} = \gamma_{xx}\,, \tag{6.12a}$$

$$\frac{\partial U}{\partial e_{yy}} = \gamma_{yy}\,, \tag{6.12b}$$

and so on.

By differentiating Eq. (6.12a) w.r.t e_{yy} and Eq. (6.12b) w.r.t e_{xx} we obtain

$$\frac{\partial \gamma_{xx}}{\partial e_{yy}} = \frac{\partial}{\partial e_{yy}}\left(\frac{\partial U}{\partial e_{xx}}\right)$$

and

$$\frac{\partial \gamma_{yy}}{\partial e_{xx}} = \frac{\partial}{\partial e_{xx}}\left(\frac{\partial U}{\partial e_{yy}}\right).$$

If the order of differentiation is not important, we can write

$$\frac{\partial}{\partial e_{yy}}\left(\frac{\partial U}{\partial e_{xx}}\right) = \frac{\partial}{\partial e_{xx}}\left(\frac{\partial U}{\partial e_{yy}}\right).$$

Physically it means that for homogeneous isotropic substances, the stress developed due to application of an external force does not depend on its direction.

Therefore, Eq. (6.12a,b) leads us to the result

$$\frac{\partial \gamma_{xx}}{\partial e_{yy}} = \frac{\partial \gamma_{yy}}{\partial e_{xx}}. \quad (6.13)$$

From Eq. (6.9) we note that

$$\frac{\partial \gamma_{xx}}{\partial e_{yy}} = C_{12},$$

and

$$\frac{\partial \gamma_{yy}}{\partial e_{xx}} = C_{21}. \quad (6.14)$$

From Eqs. (6.13) and (6.14), we find that

$$C_{12} = C_{21} \quad (6.15a)$$

You can easily generalise this result to write

$$C_{ij} = C_{ji}; \quad i, j = 1, 2, 3 \ldots 6 \quad (6.15b)$$

For a (6×6) matrix, this result shows that only twenty one elastic stiffness constants are independent, since the non-diagonal elements are equal and we have a symmetric matrix:

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{pmatrix}. \quad (6.16)$$

It may be mentioned here that the 36 elastic stiffness constants would be needed to characterize the elastic properties of only the most anisotropic bodies exhibiting entirely different elastic properties in different directions.

From your school physics you may recall the expression for the energy of a stretched spring; it is proportional to the square of elongation i.e. strain. So within elastic limits, where Hookes' law holds, we can write the elastic energy density U as a quadratic function of the strains as

$$U = \frac{1}{2} \sum_{\lambda=1}^{6} \sum_{\mu=1}^{6} C_{\lambda\mu} e_{\lambda} e_{\mu}, \quad (6.17)$$

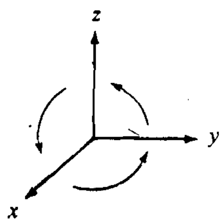


Fig.6.7: Orthogonal system

where $C_{\lambda\mu}$ are elastic stiffness constants, e_λ and e_μ are the strains. Here the indices 1 through 6 are defined as

$$1 \equiv xx;\ 2 \equiv yy;\ 3 \equiv zz;\ 4 \equiv yz;\ 5 \equiv zx;\ 6 \equiv xy$$

Moving anticlockwise, we can make use of an orthogonal cartesian coordinate system, as shown in Fig. 6.7, to write the last three indices 4, 5 and 6.

The general expression for elastic energy density can be expanded as follows:

$$U = \frac{1}{2}[C_{11}e_1^2 + C_{12}e_1e_2 + C_{13}e_1e_3 + C_{14}e_1e_4 + C_{15}e_1e_5 + C_{16}e_1e_6$$
$$+ C_{21}e_2e_1 + C_{22}e_2^2 + C_{23}e_2e_3 + C_{24}e_2e_4 + C_{25}e_2e_5 + C_{26}e_2e_6$$
$$+ C_{31}e_3e_1 + C_{32}e_3e_2 + C_{33}e_3^2 + C_{34}e_3e_4 + C_{35}e_3e_5 + C_{36}e_3e_6$$
$$+ C_{41}e_4e_1 + C_{42}e_4e_2 + C_{43}e_4e_3 + C_{44}e_4^2 + C_{45}e_4e_5 + C_{46}e_4e_6$$
$$+ C_{51}e_5e_1 + C_{52}e_5e_2 + C_{53}e_5e_3 + C_{54}e_5e_4 + C_{55}e_5^2 + C_{56}e_5e_6$$
$$+ C_{61}e_6e_1 + C_{62}e_6e_2 + C_{63}e_6e_3 + C_{64}e_6e_4 + C_{65}e_6e_5 + C_{66}e_6^2].$$

(6.18)

Since C's matrix is symmetric, of the 36 elastic stiffness constants, we need only 21 independent elements.

The number of independent elastic stiffness constants reduces further, if the crystal possesses symmetry elements. In the following section you will learn that for cubic crystals, we need only three independent stiffness constants.

6.3 ELASTIC CONSTANTS OF CUBIC CRYSTALS

In Unit 2, you learnt about symmetry elements of a cube. Since a cube has three 4-fold axes normal to each face, these axes are equivalent and can be replaced by one another by a rotation of 90°. In other words, if the crystal is rotated through 90°, it has the same physical properties. It has the same stiffness for stretching in the x-direction or in y-direction or in z-direction. The elastic energy density U is invariant under this operation. Therefore, we can write

$$C_{11} = C_{22} = C_{33}. \quad (6.19)$$

In addition to this, there are four 3-fold rotation axes along the body diagonal. The expression for elastic energy density must satisfy this requirement. We, therefore, assume that elastic energy density of a cubic crystal is given by

$$U = \frac{1}{2}C_{11}\left(e_{xx}^2 + e_{yy}^2 + e_{zz}^2\right) + \frac{1}{2}C_{44}\left(e_{yz}^2 + e_{zx}^2 + e_{xy}^2\right) + C_{12}\left(e_{yy}e_{zz} + e_{zz}e_{xx} + e_{xx}e_{yy}\right).$$

(6.20)

Let us now see how this expression satisfies the symmetry requirements. The effect of rotation of 120° about one of these four axes is to interchange the x, y and z axes according to the following scheme:

$$x \rightarrow y \rightarrow z \rightarrow x$$

Depending upon the choice of body diagonal as the axis of 3-fold rotation, the axes of the coordinate system will change as per the following schemes:

i) $x \rightarrow y \rightarrow z \rightarrow x$
ii) $-x \rightarrow y \rightarrow z \rightarrow -x$
iii) $-x \rightarrow z \rightarrow -y \rightarrow -x$
and
iv) $x \rightarrow z \rightarrow -y \rightarrow x$

Using this scheme, we can write, for example

$$e_{xx}^2 + e_{yy}^2 + e_{zz}^2 \rightarrow e_{yy}^2 + e_{zz}^2 + e_{xx}^2$$

Eq. (6.20) can be written as

$$U = \frac{1}{2}C_{11}\left(e_{yy}^2 + e_{zz}^2 + e_{xx}^2\right) + \frac{1}{2}C_{44}\left(e_{zx}^2 + e_{xy}^2 + e_{yz}^2\right) + C_{12}\left(e_{zz}e_{xx} + e_{xx}e_{yy} + e_{yy}e_{zz}\right)$$

(6.21)

You can easily convince yourself that Eqs. (6.20) and (6.21) are identical and hence invariant under the operation of 3-fold rotation. It is important to mention that if we include quadratic terms like $(e_{xx}\, e_{yz} + \ldots)$, $(e_{xx}\, e_{xy} + \ldots)$, etc. in Eq. (6.20), it will not remain invariant under rotation of 120° about one or the other of the four 3-fold axes of rotation. However, Eq. (6.20) remains invariant under rotation of 120° about all the four axes (of which invariance under rotation about one of the axes has been shown above). Hence, we are justified in assuming that Eq. (6.20) gives energy density of a cubic crystal.

You may note that Eq. (6.20) contains only three stiffness constants. In order to show that a cubic crystal possesses only three independent elastic stiffness constants ($C_{11}= C_{22} = C_{33}$, $C_{12} = C_{21} = C_{13} = C_{31} = C_{23} = C_{32}$ and $C_{44}= C_{55}= C_{66}$), we combine Eqs. (6.12a) and (6.20), to obtain

$$\gamma_{xx} = \frac{\partial U}{\partial e_{xx}} = C_{11} e_{xx} + C_{12}\left(e_{yy} + e_{zz}\right).$$

Comparing this result with that in Eq. (6.9), we get

$$C_{12} = C_{13},$$

and

$$C_{14} = C_{15} = C_{16} = 0. \tag{6.22}$$

Proceeding in the same way, you can convince yourself that

$$C_{12} = C_{21} = C_{23};\; C_{11} = C_{22};\, C_{12} = C_{31} = C_{32};\; C_{11} = C_{33};\, C_{44} = C_{55} = C_{66};$$

$$C_{24} = C_{25} = C_{26} = C_{34} = C_{35} = C_{36} = C_{41} = C_{42} = C_{43} = C_{45} = C_{46} = 0;$$

and

$$C_{51} = C_{52} = C_{53} = C_{54} = C_{56} = C_{61} = C_{62} = C_{63} = C_{64} = C_{65} = 0$$

The steps involved in deriving these relations have to be worked out in TQ 1.

Using these results in Eq. (6.16), we note that for a cubic crystal, the elastic stiffness constant matrix reduces to

$$\begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix} \tag{6.23}$$

Note that there are only three independent elastic stiffness constants for cubic crystals: C_{11}, C_{12} and C_{44}.

Using Eqs. (6.9) and (6.23), we can write the stress-strain relation for a cubic crystal in terms of matrices as:

$$\begin{pmatrix} \gamma_{xx} \\ \gamma_{yy} \\ \gamma_{zz} \\ \gamma_{yz} \\ \gamma_{zx} \\ \gamma_{xy} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix} \begin{pmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \\ e_{yz} \\ e_{zx} \\ e_{xy} \end{pmatrix} \tag{6.24}$$

Therefore, in view of Eq. (6.24), the stress-strain relation for a cubic crystal has the form

$$\gamma_{xx} = C_{11}e_{xx} + C_{12}\left(e_{yy} + e_{zz}\right),$$

$$\gamma_{yy} = C_{11}e_{yy} + C_{12}\left(e_{xx} + e_{zz}\right),$$

$$\gamma_{zz} = C_{11}e_{zz} + C_{12}\left(e_{xx} + e_{yy}\right),$$

$$\gamma_{yz} = C_{44}e_{yz},$$

$$\gamma_{zx} = C_{44}e_{zx},$$

and

$$\gamma_{xy} = C_{44}e_{xy}. \tag{6.25}$$

From the matrix in Eq. (6.24), it is clear that for a cubic crystal, the tensile stresses γ_{xx}, γ_{yy} and γ_{zz} result only in tensile strains e_{xx}, e_{yy} and e_{zz}; no shear strain is generated by these tensile stresses. Similarly, the shear stresses γ_{xy}, γ_{yz}, γ_{zx} give rise to only shear strains. Further, without going into mathematical details, we give below the relations connecting elastic stiffness constants with elastic constants of a cubic crystal:

$$C_{44} = \frac{1}{S_{44}}, \tag{6.26a}$$

$$C_{11} - C_{12} = \left(S_{11} - S_{12}\right)^{-1}, \tag{6.26b}$$

and

$$C_{11} + 2C_{12} = \left(S_{11} + 2S_{12}\right)^{-1}. \tag{6.26c}$$

You may now like to answer an SAQ before proceeding further.

SAQ 3

Spend 2 min.

In Eq. (6.25), the constant C_{44} relates the shear stress and strain in the same direction, while the constant C_{12} relates the compression stress in one direction to the strain in another. What does the constant C_{11} relate to?

Bulk Modulus

Now we consider volume elasticity which involves changes in the volume of the body when it is subjected to compressional forces. If the compressional forces of equal magnitude are applied to all faces of a cube, its volume reduces. For uniform dilation (fractional change in volume), we must have

$$e_{xx} = e_{yy} = e_{zz} = \frac{\delta}{3},$$

and

$$e_{yz} = e_{zx} = e_{xy} = 0.$$

For this case, the elastic energy density can be obtained using Eq. (6.20):

$$U = \frac{1}{2}C_{11} \times 3 \times \left(\frac{\delta^2}{9}\right) + C_{12}\left(3 \times \frac{\delta^2}{9}\right)$$

$$= \frac{1}{6}\left[C_{11} + 2C_{12}\right]\delta^2. \tag{6.27}$$

To find an expression for dilation, let us consider that a unit cube of edges $\hat{\mathbf{x}}, \hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ is deformed by external pressure and its new edges are $\mathbf{x}'$, $\mathbf{y}'$ and $\mathbf{z}'$. Then the volume of the deformed unit cube can be written as (using Eq. (6.2)):

$$V' = \mathbf{x}'.\mathbf{y}' \times \mathbf{z}' = \begin{vmatrix} 1+\varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & 1+\varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & 1+\varepsilon_{zz} \end{vmatrix}$$

$$\approx 1 + \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$$

where we have neglected products like $\varepsilon_{xy} \cdot \varepsilon_{yz}$ etc.

Thus, the fractional change in volume,

$$\delta = \frac{V' - V}{V}$$

$$= \frac{V'}{V} - 1$$

$$\cong e_{xx} + e_{yy} + e_{zz}$$

And, for uniform dilation

$$e_{xx} = e_{yy} = e_{zz} = \delta/3$$

The elastic energy density U can also be written as the quadratic function of strains (or half the product of stress × strain):

$$U = \frac{1}{2} B \delta^2 . \qquad (6.28)$$

where B is Bulk modulus. On comparing this expression with that contained in Eq. (6.27), we get the expression for Bulk Modulus

$$B = \frac{1}{3}\left(C_{11} + 2C_{12}\right). \qquad (6.29)$$

6.4 ELASTIC WAVES IN CUBIC CRYSTALS

If the forces applied on a body are suddenly withdrawn or changed, either it may be set in motion or an **elastic wave** could be generated in it. The elastic waves have small amplitude, as do sound waves.

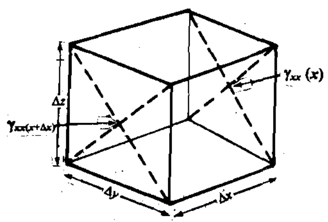


Fig.6.8: An elementary cube

To analyse the propagation of elastic waves, let us consider the forces acting on an elementary cube of volume $\Delta x\, \Delta y\, \Delta z$ (Fig. 6.8).

We recall that volume of a body, cube in the present case, can change only if it is compressed on all sides (faces of the cube). By referring to Fig.6.8, you will note that stresses $\gamma_{xx}(x)$ and $\gamma_{xx}(x+\Delta x)$ appear on faces at x and $x + \Delta x$, having area $\Delta y\, \Delta z$. These are connected through the relation

$$\gamma_{xx}(x + \Delta x) \cong \gamma_{xx} + \frac{\partial \gamma_{xx}}{\partial x} \Delta x . \qquad (6.30)$$

Therefore, the net restoring force due to the variation in γ_{xx} is given by $\left(\frac{\partial \gamma_{xx}}{\partial x} \Delta x\right) \Delta y \Delta z$.

The other contributions to the force in the x-direction shall arise from the variation in the stresses γ_{xy} and γ_{xz}. The net x-component of the force on the cube is thus

$$F_x = \left(\frac{\partial \gamma_{xx}}{\partial x} + \frac{\partial \gamma_{xy}}{\partial y} + \frac{\partial \gamma_{xz}}{\partial z}\right) \Delta x\, \Delta y\, \Delta z . \qquad (6.31)$$

This force can be equated to the product of the mass of the cube and component of the acceleration in the x-direction. If ξ is the density of the material of the cube, the mass of the cube is given by the product $\xi\, \Delta x\, \Delta y\, \Delta z$. If we denote the acceleration in the x-direction as $\frac{\partial^2 u_1}{\partial t^2}$, where u_1 is the displacement in the x-direction, the equation of motion in the x-direction is of the form

$$\xi \frac{\partial^2 u_1}{\partial t^2} = \frac{\partial \gamma_{xx}}{\partial x} + \frac{\partial \gamma_{xy}}{\partial y} + \frac{\partial \gamma_{xz}}{\partial z} . \qquad (6.32a)$$

You can write similar expressions for y- and z-directions:

$$\xi \frac{\partial^2 u_2}{\partial t^2} = \frac{\partial \gamma_{yx}}{\partial x} + \frac{\partial \gamma_{yy}}{\partial y} + \frac{\partial \gamma_{yz}}{\partial z} \qquad (6.32b)$$

and

$$\xi \frac{\partial^2 u_3}{\partial t^2} = \frac{\partial \gamma_{zx}}{\partial x} + \frac{\partial \gamma_{zy}}{\partial y} + \frac{\partial \gamma_{zz}}{\partial z}, \quad (6.32c)$$

where u_2 and u_3 are components of displacement in the y- and z-directions, respectively. Substituting the values of stress components γ_{xx}, γ_{xy} and γ_{xz} from Eq. (6.25) in Eq. (6.32a), we get

$$\xi \frac{\partial^2 u_1}{\partial t^2} = C_{11} \frac{\partial e_{xx}}{\partial x} + C_{12}\left(\frac{\partial e_{yy}}{\partial x} + \frac{\partial e_{zz}}{\partial x}\right) + C_{44}\left(\frac{\partial e_{xy}}{\partial y} + \frac{\partial e_{zx}}{\partial z}\right)$$

Note that we have taken x, y and z directions to be parallel to edges of the cube. Using the definitions of strain components given in Eqs. (6.5) and (6.6), we have

$$\xi \frac{\partial^2 u_1}{\partial t^2} = C_{11} \frac{\partial^2 u_1}{\partial x^2} + C_{44}\left(\frac{\partial^2 u_1}{\partial y^2} + \frac{\partial^2 u_1}{\partial z^2}\right) + (C_{12} + C_{44})\left(\frac{\partial^2 u_2}{\partial x \partial y} + \frac{\partial^2 u_3}{\partial x \partial z}\right). \quad (6.33a)$$

You can write the corresponding equations of motion for $\frac{\partial^2 u_2}{\partial t^2}$ and $\frac{\partial^2 u_3}{\partial t^2}$ directly by symmetry, i.e. changing $u_1 \to u_2 \to u_3$ and $x \to y \to z$

$$\xi \frac{\partial^2 u_2}{\partial t^2} = C_{11} \frac{\partial^2 u_2}{\partial y^2} + C_{44}\left(\frac{\partial^2 u_2}{\partial z^2} + \frac{\partial^2 u_2}{\partial x^2}\right) + (C_{12} + C_{44})\left(\frac{\partial^2 u_3}{\partial y \partial z} + \frac{\partial^2 u_1}{\partial y \partial x}\right), \quad (6.33b)$$

and

$$\xi \frac{\partial^2 u_3}{\partial t^2} = C_{11} \frac{\partial^2 u_3}{\partial z^2} + C_{44}\left(\frac{\partial^2 u_3}{\partial x^2} + \frac{\partial^2 u_3}{\partial y^2}\right) + (C_{12} + C_{44})\left(\frac{\partial^2 u_1}{\partial z \partial x} + \frac{\partial^2 u_2}{\partial z \partial y}\right) \quad (6.33c)$$

These equations of motion are solved for special directions of propagation of the waves in a crystal.

In simple isotropic solids, there can be three basic directions of displacement – one along the axis of the propagation and two transverse to the axis of propagation. In the former case, the wave is termed as the *longitudinal* or *compression wave* and in the latter case, the waves are termed *transverse* or *shear waves*; the two shear waves themselves have orthogonal displacements.

We shall now discuss the propagation of transverse and longitudinal waves along a few specified directions in a cubic crystal.

6.4.1 Wave Propagation in the [100] Direction

Consider a transverse wave having wave vector k propagating along the x-direction. The particle displacement u_2 in the y-direction is represented by:

$$u_2 = u_{02} \exp[i(kx - \omega t)], \quad (6.34)$$

where wave number $k = 2\pi/\lambda$; λ being the wavelength of elastic wave and ω is angular frequency. The motion in y-direction is, in general, described by Eq. (6.33b).

However, in the instant case, this expression simplifies considerably, since we have to consider only variations in u_2 along x:

$$\xi \frac{\partial^2 u_2}{\partial t^2} = C_{44} \frac{\partial^2 u_2}{\partial x^2}$$

From Eq. (6.34), we can write

$$\frac{\partial u_2}{\partial x} = u_{02} ik \exp[i(kx - \omega t)]$$

and

$$\frac{\partial^2 u_2}{\partial x^2} = u_{02}\, i^2 k^2 \exp[i(kx - \omega t)] = i^2 k^2 u_2 \quad \text{(i)}$$

Similarly

$$\frac{\partial u_2}{\partial t} = -u_{02}\, i\omega \exp[i(kx - \omega t)]$$

$$\frac{\partial^2 u_2}{\partial t^2} = +u_{02}\, i^2 \omega^2 \exp[i(kx - \omega t)] = i^2 \omega^2 u_2 \quad \text{(ii)}$$

On substituting the values of $\frac{\partial^2 u_2}{\partial x^2}$ and $\frac{\partial^2 u_2}{\partial t^2}$ (using Eq. (6.34)) in this expression and simplifying the resultant expression, we get

$$\xi\, \omega^2 = C_{44}\, k^2 ,$$

which tells us that

$$\frac{\omega}{k} = \left(\frac{C_{44}}{\xi} \right)^{1/2} .$$

But $\left(\frac{\omega}{k} \right)$ defines the velocity of the wave. Therefore the velocity v_t of the transverse wave in the [100] direction is given by

$$v_t = \sqrt{C_{44}/\xi} . \quad (6.35)$$

You may now like to answer an SAQ.

Spend 5 min.

SAQ 4

Consider a transverse wave with the wave vector along the x-direction and the particle displacement u_3 along the z-direction represented by

$$u_3 = u_{03} \exp[i(kx - \omega t)].$$

Derive an expression for its velocity.

Longitudinal Wave

Next let us consider longitudinal or compression wave propagation along [100] direction in a cubic crystal. Obviously, both the wave vector and the particle displacement shall be along the same direction. Let us choose it to be along x-axis. Suppose that the particle displacement along x-axis is represented by

$$u_1 = u_{01} \exp[i(kx - \omega t)] \quad (6.36)$$

Eq. (6.33a) in this case simplifies to

$$\xi \frac{\partial^2 u_1}{\partial t^2} = C_{11} \frac{\partial^2 u_1}{\partial x^2} . \quad (6.37)$$

On substituting the values of $\frac{\partial^2 u_1}{\partial t^2}$ and $\frac{\partial^2 u_1}{\partial x^2}$, we get

$$\omega^2 \xi = C_{11}\, k^2 .$$

or

$$\frac{\omega}{k} = \sqrt{C_{11}/\xi}$$

This shows that velocity of the longitudinal wave in the [100] direction is given by

$$v_l = \sqrt{C_{11}/\xi}\,. \tag{6.38}$$

The longitudinal and the transverse wave velocities in [100] direction of a cubic crystal can be measured experimentally. Thus, it is possible to use Eqs. (6.35) and (6.38) to determine the elastic stiffness constants C_{11} and C_{44}.

Further the waves which propagate along the [110] direction (i.e. in the face diagonal direction) are of special interest, because determination of their propagation velocities enables us to determine all the three elastic stiffness constants C_{11}, C_{12} and C_{44} of a cubic crystal. The expressions for velocities of transverse and longitudinal waves along [110] directions have been derived in Appendix B. Here, we simply quote the results. For longitudinal wave along [110] direction

$$v_l = \sqrt{\frac{C_{11} + C_{12} + 2C_{44}}{2\xi}} \tag{6.39}$$

and for a transverse wave

$$v_t = \sqrt{\frac{C_{11} - C_{12}}{2\xi}}\,. \tag{6.40}$$

Further, it is important to mentioned here that velocity of waves in an isotropic medium propagating along [100] or [110] direction will be same. It implies that there must be some relation amongst the three elastic constants C_{11}, C_{12} and C_{44} for such a medium.

On comparing Eqs. (6.38) and (6.39) we have

$$\sqrt{\frac{C_{11}}{\xi}} = \sqrt{\frac{C_{11} + C_{12} + 2C_{44}}{2\xi}}$$

which on simplification leads to the result

$$C_{11} - C_{12} = 2\, C_{44}. \tag{6.41}$$

You will obtain the same relation if you compare Eqs. (6.35) and (6.40) for transverse waves along [100] and [110] directions.

The three independent elastic constants C_{11}, C_{12} and C_{44} are determined by measuring velocity of sound in particular directions of the crystal. The velocities of longitudinal and shear waves along the [100] direction enable us to determine C_{11} and C_{44}, respectively. Then we can make use Eq. (6.41) to obtain the value of C_{12}.

You can also consider the waves propagating along the body diagonal direction [111] but this does not reveal any new information regarding C_{11}, C_{12} and C_{44}. We shall therefore not consider it here.

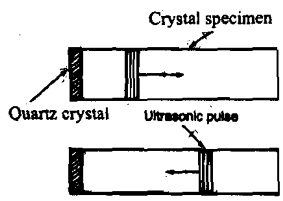


Fig.6.9: A pulse of sound is generated by piezoelectric transducer; the pulse undergoes successive reflections and is detected each time it reaches back to the transducer.

Experimental Determination of Elastic Constants

As discussed above, the elastic constants of a crystalline solid can be determined by the measurement of longitudinal and transverse wave velocities. The method discussed in following paragraphs involves excitation of elastic waves in the crystal specimen. The measurements are often made in the ultrasonic frequency range, where the wavelengths are sufficiently large and the crystal can be treated as a continuous and homogeneous medium. The schematics of this method is depicted in Fig. 6.9.

A quartz crystal acting as a transducer is cemented to one of the parallel surfaces of the experimental crystal taken in the form of a plate. The quartz crystal is in the form of a slab cut in such a way that either a longitudinal or a transverse wave is excited in it by the application of an electric field across its opposite faces. An ultrasonic pulse of short duration (~ 1 μs) is generated and transmitted through the crystal (length of the order of 1 cm) in a particular direction. The pulse gets reflected from the opposite surface of the crystal and is received by the transmitting quartz crystal, which now acts as a receiver.

Quartz crystal is piezoelectric in nature. It can be mechanically deformed when electric pulse is applied to it, and it can generate electrical signal when it is mechanically deformed. Hence it can be used as both, mechanical wave generator as well as its detector.

The time elapsed between the generation of pulse and receipt of reflected pulse is measured with the help of a cathode ray oscillograph. The velocity is then obtained by dividing the round trip distance by the time elapsed. In a representative arrangement, the experimental frequency may be 15 MHz (wavelength 0.03 cm). This method is considered fairly accurate.

6.5 ELASTIC PROPERTIES OF NON-CUBIC CRYSTALS

In the previous section, we have considered the deformation of cubic crystals in [100] direction. Since the cubic structure exhibits a large number of symmetry elements, only three elastic stiffness constants C_{11}, C_{12} and C_{44} are sufficient to study its elastic properties. However, a large number of elastic constants will be required to study the deformation of non-cubic crystals such as triclinic, orthorhombic and monoclinic systems.

Let us consider an orthorhombic crystal and determine the number of independent elastic constants required to study its elastic properties. We again start with the elastic energy density expression given in Eq. (6.17).

In an orthorhombic lattice, all the three sides are unequal, that is, $a \neq b \neq c$. Therefore, the condition $C_{11} = C_{22} = C_{33}$ does not hold in this case.

We start by considering reflection symmetries possessed by an orthorhombic lattice. It can be cut into two equal halves in planes perpendicular to x-axis, y-axis and z-axis. The linear strain component terms, e_1, e_2 and e_3 do not change due to reflection. Let us consider three different cases:

$e_1 = e_{xx}$
$e_2 = e_{yy}$
$e_3 = e_{zz}$

Case I: Orthorhombic lattice is cut by a plane perpendicular to the x-axis. It means that yz-plane is cutting the lattice into two equal halves. Shear strain component $e_4 \equiv e_{yz}$ remains unaffected while

$$e_5 \equiv e_{zx} \to -e_{zx}$$

and

$$e_6 \equiv e_{xy} \to -e_{xy}.$$

Since the expression of elastic energy density remains invariant under the transformation, the coefficients involving e_5 and e_6 i.e. e_1e_5, e_1e_6, e_2e_5, e_2e_6, e_3e_5, e_3e_6, e_4e_5, and e_4e_6 must be zero. Thus, Eq. (6.18) takes somewhat simpler form:

$$U = \frac{1}{2}\Big[C_{11}e_1^2 + C_{22}e_2^2 + C_{33}e_3^2 + C_{44}e_4^2 + C_{55}e_5^2 + C_{66}e_6^2 + C_{12}e_1e_2 + C_{13}e_1e_3 + C_{14}e_1e_4 + C_{23}e_2e_3 + C_{24}e_2e_4 + C_{34}e_3e_4 + C_{56}e_5e_6\Big]. \tag{6.42}$$

Case II: Orthorhombic lattice is cut by a plane perpendicular to y-axis i.e. zx-plane cuts the lattice into two equal halves. Shear strain component $e_5 \equiv e_{zx}$ remains unaffected while

$$e_4 \equiv e_{yz} \rightarrow -e_{yz}$$

$$e_6 \equiv e_{xy} \rightarrow -e_{xy}.$$

This implies that all coefficients involving e_4 and e_6 i.e. e_1e_4, e_2e_4, e_3e_4, and e_5e_6 in Eq. (6.42) are zero:

$$C_{14} = C_{24} = C_{34} = C_{56} = 0$$

Hence, Eq. (6.42) reduces to

$$U = \frac{1}{2}\Big[C_{11}\, e_1^2 + C_{22}\, e_2^2 + C_{33}\, e_3^2 + C_{44}\, e_4^2 + C_{55}\, e_5^2 + C_{66}\, e_6^2$$

$$+ C_{12}e_1e_2 + C_{13}e_1e_3 + C_{23}e_2e_3\Big]. \qquad (6.43)$$

Case III: Orthorhombic lattice is cut by a plane perpendicular to z-axis i.e. xy-plane cuts the lattice into two equal halves. In this case, shear strain component $e_6 \equiv e_{xy}$ remains unaffected while

$$e_4 \equiv e_{yz} \rightarrow -e_{yz}$$

$$e_5 \equiv e_{zx} \rightarrow -e_{zx}.$$

This implies that all coefficients involving e_4 and e_5 in Eq. (6.43) must be zero. However, no such term exists in Eq. (6.43) because they have already been eliminated in view of Case I and II above. Thus, the reflection symmetry of orthorhombic crystals reduces the number of independent elastic stiffness constants from 36 to 9. We may conclude that *for an orthorhombic system, we have to determine nine elastic stiffness constants in order to study its elastic property*. From Eq. (6.43), the matrix of these elastic stiffness constants, $C_{\lambda\mu}$ is given as:

$$C_{\lambda\mu} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{pmatrix} \qquad (6.44)$$

Let us now summarise what you have learnt in this unit.

6.6 SUMMARY

- Elastic properties of solids are analysed on the basis of Hookes' law.

- Linear strain components give a measure of change in the volume of the crystal keeping its shape unaffected, whereas shear strain components refer to change in shape of the crystal keeping its volume unaltered.

- The elastic energy density U is defined as the potential energy stored in a solid per unit volume. It can be expressed in terms of stress and strain components:

$$U = \gamma_{xx} e_{xx} + \gamma_{yy} e_{yy} + \gamma_{zz} e_{zz} + \gamma_{yz} e_{yz} + \gamma_{zx} e_{zx} + \gamma_{xy} e_{xy}$$

  Using the concept of elastic energy density, the number of independent elastic stiffness constants reduces from 36 to 21.

- For cubic crystals, the number of independent elastic stiffness constants reduces to only three because of symmetry elements.

- Bulk modulus of elasticity is given by $\frac{1}{3}(C_{11} + 2C_{12})$.

- The velocity of transverse and longitudinal elastic waves propagating in a cubic crystal along [100] direction is given by

$$v_t = \sqrt{C_{44}/\xi}$$

  and

$$v_l = \sqrt{C_{11}/\xi}\,.$$

- The velocity of propagation of transverse and longitudinal elastic waves in a cubic crystal along [110] direction is given by

$$v_t = \sqrt{\frac{C_{11} - C_{12}}{2\xi}}$$

  and

$$v_l = \sqrt{\frac{C_{11} + C_{12} + 2C_{44}}{2\xi}}\,.$$

- Measurement of the velocity of propagation of elastic waves in solids is a standard technique to determine its elastic stiffness constants.

6.7 TERMINAL QUESTIONS

Spend 20 *min.*

1. Show that for a cubic crystal, there are only three independent elastic stiffness constant.

2. At room temperature, the values of elastic stiffness constants C_{11}, C_{12} and C_{44} for copper are $1.684 \times 10^{11} \text{Nm}^{-2}$, $1.214 \times 10^{11} \text{Nm}^{-2}$ and $0.754 \times 10^{11} \text{Nm}^{-2}$ respectively. If density of copper is 9.018×10^{3} kg m^{-3}, calculate the velocity of longitudinal and transverse elastic waves along [110] direction.

6.8 SOLUTIONS AND ANSWERS

Self-Assessment Questions (SAQs)

1. The self dot product of strained vector $\mathbf{x}'$ is

$$\mathbf{x}'.\mathbf{x}' = \left[(1+\varepsilon_{xx})\,\hat{\mathbf{x}} + \varepsilon_{xy}\,\hat{\mathbf{y}} + \varepsilon_{xz}\,\hat{\mathbf{z}}\right].\left[(1+\varepsilon_{xx})\,\hat{\mathbf{x}} + \varepsilon_{xy}\,\hat{\mathbf{y}} + \varepsilon_{xz}\,\hat{\mathbf{z}}\right]$$

$$= (1+\varepsilon_{xx})^2\,\hat{\mathbf{x}}.\hat{\mathbf{x}} + 0 + 0 + 0 + \varepsilon_{xy}^2\,\hat{\mathbf{y}}.\hat{\mathbf{y}} + 0 + 0 + 0 + \varepsilon_{xz}^2\,\hat{\mathbf{z}}.\hat{\mathbf{z}}$$

so that

$$x'^2 = (1+\varepsilon_{xx})^2 + \varepsilon_{xy}^2 + \varepsilon_{xz}^2 . \qquad \text{(i)}$$

Since deformation coefficients $\varepsilon_{\alpha\beta}$ is much less than unity, we can neglect the quantities in their second power. Hence we can write

$$x' = 1 + \varepsilon_{xx} . \qquad \text{(ii)}$$

This shows that the fractional change in the length of $\hat{\mathbf{x}}$, to the first order approximation, is ε_{xx}. Since we are considering uniform deformation, the same should hold for $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ as well.

2. To verify whether or not the deformed coordinate axes are orthogonal to each other, let us compute $\mathbf{x}'.\mathbf{y}'$:

$$\mathbf{x}'.\mathbf{y}' = \left[(1+\varepsilon_{xx})\hat{\mathbf{x}} + \varepsilon_{xy}\,\hat{\mathbf{y}} + \varepsilon_{xz}\,\hat{\mathbf{z}}\right].\left[\varepsilon_{yx}\,\hat{\mathbf{x}} + (1+\varepsilon_{yy})\,\hat{\mathbf{y}} + \varepsilon_{yz}\,\hat{\mathbf{z}}\right]$$

Since $\hat{\mathbf{x}}.\hat{\mathbf{y}} = 0 = \hat{\mathbf{x}}.\hat{\mathbf{z}} = \hat{\mathbf{y}}.\hat{\mathbf{z}}$, this expression simplifies to

$$\mathbf{x}'.\mathbf{y}' = (1+\varepsilon_{xx})\,\varepsilon_{yx}\,\hat{\mathbf{x}}.\hat{\mathbf{x}} + (1+\varepsilon_{yy})\,\varepsilon_{xy}\,\hat{\mathbf{y}}.\hat{\mathbf{y}} + \varepsilon_{xz}\varepsilon_{yz}\,\hat{\mathbf{z}}.\hat{\mathbf{z}}$$

Neglecting the products $\varepsilon_{xx}\,\varepsilon_{yx}, \varepsilon_{yy}\,\varepsilon_{xy}$ and $\varepsilon_{xz}\,\varepsilon_{yz}$ because the individual coefficients are very small, we get

$$\mathbf{x}'.\mathbf{y}' \cong \varepsilon_{yx} + \varepsilon_{xy}$$

Since ε_{yx} and ε_{xy} are finite, the dot product $\mathbf{x}'.\mathbf{y}'$ is non-zero. This means that $\mathbf{x}'$ and $\mathbf{y}'$ are not mutually orthogonal.

3. The constant C_{11} relates the compression stress and strain along the x-, y- or z-axis.

4. The relevant terms in Eq. (6.33c) for this case are

$$\xi\frac{\partial^2 u_3}{\partial t^2} = C_{44}\frac{\partial^2 u_3}{\partial x^2} \qquad \text{(i)}$$

we have

$$u_3 = u_{03}\exp\left[i\,(kx - wt)\right]$$

Evaluating $\frac{\partial^2 u_3}{\partial t^2}$ and $\frac{\partial^2 u_3}{\partial x^2}$ using above expression for w and substituting them in (i) above, we get:

$$\omega^2 \xi = C_{44} k^2$$

$$v_t = \left(\frac{\omega}{k}\right) = \sqrt{C_{44}/\xi} \qquad \text{(ii)}$$

This expression is identical to that contained in Eq. (6.35). It means that two independent shear waves have equal velocities.

Terminal Questions (TQs)

1. In order to show that we need only three elastic stiffness constants to describe a cubic crystal, let us first combine Eqs. (6.12a) and (6.20) to obtain:

$$\gamma_{xx} = \frac{\partial U}{\partial e_{xx}}$$

$$= C_{11} e_{xx} + C_{12}\left(e_{yy} + e_{zz}\right)$$

If we compare above expression for γ_{xx} with the one given by Eq. (6.9), we get:

$$C_{12} = C_{13}$$

and

$$C_{14} = C_{15} = C_{16} = 0.$$

Similarly, from Eqs. (6.12b) and (6.21), we have

$$\gamma_{yy} = \frac{\partial U}{\partial e_{yy}} = C_{11} e_{yy} + C_{12}\left(e_{zz} + e_{xx}\right)$$

Now comparing with expression of stress components γ_{yy} (Eq. (6.9))

$$\gamma_{yy} = C_{21} e_{xx} + C_{22} e_{yy} + C_{23} e_{zz} + C_{24} e_{yz} + C_{25} e_{zx} + C_{26} e_{xy}$$

we get,

$$C_{12} = C_{21} = C_{23};\ C_{24} = C_{25} = C_{26} = 0;\ \text{and}\ C_{11} = C_{22}$$

Comparison of the stress components γ_{zz} :

$$\gamma_{zz} = C_{31} e_{xx} + C_{32} e_{yy} + C_{33} e_{zz} + C_{34} e_{yz} + C_{35} e_{zx} + C_{36} e_{xy}$$

and

$$\gamma_{zz} = \frac{\partial U}{\partial e_{zz}} = C_{11} e_{zz} + C_{12}\left(e_{yy} + e_{xx}\right)$$

would give

$$C_{12} = C_{32} = C_{31};\ C_{11} = C_{33};\ C_{34} = C_{35} = C_{36} = 0$$

Let us consider the expression of γ_{yz}:

$$\gamma_{yz} = C_{41}e_{xx} + C_{42}e_{yy} + C_{43}e_{zz} + C_{44}e_{yz} + C_{45}e_{zx} + C_{46}e_{xy}$$

From Eqs. (6.11) and (6.20):

$$\gamma_{yz} = \frac{\partial U}{\partial e_{yz}} = C_{44}e_{yz}$$

On comparison of above expressions for γ_{yz} (Eq. (6.9)) we find

$$C_{41} = C_{42} = C_{43} = C_{45} = C_{46} = 0$$

Next, from Eqs. (6.11) and (6.20) we have stress component:

$$\gamma_{zx} = \frac{\partial U}{\partial e_{zx}} = C_{44}e_{zx}$$

It can be compared with the expression:

$$\gamma_{zx} = C_{51}e_{xx} + C_{52}e_{yy} + C_{53}e_{zz} + C_{54}e_{yz} + C_{55}e_{zx} + C_{56}e_{xy}$$

which gives

$$C_{44} = C_{55}\ ;\ C_{51} = C_{52} = C_{53} = C_{54} = C_{56} = 0$$

Again considering the stress component γ_{xy} from Eqs. (6.11) and (6.20):

$$\gamma_{xy} = \frac{\partial U}{\partial e_{xy}} = C_{44}e_{xy}$$

It can be compared with the expression for γ_{xy} given as (Eq. (6.9))

$$\gamma_{xy} = C_{61}e_{xx} + C_{62}e_{yy} + C_{63}e_{zz} + C_{64}e_{yz} + C_{65}e_{zx} + C_{66}e_{xy}$$

and we get:

$$C_{44} = C_{66}\ ;\ C_{61} = C_{62} = C_{63} = C_{64} = C_{65} = 0$$

Thus for a cubic crystal, we have the relation

$$C_{44} = C_{55} = C_{66}$$

Therefore, for a cubic crystal, we have only three independent elastic stiffness constants namely C_{11}, C_{12} and C_{44}.

2. For elastic waves propagating along [110] direction, expression for the velocities of longitudinal and transverse waves are given by (Eqs. (6.39) and (6.40)):

$$v_l = \sqrt{\frac{C_{11} + C_{12} + 2C_{44}}{2\xi}}$$

and

$$v_t = \sqrt{\frac{C_{11} - C_{12}}{2\xi}}$$

We have

$$C_{11} = 1.684 \times 10^{11}\ \text{Nm}^{-2}$$

$$C_{12} = 1.214 \times 10^{11}\ \text{Nm}^{-2}$$

$$C_{44} = 0.754 \times 10^{11}\ \text{Nm}^{-2}$$

$$\xi = 9.018 \times 10^{3}\ \text{kg m}^{-3}$$

Thus,

$$v_l = \sqrt{\frac{(1.684 \times 10^{11}\ \text{Nm}^{-2}) + (1.214 \times 10^{11}\ \text{Nm}^{-2}) + (0.754 \times 10^{11}\ \text{Nm}^{-2})}{2 \times (9.018 \times 10^{3}\ \text{kg m}^{-3})}}$$

$$= 4 \times 10^{3}\ \text{ms}^{-1}$$

and

$$v_t = \sqrt{\frac{C_{11} - C_{12}}{2\xi}}$$

$$= \sqrt{\frac{(1.684 \times 10^{11}\ \text{Nm}^{-2}) - (1.214 \times 10^{11}\ \text{Nm}^{-2})}{2 \times (9.018 \times 10^{3}\ \text{kg m}^{-3})}}$$

$$= 1.6 \times 10^{3}\ \text{ms}^{-1}$$

APPENDIX *A:* INDICIAL NOTATION AND SUMMATION CONVENTION

A set of n variables, namely, $x_1, x_2, x_3 \ldots\ldots x_n$ is denoted by x_i where the index $i = 1, 2, 3, \ldots\ldots n$. Two or more indices are also used to denote a set of quantities. Thus, A_{ij} ($i, j = 1, 2, 3$) represents a set of $3^2 = 9$ quantities namely, $A_{11}, A_{12}, A_{13}, A_{21}, A_{22}, A_{23}, A_{31}, A_{32}\ A_{33}$,. Similarly B_{ijk}, ($i, j, k = 1, 2, 3$) represents 27 quantities, C_{ijkl} ($i, j, k, l = 1, 2, 3$) stands for 81 quantities and so on. In general, if a term has r indices and each of the indices takes values $1, 2, 3, \ldots, n$, it denotes n^r quantities.

The summation convention proposed by Albert Einstein is as follows: "The repetition of an index in a term denote the summation over the entire range of the index". Thus $a_i x_i$ (for $i = 1, 2, 3, 4$) means $a_1x_1 + a_2x_2 + a_3x_3 + a_4x_4$. The repeated index, that is to be summed over, is called a 'dummy' or 'bound' index and the one that is not to be summed over is called a 'free' index. For example, in the term $\tau_{ij}\, v_j$, j is the dummy index while i is the free index.

To illustrate it further, let us write the Cartesian form of a few expressions. Take $i, j, k = 1, 2, 3$.

i) $a_i x_i = a_1x_1 + a_2x_2 + a_3x_3$;

ii) $\sigma_{ii} = \sigma_{11} + \sigma_{22} + \sigma_{33}$;

iii) $\dfrac{\partial u_i}{\partial x_i} = \dfrac{\partial u_1}{\partial x_1} + \dfrac{\partial u_2}{\partial x_2} + \dfrac{\partial u_3}{\partial x_3}$;

iv) $\sigma_{ij}\sigma_{ji} = \sigma_{11}^2 + \sigma_{22}^2 + \sigma_{33}^2 + 2(\sigma_{12}\sigma_{21} + \sigma_{13}\sigma_{31} + \sigma_{23}\sigma_{32})$;

v) $\sigma_{ij}\sigma_{jk}\sigma_{ki} = \sigma_{11}^3 + \sigma_{22}^3 + \sigma_{33}^3 + 3(\sigma_{11}\sigma_{12}\sigma_{21} + \sigma_{11}\sigma_{13}\sigma_{31} + \sigma_{21}\sigma_{12}\sigma_{22} +$
$\sigma_{21}\sigma_{13}\sigma_{32} + \sigma_{31}\sigma_{12}\sigma_{23} + \sigma_{31}\sigma_{13}\sigma_{33} + \sigma_{22}\sigma_{23}\sigma_{32} + \sigma_{32}\sigma_{23}\sigma_{33})$;

vi) $\sigma_{ik}\dfrac{\partial u_i}{\partial x_k} = \sigma_{12}\dfrac{\partial u_1}{\partial x_2} + \sigma_{13}\dfrac{\partial u_1}{\partial x_3} + \sigma_{21}\dfrac{\partial u_2}{\partial x_1} + \sigma_{22}\dfrac{\partial u_2}{\partial x_2} + \sigma_{23}\dfrac{\partial u_2}{\partial x_3} + \sigma_{31}\dfrac{\partial u_3}{\partial x_1} +$
$\sigma_{32}\dfrac{\partial u_3}{\partial x_2} + \sigma_{33}\dfrac{\partial u_3}{\partial x_3}$

APPENDIX *B:* WAVE PROPAGATION IN THE [110] DIRECTION

Transverse waves

Let us first consider a shear wave which propagates in the *xy*-plane with particle displacement u_3 in the *z*-direction. It can be represented as

$$u_3 = u_{03} \exp [i(k_x x + k_y y - \omega t)], \tag{B.1}$$

where k_x and k_y are the *x* and *y* components of wave vector *k*. In this case, the relevant terms in the equation of motion (Eq. 6.33c) are

$$\xi \frac{\partial^2 u_3}{\partial t^2} = C_{44}\left(\frac{\partial^2 u_3}{\partial x^2} + \frac{\partial^2 u_3}{\partial y^2}\right)$$

On substituting for $\frac{\partial^2 u_3}{\partial t^2}, \frac{\partial^2 u_3}{\partial x^2}$ and $\frac{\partial^2 u_3}{\partial y^2}$ from Eq. (B.1), we get

$$\omega^2 \xi = C_{44}\left(k_x^2 + k_y^2\right) = C_{44}\, k^2 ,$$

where $k^2 = k_x^2 + k_y^2$.

This result shows that the velocity of the transverse wave propagating in *xy*-plane is given by

$$v_t = \frac{\omega}{k} = \sqrt{C_{44}/\xi}\, . \tag{B.2}$$

Note that the velocity of the shear wave given by Eq. (B.2) is independent of propagation direction; it can propagate along any direction in the *xy*-plane.

Next we consider other waves which propagate in the *xy*-plane with particle motion in the *xy* plane. Let the particle displacements along the *x* and *y* directions be represented by:

$$u_1 = u_{01} \exp [i\,(k_x x + k_y y - \omega t)] \tag{B.3}$$

and

$$u_2 = u_{02} \exp [i\,(k_x x + k_y y - \omega t)]. \tag{B.4}$$

From Eqs. (6.33a) and (6.33b), we note that the relevant terms are

$$\xi \frac{\partial^2 u_1}{\partial t^2} = C_{11}\frac{\partial^2 u_1}{\partial x^2} + C_{44}\left(\frac{\partial^2 u_1}{\partial y^2}\right) + \left(C_{12} + C_{44}\right)\frac{\partial^2 u_2}{\partial x \partial y} \tag{B.5a}$$

and

$$\xi \frac{\partial^2 u_2}{\partial t^2} = C_{11}\frac{\partial^2 u_2}{\partial x^2} + C_{44}\frac{\partial^2 u_2}{\partial y^2} + \left(C_{12} + C_{44}\right)\frac{\partial^2 u_1}{\partial y \partial x}. \tag{B.5b}$$

Substituting Eqs. (B.3) and (B.4) in Eqs. (B.5a) and (B.5b), we get

$$\omega^2 \xi u_1 = \left(C_{11}k_x^2 + C_{44}k_y^2\right)u_1 + (C_{12} + C_{44})k_x k_y u_2$$

and

$$\omega^2 \xi u_2 = \left(C_{11}k_x^2 + C_{44}k_y^2\right)u_2 + (C_{12} + C_{44})k_x k_y u_1 .$$

These equations can be readily solved for a wave travelling in the [110] direction if we take $k_x = k_y = \dfrac{k}{\sqrt{2}}$. Then these equations simplify to:

$$\omega^2 \xi u_1 = (C_{11} + C_{44})\frac{k^2}{2}u_1 + (C_{12} + C_{44})\frac{k^2}{2}u_2 \qquad \text{(B.6a)}$$

and

$$\omega^2 \xi u_2 = (C_{11} + C_{44})\frac{k^2}{2}u_2 + (C_{12} + C_{44})\frac{k^2}{2}u_1 \qquad \text{(B.6b)}$$

To obtain non-zero solutions of these equations, we equate the determinant of coefficients of u_1 and u_2 to zero:

$$\begin{vmatrix} -\omega^2\xi + \frac{1}{2}(C_{11} + C_{44})k^2 & \frac{1}{2}(C_{12} + C_{44})k^2 \\ \frac{1}{2}(C_{12} + C_{44})k^2 & -\omega^2\xi + \frac{1}{2}(C_{11} + C_{44})k^2 \end{vmatrix} = 0$$

If we introduce two new variables by defining

$$A = -\omega^2\xi + \frac{1}{2}(C_{11} + C_{44})\ k^2$$

and

$$B = \frac{1}{2}(C_{12} + C_{44})k^2 ,$$

the determinant reduces to

$$\begin{vmatrix} A & B \\ B & A \end{vmatrix} = 0$$

This gives

$$A^2 - B^2 = 0$$

or

$$(A + B)\,(A - B) = 0$$

This result shows that either $A = B$ or $A = -B$. Let us first consider the case $A = B$. In terms of ω, ξ, C's and k, this leads to

$$-\omega^2\xi + \frac{k^2}{2}(C_{11} + C_{44}) = \frac{k^2}{2}(C_{12} + C_{44})$$

or

$$\omega^2\xi = \frac{k^2}{2}(C_{11} - C_{12}) \qquad \text{(B.7a)}$$

Similarly, the case $A = -B$ leads us to the result

$$\omega^2\xi = \frac{1}{2}(C_{11} + C_{12} + 2C_{44})k^2. \qquad \text{(B.7b)}$$

The nature — transverse or longitudinal — of waves represented by Eqs. (B.7a, b) can be ascertained by determining the direction of corresponding particle displacements. To do so, we substitute Eq. (B.7a) in Eq. (B.6a). This gives

$$\frac{1}{2}(C_{11} - C_{12})k^2u_1 = \frac{1}{2}(C_{11} + C_{44})k^2u_1 + \frac{1}{2}(C_{12} + C_{44})k^2u_2$$

This equation will be satisfied only if we have $u_1 = -u_2$, indicating that the particle displacement in this case is along $[1\bar{1}0]$ and thus perpendicular to k vector. Therefore, Eq. (B.7a) describes a transverse wave.

Similarly, if we combine Eqs. (B.6b) and (B.7b), we find that the resultant equation will hold only if we have $u_1 = u_2$. That is, the particle displacement is along [110] and thus parallel to k vector. Therefore, Eq. (B.7b) describes a longitudinal wave.

Hence, from Eq. (B.7a, b), we can write the expressions for the velocities of longitudinal and transverse waves travelling along [110] direction as:

$$v_l = \frac{\omega}{k} = \sqrt{\frac{C_{11} + C_{12} + 2C_{44}}{2\xi}} \qquad \text{(B.8)}$$

$$v_t = \frac{\omega}{k} = \sqrt{\frac{C_{11} - C_{12}}{2\xi}} \qquad \text{(B.9)}$$