Wave Speed in Cubic Crystals

by Dr. Colton, Physics 581 (last updated: Fall 2020)

Objective

The purpose of this handout is to demonstrate how to use Eq. 3.57(a)(b)(c) to solve for the wave speed in a cubic crystal in any arbitrary direction, with any arbitrary polarization (oscillation direction).

General Wave Information

1) General exponential dependence is $e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$
2) Direction of travel tells you what $\mathbf{k}$ components are present. I.e. $\mathbf{k}$ points in the direction the wave is travelling.
3) Direction of oscillation (i.e. longitudinal vs. transverse, and which specific transverse direction) tells you which $\mathbf{u}$ components are present. Remember the components of $\mathbf{u}$ are what I call u_x, u_y, u_z and what the book calls u, v, w.

How to use Eq. 3.57 (a),(b),(c)

1) The Easy Way – If you know the specifics of u_x, u_y, u_z, plug them in from the start.

   - Example 1. (100) wave direction, longitudinal wave (i.e. the wave displacement $\mathbf{u}$ is also in $\mathbf{x}$ direction).

     The given info means that $\mathbf{k} = (k, 0,0)$ and $\mathbf{u} = u_x\hat{\mathbf{x}}e^{i(kx-\omega t)}$.

     Eq. 3.57(a) becomes

$$\rho\frac{\partial^2 u_x}{\partial t^2} = C_{11}\frac{\partial^2 u_x}{\partial x^2}$$

$$\rho w^2 u_x\hat{\mathbf{x}}e^{i(kx-wt)} = C_{11}k^2 u_x\hat{\mathbf{x}}e^{i(kx-\omega t)}$$

$$v = \frac{\omega}{k} = \sqrt{\frac{C_{11}}{\rho}}$$

     Note that the exponentials always cancel. I will not include them in the other examples, except inasmuch as $\frac{\partial^2}{\partial t^2}$ yields factors of $-\omega^2$.

   - Example 2. (100) wave direction transverse wave in the (0,1,0) direction

     The given info means that $\mathbf{k} = (k, 0,0)$ and $\mathbf{u} = (0, u_y, 0) = u_y\hat{\mathbf{y}}e^{i(kx-\omega t)}$.

     Eq. 3.57(b) becomes

$$\rho\frac{\partial^2 u_y}{\partial t^2} = C_{44}\frac{\partial^2 u_y}{\partial x^2}$$
$$\rho\omega^2 u_y = C_{44}k^2 u_y$$
$$v = \frac{\omega}{k} = \sqrt{\frac{C_{44}}{\rho}}$$

- Example 3. (110) wave direction, longitudinal wave

The given info means that $\mathbf{k} = k\left(\frac{\hat{\mathbf{x}}+\hat{\mathbf{y}}}{\sqrt{2}}\right)$ and $\mathbf{u} = u\left(\frac{\hat{\mathbf{x}}+\hat{\mathbf{y}}}{\sqrt{2}}\right)e^{i\left(k\left(\frac{\mathrm{x}+\mathrm{y}}{\sqrt{2}}\right)-\omega t\right)}$.

The exponential factor looks like that because

$$\begin{aligned}\mathbf{k}\cdot\mathbf{r} &= k_x x + k_y y + k_z z\\ &= \left(\frac{k}{\sqrt{2}}\right)x + \left(\frac{k}{\sqrt{2}}\right)y\\ &= \frac{k(x+y)}{\sqrt{2}}\end{aligned}$$

Eq. 3.57(a) becomes: (note I put both u_x and u_y in terms of u)

$$\rho\omega^2 u = C_{11}\frac{k^2}{2}u + C_{44}\frac{k^2}{2}u + (C_{12}+C_{44})\left(\frac{k^2}{2}u\right)$$
$$v = \frac{\omega}{k} = \sqrt{\frac{1}{2p}(C_{11}+C_{12}+2C_{44})}$$

2) <u>The Hard Way</u> – if you don't know all of the specifics, you will need to solve Eq. 3.57 (a),(b), and/or (c) as multiple simultaneous equations. They actually turn into an **eigenvalue matrix equation**.

- Example 4. (110) wave direction, unknown polarization direction in the x-y plane. (As we will find in the end, there are actually two possible polarizations in that plane—one longitudinal and the other transverse.)

The given info means that $\mathbf{k} = k\left(\frac{\hat{x}+\hat{y}}{\sqrt{2}}\right)$ and $\mathbf{u} = \underbrace{(u_x\hat{x} + u_y\hat{y})}_{u_z=0\text{ is known}}\underbrace{e^{i\left(k\left(\frac{x+y}{\sqrt{2}}\right)-\omega t\right)}}_{\text{known by }\mathbf{k}}$.

Eq. 3.57(a) becomes:

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

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

Eq. 3.57(b) becomes:

$$\rho\omega^2 u_y = \tfrac{1}{2}k^2(C_{11}+C_{44})u_y + \tfrac{1}{2}k^2(C_{12}+C_{44})u_x$$

Combine the two in matrix form,

$$\begin{pmatrix}\rho\omega^2 & 0\\ 0 & \rho\omega^2\end{pmatrix}\begin{pmatrix}u_x\\ u_y\end{pmatrix} = \frac{1}{2}k^2\begin{pmatrix}C_{11}+C_{44} & C_{12}+C_{44}\\ C_{12}+C_{44} & C_{11}+C_{44}\end{pmatrix}\begin{pmatrix}u_x\\ u_y\end{pmatrix}$$

This is an eigenvalue equation! That can be seen more easily by writing it like this:

$$\begin{pmatrix}\dfrac{C_{11}+C_{44}}{2\rho} & \dfrac{C_{12}+C_{44}}{2\rho}\\ \dfrac{C_{12}+C_{44}}{2\rho} & \dfrac{C_{11}+C_{44}}{2\rho}\end{pmatrix}\begin{pmatrix}u_x\\ u_y\end{pmatrix} = \frac{\omega^2}{k^2}\begin{pmatrix}u_x\\ u_y\end{pmatrix}$$

This is of the form $\mathbf{Av} = \lambda\mathbf{v}$. The eigenvalues λ are ω^2/k^2; i.e. in this example the two wave speeds for the two polarizations will be the square roots of the two eigenvalues of that matrix.

To solve for $v = \omega/k$ we do:

$$\begin{pmatrix}\dfrac{C_{11}+C_{44}}{2\rho} - \dfrac{\omega^2}{k^2} & \dfrac{C_{12}+C_{44}}{2\rho}\\ \dfrac{C_{12}+C_{44}}{2\rho} & \dfrac{C_{11}+C_{44}}{2\rho} - \dfrac{\omega^2}{k^2}\end{pmatrix}\begin{pmatrix}u_x\\ u_y\end{pmatrix} = 0$$

To have nonzero solutions, the determinant of the matrix must equal 0:

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

(that's called the "characteristic equation")

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

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

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

The two solution are either:

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

or

$$v = \frac{\omega}{k} = \sqrt{\frac{1}{2\rho}(C_{11} - C_{12})}$$

To determine the direction of oscillation for each of these velocities, plug the $\frac{\omega}{k}$ value back into Eq. 3.57 (either (a) or (b)) and solve for the $\frac{u_y}{u_x}$ ratio. One $\frac{\omega}{k}$ value turns out to give you $u_y = u_x$, the other gives you $u_y = -u_x$. The first is a longitudinal wave because (110) is the direction of travel; the second is a transverse wave because (–110) is perpendicular to the direction of travel. (This is exactly analogous to finding the eigenvectors once the eigenvalues are known.)

In general you might have to use all three of the Eq. 3.57 equations, and will end up with a 3×3 matrix equation, with three different wave speeds (three eigenvalues) and three different types of oscillations (three eigenvectors).