Solid State Physics

Presentation

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Summary

- Elastic wave in [111] direction
- Experimental determination of elastic constants

The [111] Direction

- Miller indices like [100], [110], and [111] describe crystal orientations.
- The [111] direction in a cubic crystal (FCC or BCC) is along a body diagonal.
- For an FCC crystal, the [111] direction cuts through atoms equally along the x, y, and z axes.

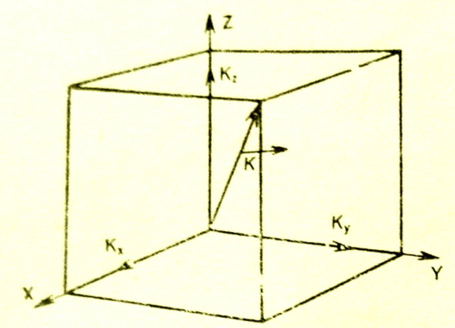
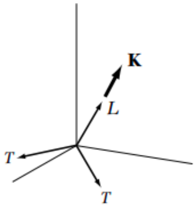


Figure: Wave vector $\vec{k}$ along [111] direction

Waves in the [111] Direction

- Phonon propagation in the [111] crystallographic direction.
- Waves can be longitudinal (compression) or transverse (shear).
- There are two degenerate transverse modes and a longitudinal mode.



Wave in [111] direction

$L : \frac{1}{3}(C_{11} + 2C_{12} + 4C_{44})$

$T : \frac{1}{3}(C_{11} - C_{12} + C_{44})$

Types of Waves in [111] Direction

For longitudinal waves:

- Particle motion and wave velocity are both along the [111] direction.
- Displacement components: $U = V = W$.

For transverse waves:

- Particle motion and wave velocity are perpendicular to each other.
- Displacement components: $U = -V$ and $W = 0$.

Equations of an elastic wave

Equation of motion:

$$\rho \frac{\partial^2 U}{\partial t^2} = C_{11} \frac{\partial^2 U}{\partial x^2} + C_{44} \left(\frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} \right) + (C_{12} + C_{44}) \left(\frac{\partial^2 V}{\partial x \partial y} + \frac{\partial^2 W}{\partial x \partial z} \right)$$

Displacement equations:

$$U = U_0 e^{i(k_x x + k_y y + k_z z - \omega t)} \quad (1)$$

$$V = V_0 e^{i(k_x x + k_y y + k_z z - \omega t)} \quad (2)$$

$$W = W_0 e^{i(k_x x + k_y y + k_z z - \omega t)} \quad (3)$$

Wave vector

In a cubic crystal, wave vector components are related: $k_x = k_y = k_z$
Therefore,

$$k_x^2 + k_y^2 + k_z^2 = 3k_x^2 = k^2$$

$$k_x^2 = \frac{k^2}{3}$$

$$k_x = \frac{k}{\sqrt{3}}$$

Now, the displacement equations are:

$$U = U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \tag{3}$$

$$V = V_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \tag{4}$$

$$W = W_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \tag{5}$$

The equation of motion of a particle is given by

$$\rho \frac{\partial^2 U}{\partial t^2} = C_{11} \frac{\partial^2 U}{\partial x^2} + C_{44} \left(\frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} \right) + (C_{12} + C_{44}) \left(\frac{\partial^2 V}{\partial x \partial y} + \frac{\partial^2 W}{\partial x \partial z} \right) \tag{1}$$

From equation (3), we get:

$$\frac{\partial U}{\partial t} = -i\omega U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \Rightarrow \frac{\partial^2 U}{\partial t^2} = (-i\omega)^2 U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} = -\omega^2 U$$

$$\frac{\partial U}{\partial x} = -i\frac{k_x}{\sqrt{3}} U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \Rightarrow \frac{\partial^2 U}{\partial x^2} = (-i\frac{k_x}{\sqrt{3}})^2 U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} = -\frac{k_x^2}{3}U = -\frac{k^2}{3}U$$

$$\frac{\partial U}{\partial y} = -i\frac{k_y}{\sqrt{3}} U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \Rightarrow \frac{\partial^2 U}{\partial y^2} = (-i\frac{k_y}{\sqrt{3}})^2 U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} = -\frac{k_y^2}{3}U = -\frac{k^2}{3}U$$

$$\frac{\partial U}{\partial z} = -i\frac{k_z}{\sqrt{3}} U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \Rightarrow \frac{\partial^2 U}{\partial z^2} = (-i\frac{k_z}{\sqrt{3}})^2 U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} = -\frac{k_z^2}{3}U = -\frac{k^2}{3}U$$

Now, from equation(4), we get:

$$\frac{\partial^2 V}{\partial x \partial y} = \frac{\partial}{\partial y}\frac{\partial V}{\partial x} = \frac{\partial}{\partial y}\left(\frac{ik}{\sqrt{3}}V\right) = \frac{ik}{\sqrt{3}}\left(\frac{\partial V}{\partial y}\right) = \frac{ik}{\sqrt{3}}\left(\frac{ik}{\sqrt{3}}V\right) = -\frac{k^2}{3}V = -\frac{k^2}{3}U \qquad (\because U = V)$$

And, now from equation (5)

$$\frac{\partial^2 W}{\partial x \partial z} = \frac{\partial}{\partial z}\frac{\partial W}{\partial x} = \frac{\partial}{\partial z}\left(\frac{ik}{\sqrt{3}}W\right) = \frac{ik}{\sqrt{3}}\left(\frac{\partial W}{\partial z}\right) = \frac{ik}{\sqrt{3}}\left(\frac{ik}{\sqrt{3}}W\right) = -\frac{k^2}{3}W = -\frac{k^2}{3}U \qquad (\because U = V = W)$$

Now, putting the values of $\frac{\partial^2 U}{\partial t^2}, \frac{\partial^2 U}{\partial x^2}, \frac{\partial^2 U}{\partial y^2}, \frac{\partial^2 U}{\partial z^2}, \frac{\partial^2 V}{\partial x \partial y}, \frac{\partial^2 W}{\partial x \partial z}$ in equation (1), we get:

$$-\rho\omega^2 U = C_{11}\left(\frac{-k^2}{3}U\right) + C_{44}\left(\frac{-k^2}{3}U + \frac{-k^2}{3}U\right) + (C_{12}+C_{44})\left(\frac{-k^2}{3}U + \frac{-k^2}{3}U\right)$$

$$\rho\omega^2 U = C_{11}\left(\frac{k^2}{3}U\right) + C_{44}\left(\frac{k^2}{3}U + \frac{k^2}{3}U\right) + (C_{12}+C_{44})\left(\frac{k^2}{3}U + \frac{k^2}{3}U\right)$$

$$\rho\omega^2 \cancel{U} = \frac{k^2}{3}\cancel{U}[C_{11} + C_{44}(1+1) + C_{12} + C_{44}(1+1)]$$

$$\rho\omega^2 = \frac{k^2}{3}[C_{11} + 2C_{44} + 2C_{12} + 2C_{44}]$$

$$\rho\omega^2 = (C_{11} + 2C_{12} + 4C_{44})\frac{k^2}{3}$$

Now, we know that the velocity of the wave is given by $v = \frac{\omega}{k}$, therefore:

$$\frac{\omega^2}{k^2} = (C_{11} + 2C_{12} + 4C_{44})\frac{1}{3\rho}$$

$$v = \frac{\omega}{k} = \sqrt{(C_{11} + 2C_{12} + 4C_{44})\frac{1}{3\rho}}$$

This is the velocity of a longitudinal elastic wave in [111] direction of a cubic crystal

Transverse wave in [111] direction

From equation (3), we get:

$$\frac{\partial U}{\partial t} = -i\omega U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \Rightarrow \frac{\partial^2 U}{\partial t^2} = (-i\omega)^2 U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \qquad = -\omega^2 U$$

$$\frac{\partial U}{\partial x} = -i\frac{k_x}{\sqrt{3}} U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \Rightarrow \frac{\partial^2 U}{\partial x^2} = (-i\frac{k_x}{\sqrt{3}})^2 U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \qquad = -\frac{k_x^2}{3} U = -\frac{k^2}{3} U$$

$$\frac{\partial U}{\partial y} = -i\frac{k_y}{\sqrt{3}} U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \Rightarrow \frac{\partial^2 U}{\partial y^2} = (-i\frac{k_y}{\sqrt{3}})^2 U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \qquad = -\frac{k_y^2}{3} U = -\frac{k^2}{3} U$$

$$\frac{\partial U}{\partial z} = -i\frac{k_z}{\sqrt{3}} U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \Rightarrow \frac{\partial^2 U}{\partial z^2} = (-i\frac{k_z}{\sqrt{3}})^2 U_0 e^{i\left(\frac{k}{\sqrt{3}}(x+y+z)-\omega t\right)} \qquad = -\frac{k_z^2}{3} U = -\frac{k^2}{3} U$$

From equation(4) we get:

$$\frac{\partial^2 V}{\partial x \partial y} = \frac{\partial}{\partial y}\frac{\partial V}{\partial x} = \frac{\partial}{\partial y}\left(\frac{ik}{\sqrt{3}}V\right) = \frac{ik}{\sqrt{3}}\left(\frac{\partial V}{\partial y}\right) = \frac{ik}{\sqrt{3}}\left(\frac{ik}{\sqrt{3}}V\right) = -\frac{k^2}{3}V = \frac{k^2}{3}U \qquad (\because V = -U)$$

From equation(5) we get:

$$\frac{\partial^2 W}{\partial x \partial z} = 0(\because W = 0)$$

Now, putting the values of $\frac{\partial^2 U}{\partial t^2}, \frac{\partial^2 U}{\partial x^2}, \frac{\partial^2 U}{\partial y^2}, \frac{\partial^2 U}{\partial z^2}, \frac{\partial^2 V}{\partial x \partial y}, \frac{\partial^2 W}{\partial x \partial z}$ in equation (1), we get:

$$-\rho\omega^2 U = C_{11}\left(\frac{-k^2}{3}U\right) + C_{44}\left(\frac{-k^2}{3}U + \frac{-k^2}{3}U\right) + (C_{12}+C_{44})\left(\frac{k^2}{3}U + 0\right)$$

$$-\rho\omega^2 \cancel{U} = \frac{k^2}{3}\cancel{U}\left[C_{11}(-1) + C_{44}(-1+-1) + (C_{12}+C_{44})(1)\right]$$

$$\rho\omega^2 = \frac{k^2}{3}\left(C_{11} + 2C_{44} - (C_{12}+C_{44})\right)$$

$$\rho\omega^2 = (C_{11} - C_{12} + C_{44})\frac{k^2}{3}$$

Now, we know that the velocity of the wave is given by $v = \frac{\omega}{k}$, therefore:

$$\frac{\omega^2}{k^2} = (C_{11} - C_{12} + C_{44})\frac{1}{3\rho}$$

$$v = \frac{\omega}{k} = \sqrt{(C_{11} - C_{12} + C_{44})\frac{1}{3\rho}}$$

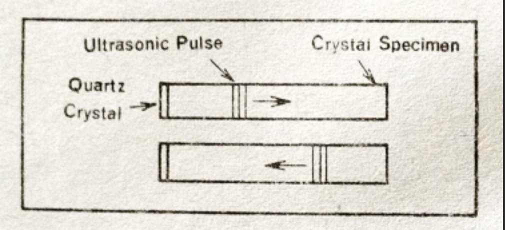
This is the velocity of transverse wave in [111] direction

Relation Between Velocities and Elastic Constants

- Elastic waves' velocities and elastic moduli help in determining elastic constants.
- Elastic waves are excited in a crystal, and their velocity is measured.

Ultrasonic Pulse Method

- Frequencies are in the ultrasonic range, where the crystal behaves as a continuous elastic medium.
- The waves are pulsed; this is known as the ultrasonic pulse method.



Crystal Specimen Setup

- The crystal specimen has flat ends for proper pulse reflection.
- A piezoelectric quartz transducer is attached to one end.

Pulse Reflection and Velocity Measurement

- The ultrasonic pulse is reflected from the rear surface back to the transducer.
- Time taken for the pulse to travel round-trip is measured electronically.
- Velocity is calculated using distance divided by time.

Apparatus of ultrasonic pulse-echo method

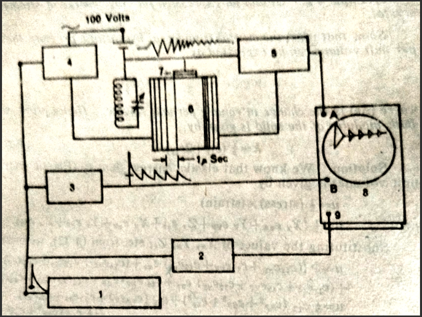


Figure: Block diagram of apparatus for ultrasonic pulse-echo method. 1.trigger generator(1000μ s period, 2. delay circuit, 3. time mark generator, 4. thyratron switch, 5. wide band rf amplifier, 6.specimen, 7.quartz, 8.oscilloscope, 9.sweep trigger

Electronic Apparatus and Measurement Process

- The trigger generator initiates the process by discharging a condenser through an LC network.
- A voltage wave is imposed on the quartz transducer glued to the specimen.

Measurement Accuracy

- The time mark generator and delay circuit ensure precise measurement of pulse arrival.
- This method is highly accurate and uses only small specimen sizes.

Applications and Elastic Constants

- This method can determine elastic constants at various temperatures and pressures.
- Elastic stiffness constants C_{11}, C_{12}, C_{44} of a cubic crystal can be calculated.

References

- Hemarajini and Kakani, Solid State Physics
- Charles Kittel, Solid State Physics
- Circus of Physics Channel

The End