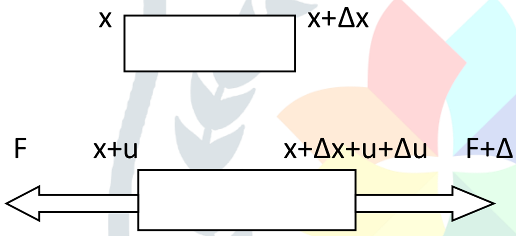
Determination of velocities of elastic waves through cubic crystal in different directions in terms of elastic constants

Vishal Sharma
Assistant professor of Physics
D.A.V. College, Hoshiarpur (Punjab)

Abstract : The velocities of elastic waves through the cubic crystal along different orientations are theoretically, calculated using stress-strain relationship in tensor form and secular determinant. These velocities are determined in terms of three elastic constants C_{11}, C_{12} &C_{44} of cubic crystal. Three values of wave velocities are obtained:one value corresponds to longitudinal velocity and other two identical values corresponds to transverse velocities.The wave velocities along different orientations can be measured experimentally. Using these velocity values, elastic constants for cubic crystal can be obtained.

Keywords*: Elastic constants, secular determinant, symmetry direction, stress and strain tensor, wave velocity*.

I.Introduction



We consider a state of strain which is caused to exist in the crystal in x-direction only and this disturbance is allowed to be moved along the crystal. In the first figure, the equilibrium position is shown where an isolated portion of undisturbed crystal is defined by the co-ordinates x and x+Δx. When a plane wave passes through the crystal, each point x is associated with a displacement u. This u is a function of both position and time. The disturbed position is shown in second figure where the isolated portion is now bounded by planes at x+u and x+ Δx+u+Δu. The corresponding tensions are F and F+ΔF as represented in the figure. By Hooke's law, the tension ΔF on the area of cross-section A can be expressed as$\Delta F = CA\Delta\left(\frac{\partial u}{\partial x}\right)$. If ρ is the density of crystal, then dividing by AΔx and taking limit as $\Delta x \to 0$, we get $\rho\frac{\partial^2 u}{\partial t^2} = C\left(\frac{\partial^2 u}{\partial x^2}\right)$. The displacement u can be written in terms of strain tensorγ as $u_m = \gamma_{mn}x_n$ where $x_n = x, y, z$ for n=1,2,3 respectively. The stress tensor can be written as $\tau_{ik} = C_{ikmn}\frac{\partial u_m}{\partial x_n}$ .On differentiating this equation and using earlier equation, the equation of propagation of elastic wave through crystal becomes $\rho\frac{\partial^2 u_i}{\partial t^2} = C_{ikmn}\frac{\partial^2 u_m}{\partial x_k \partial x_n}$.A plane wave solution for above propagation is represented as $u_i = \xi_i e^{i(\vec{q}.\vec{r}-\omega t)}$ where $\vec{r}$ = x$\vec{a}$ + y$\vec{b}$ + z$\vec{c}$. Also, $\vec{q} = q(\zeta_1\vec{a}^* + \zeta_2\vec{b}^* + \zeta_3\vec{c}^*)$. Here ξ_i represents the amplitude and ζ_i the direction cosines. Differentiating the plane wave equation and substituting in equation of propagation, one gets

$$-\rho\omega^2\xi_i = -\xi_m C_{ikmn}(q\zeta_k)(q\zeta_n)$$

Putting $C_{ikmn}\zeta_k\zeta_n = f_{im}$ *and* ${\omega^2}/{q^2} = v^2$ where v is the velocity of the elastic wave in the crystal, we have $\rho v^2\xi_i = f_{im}\xi_m$. Putting i and m as 1,2 and 3, the equations are

$$\xi_1(f_{11}-\rho v^2)+\xi_2 f_{12}+\xi_3 f_{13}=0$$

$$\xi_1 f_{21}+\xi_2(f_{22}-\rho v^2)+\xi_3 f_{23}=0$$

$$\xi_1 f_{31}+\xi_2 f_{32}+\xi_3(f_{33}-\rho v^2)=0$$

The above equations have a real solution only if the determinant obtained from the coefficients of the ξ_1 ,ξ_2 , $\xi_3$is equal to zero. This secular determinant is termed as Christofell determinant.

$$\begin{vmatrix} f_{11}-\rho v^2 & f_{12} & f_{13} \\ f_{21} & f_{22}-\rho v^2 & f_{23} \\ f_{31} & f_{32} & f_{33}-\rho v^2 \end{vmatrix} = 0$$

The above determinant is a general condition for crystals. Solving this determinant for different crystal structures and different orientations, we can find velocity of elastic waves through crystal for those cases.

II. For Cubic crystal

1. Along symmetry direction [100]

   Direction cosines along this direction are $\zeta_1 = 1, \zeta_2 = 0, \zeta_3 = 0$.Also, we make replacements : 11→1, 22→2, 33→3, 23→4, 13→5, 12→6.

$$f_{11} = C_{1111} = C_{11}$$

$$f_{22} = C_{2121} = C_{66} = C_{44}$$

$$f_{33} = C_{3131} = C_{55} = C_{44}$$

   And all other f ‘s are zero. The Secular determinant becomes

$$\begin{vmatrix} C_{11}-\rho v^2 & 0 & 0 \\ 0 & C_{44}-\rho v^2 & 0 \\ 0 & 0 & C_{44}-\rho v^2 \end{vmatrix} = 0$$

   This provides three wave velocities along the direction along [100] are $\sqrt{C_{11}/\rho}$, $\sqrt{C_{44}/\rho}$, $\sqrt{C_{44}/\rho}$.

   The first velocity $\sqrt{C_{11}/\rho}$ corresponds to a longitudinal wave and the other two identical ones correspond to transverse wave in terms of elastic constants C_{11} andC_{44}.

2. Along symmetry direction [010]

   Direction cosines along this direction are $\zeta_1 = 0 , \zeta_2 = 1, \zeta_3 = 0$.

$$f_{11} = C_{1212} = C_{66} = C_{44}$$

$$f_{22} = C_{2222} = C_{22} = C_{11}$$

$$f_{33} = C_{3232} = C_{44}$$

   And all other f ‘s are zero. This gives the Secular determinant as

$$\begin{vmatrix} C_{44}-\rho v^2 & 0 & 0 \\ 0 & C_{11}-\rho v^2 & 0 \\ 0 & 0 & C_{44}-\rho v^2 \end{vmatrix} = 0$$

   This provides the same values of three velocities as along direction [100].

3. Along symmetry direction [001]

Direction cosines along this direction are $\zeta_1 = 0$, $\zeta_2 = 0$, $\zeta_3 = 1$.

$$f_{11} = C_{1313} = C_{55} = C_{44}$$

$$f_{22} = C_{2323} = C_{44}$$

$$f_{33} = C_{3333} = C_{33} = C_{11}$$

And all other f 's are zero. The Secular determinant is now given by

$$\begin{vmatrix} C_{44} - \rho v^2 & 0 & 0 \\ 0 & C_{44} - \rho v^2 & 0 \\ 0 & 0 & C_{11} - \rho v^2 \end{vmatrix} = 0$$

This provides the same values of three velocities as along direction [100] and [010].

4. Along symmetry direction [110]

Direction cosines along this direction are $\zeta_1 = 1/\sqrt{2}$, $\zeta_2 = 1/\sqrt{2}$, $\zeta_3 = 0$.

$$f_{11} = C_{1111}\zeta_1^2 + C_{1212}\zeta_2^2 = \frac{1}{2}(C_{11} + C_{44})$$
$$f_{22} = C_{2121}\zeta_1^2 + C_{2222}\zeta_2^2 = \frac{1}{2}(C_{11} + C_{44})$$
$$f_{33} = C_{3131}\zeta_1^2 + C_{3232}\zeta_2^2 = C_{44}$$
$$f_{12} = C_{1122}\zeta_1\zeta_2 + C_{1221}\zeta_2\zeta_1 = \frac{1}{2}(C_{12} + C_{44}) = f_{21}$$
$$f_{13} = f_{31} = 0$$
$$f_{23} = f_{32} = 0$$

Secular determinant is

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

The solution of this determinant provides

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

First of the three equations provide velocity corresponding to longitudinal wave whereas the rest two equations yield velocities for transverse waves in terms of elastic constants C_{11}, C_{12} and C_{44} .

5. Along symmetry direction [011]

Direction cosines along this direction are $\zeta_1 = 0$, $\zeta_2 = 1/\sqrt{2}$, $\zeta_3 = 1/\sqrt{2}$.

$$f_{11} = C_{1212}\zeta_2^2 + C_{1313}\zeta_3^2 = C_{44}$$
$$f_{22} = C_{2222}\zeta_2^2 + C_{2323}\zeta_3^2 = \frac{1}{2}(C_{11} + C_{44})$$
$$f_{33} = C_{3232}\zeta_2^2 + C_{3333}\zeta_3^2 = \frac{1}{2}(C_{11} + C_{44})$$
$$f_{12} = f_{21} = 0$$
$$f_{13} = f_{31} = 0$$
$$f_{23} = C_{2233}\zeta_2\zeta_3 + C_{2332}\zeta_3\zeta_2 = \frac{1}{2}(C_{12} + C_{44}) = f_{32}$$

Secular determinant becomes

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

The solution of this determinant provides the same equations containing wave velocities as in case of symmetry direction [110]

6. Along symmetry direction [101]

Direction cosines along this direction are $\zeta_1 = 1/\sqrt{2}$, $\zeta_2 = 0$, $\zeta_3 = 1/\sqrt{2}$.

$$f_{11} = C_{1111}\zeta_1^2 + C_{1313}\zeta_3^2 = \frac{1}{2}(C_{11}+C_{44})$$
$$f_{22} = C_{2121}\zeta_1^2 + C_{2323}\zeta_3^2 = C_{44}$$
$$f_{33} = C_{3131}\zeta_2^2 + C_{3333}\zeta_3^2 = \frac{1}{2}(C_{11}+C_{44})$$
$$f_{12} = f_{21} = 0$$
$$f_{13} = C_{1133}\zeta_1\zeta_3 + C_{1331}\zeta_3\zeta_1 = \frac{1}{2}(C_{12}+C_{44}) = f_{31}$$
$$f_{23} = f_{32} = 0$$

Secular determinant is given as

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

The solution of this determinant provides the same equations containing wave velocities as along directions [110] and [011].

7. Along symmetry direction [111]

Direction cosines along this direction are $\zeta_1 = \zeta_2 = \zeta_3 = 1/\sqrt{3}$

$$f_{11} = C_{1111}\zeta_1^2 + C_{1212}\zeta_2^2 + C_{1313}\zeta_3^2 = \frac{1}{3}(C_{11}+2C_{44})$$
$$f_{22} = C_{2121}\zeta_1^2 + C_{2222}\zeta_2^2 + C_{2323}\zeta_3^2 = \frac{1}{3}(C_{11}+2C_{44})$$
$$f_{33} = C_{3131}\zeta_1^2 + C_{3232}\zeta_2^2 + C_{3333}\zeta_3^2 = \frac{1}{3}(C_{11}+2C_{44})$$
$$f_{12} = C_{1122}\zeta_1\zeta_2 + C_{1221}\zeta_2\zeta_1 + C_{1123}\zeta_1\zeta_3 + C_{1321}\zeta_3\zeta_1 + C_{1223}\zeta_2\zeta_3 + C_{1322}\zeta_3\zeta_2$$
$$= \frac{1}{3}(C_{12}+C_{44}) = f_{21}$$
$$f_{13} = \frac{1}{3}(C_{12}+C_{44}) = f_{31}$$
$$f_{23} = \frac{1}{3}(C_{12}+C_{44}) = f_{32}$$

Secular determinant becomes

$$\begin{vmatrix} \frac{1}{3}(C_{11}+2C_{44})-\rho v^2 & \frac{1}{3}(C_{12}+C_{44}) & \frac{1}{3}(C_{12}+C_{44}) \\ \frac{1}{3}(C_{12}+C_{44}) & \frac{1}{3}(C_{11}+2C_{44})-\rho v^2 & \frac{1}{3}(C_{12}+C_{44}) \\ \frac{1}{3}(C_{12}+C_{44}) & \frac{1}{3}(C_{12}+C_{44}) & \frac{1}{3}(C_{11}+2C_{44})-\rho v^2 \end{vmatrix}=0$$

The solution of this determinant gives

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

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

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

First of the three equations provide velocity corresponding to longitudinal wave whereas the rest two equations yield velocities for transverse waves in terms of elastic constants C_{11}, C_{12} and C_{44}.

III. Conclusion

- Velocity of elastic waves through cubic crystal is same along symmetry directions [100],[010] and [001]. Also, wave velocity is same along orientations [110],[011] and [101].
- Velocities of longitudinal and transverse waves are different along a particular direction.
- Values of elastic constants C_{11}, C_{12} *and* C_{44} can be obtained by experimental measurement of velocity of elastic waves along different directions.

References

1) A.K.Ghatak & L.S.Kothari, An Introduction to Lattice Dynamics, Addison-Wesley Publishing Company(1990)
2) P.D.S.Verma, Theory of Elasticity, Vikas Publishing House(1997)
3) J. Rychlewski, On Hooke's law, Journal of Applied Mathematics and Mechanics, Volume 48, Issue 3, Pages 303-314(1984)
4) C.Kittel, Introduction to Solid State Physics, Wiley Eastern Ltd.(1993)