Lecture notes 9: Elastic waves in cubic solids

Outline:

- **Review: elastic stiffness constants in cubic solids**
- **Elastic waves in cubic crystals**
  - **Derivation of wave equation**
  - **Waves in two specific directions in a cubic crystal**

Review

Definitions:

- Stress: force per unit area
- Strain: dimensionless displacement due to applied stress

The displacement, **R**, of a volume element of a solid upon an arbitrary deformation is defined by

$$\boldsymbol{R}(\boldsymbol{r}) = u(\boldsymbol{r})\hat{\boldsymbol{x}} + v(\boldsymbol{r})\hat{\boldsymbol{y}} + w(\boldsymbol{r})\hat{\boldsymbol{z}}$$

Where the vector **r** defines the original position of that volume element, and **u,v,w** are continuous variables which are used to determine local strain

Local **strain** is given by variables e_{ij} where I,j=x,y,orz

Diagonal components of strain:

$$e_{xx} \equiv \frac{\partial u}{\partial x}$$
$$e_{yy} \equiv \frac{\partial v}{\partial y}$$

$$e_{zz} \equiv \frac{\partial w}{\partial z}$$

Off-diagonal components of strain:

$$e_{xy} \cong \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}$$

$$e_{yz} \cong \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}$$

$$e_{zx} \cong \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}$$

There are 6 distinct **stress** components: $X_x, X_y, Z_z, Y_z, Z_x, X_z$

The capital letter is the **direction of the force**, and the subscript is the **normal of the plane that the force is being applied to**. For example, the Y_z stress component is a sheer stress in the y direction, applied to the xy plane (to which the z axis is normal).

The stress and strain are connected to one another via a 3D generalization of Hooke's law.

Via **elastic compliance matrix (S):** $\boldsymbol{e} = \boldsymbol{SX}$ (analogous to x=F/k)

Via **elastic stiffness matrix C (more common in this class):** $\boldsymbol{X} = \boldsymbol{Ce}$ (analogous to F=kx)

C is a 6x6 matrix with 36 elements.

By symmetry considerations which apply to all crystal classes, **C** can be reduced to only having 21 unique elements.

Finally, for cubic crystal systems (which are the most symmetric), there are only **4** unique elements of **C**. This is the case that we will deal with explicitly.

$$\begin{pmatrix} X_x \\ Y_y \\ Z_z \\ Y_z \\ Z_x \\ X_y \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix} \begin{pmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \\ e_{yz} \\ e_{zx} \\ e_{xy} \end{pmatrix}$$

C_{11}: these terms are on the diagonal in the top left quadrant, and they denote elastic constants relevant when one pushed on one face and considers displacement in the same direction as the force. For a cubic crystal, this 'spring constant' is clearly the same whether the force is applied along x, y, z.

C_{12}: these terms are off diagonal in the top left quadrant. They are the elastic constants involved, for example, when you push/pull the cube in the x direction, and the cube bulges in the y and z direction. Clearly, the amount of bulging in that direction will be the same in both y and z (because it is a cube), and when an identical force is applied along the y or z direction, the other two dimensions will bulge or contract in the same way.

C_{44}: these are the components of sheer moduli. They are the same because sheering one plane in a cube is equivalent to sheering an orthogonal plane.

The compliance matrix (**S**) is the inverse of the stiffness matrix (**C**), and for a cubic system, its elements can be calculated pretty straighforwardly:

$$C_{44} = 1/S_{44}$$

$$C_{11} - C_{12} = (S_{11} - S_{12})^{-1}$$

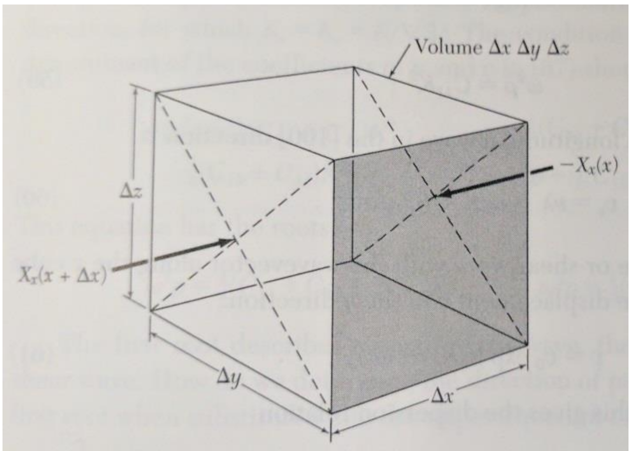
$$C_{11} + 2C_{12} = (S_{11} + 2S_{12})^{-1}$$

Elastic waves in cubic crystals

In this portion of the chapter we approach waves in elastic solids from a top down approach: we consider a continuous medium (ignore atoms) and only use the microscopic atomic structure to make symmetry constraints which make our equations easier. In the next chapter, we will use a bottom up approach where we begin with atoms, treat them like masses on a spring (which mathematically, they basically are because atomic potentials look like a harmonic oscillator at small displacements), and find that in aggregate this structure can be used to propagate elastic waves.

Both approaches to the problem reproduce the most significant way that non-electromagnetic information is transmitted in a solid. So if you shine light on a solid or apply a potential different between the two ends, that information will be transmitted at the speed of light. But if you wack one side of a solid with a hammer or heat up only one side of a solid, that information will be transmitted to the other side (primarily) by propagating elastic waves.

We begin the derivation by considering an **inhomogenous** force on a volume element. It should be noted that a uniform stretching or compression will **not** produce a propagating wave.



The volume element is expressed as a cube with lengths $\Delta x, \Delta y, \Delta z$

A stress $-X_x(x)$ acts on the front face, and a stresss $X_x(x+\Delta x) \approx X_x(X) + \frac{\partial X_x}{\partial x}\Delta x$ acts on the back face (the approximation is just the first two terms in an expansion about $\Delta x = 0$).

The net **force** on the **entire unit cube** is given by $\left(\frac{\partial X_x}{\partial x}\Delta \mathrm{x}\right)\Delta \mathrm{y}\Delta \mathrm{z}$, where the terms inside the parenthesis come from adding the stresses on the front and back face, and the other terms come from multiplying the stress by the area of the face that it is acting upon to get an answer in units of force

Other forces in the x-direction are provided by stresses X_y and X_z (forces applied in X direction to planes whose normal is in the y and z direction, respectively). These give forces of the form:

$X_y \rightarrow F = \left(\frac{\partial X_y}{\partial y}\Delta \mathrm{y}\right)\Delta x\Delta z$ (area of plane normal to y direction is $\Delta x\Delta z$)

$X_z \rightarrow F = \left(\frac{\partial X_z}{\partial z}\Delta \mathrm{z}\right)\Delta x\Delta y$ (area of plane normal to z direction is $\Delta x\Delta y$)

Thus, the **net** force acting in the x direction is given by:

$$F_x = \left(\frac{\partial X_x}{\partial x} + \frac{\partial X_y}{\partial y} + \frac{\partial X_z}{\partial z}\right)\Delta x\Delta y\Delta z$$

Force=mass*acceleration, and we consider the effect of these forces on a displacement variable, u. This u is the same u we used earlier to describe continuous deformations of a volume element of a solid

$$m\frac{\partial^2 u}{\partial t^2} = \left(\frac{\partial X_x}{\partial x} + \frac{\partial X_y}{\partial y} + \frac{\partial X_z}{\partial z}\right)\Delta x\Delta y\Delta z$$

Divide both sides by volume to make density, ρ, the prefactor in front of acceleration

$$\rho\frac{\partial^2 u}{\partial t^2} = \left(\frac{\partial X_x}{\partial x} + \frac{\partial X_y}{\partial y} + \frac{\partial X_z}{\partial z}\right)$$

From earlier, we have expressions for X_x, X_y, X_z in terms of strains e_{ij}. Again, we are only working in a cubic crystal system, so the matrix connecting stresses to strains is fairly sparse

$$X_x = C_{11}e_{xx} + C_{12}e_{yy} + C_{12}e_{zz}$$

$$X_y = C_{44}e_{xy}$$

$$X_z = Z_x = C_{44}e_{zx}$$

Plugging this in to the equation for acceleration above, we get:

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

Collect terms in front of common C components:

$$\rho\frac{\partial^2 u}{\partial t^2} = C_{11}\frac{\partial e_{xx}}{\partial x} + C_{12}(\frac{\partial e_{yy}}{\partial x} + \frac{\partial e_{zz}}{\partial x}) + C_{44}(\frac{\partial e_{xy}}{\partial y} + \frac{\partial e_{xz}}{\partial z})$$

Earlier, we had defined e_{ij} in terms of derivatives of u,v, and w, continuous variables describing local strain in the x, y, and z directions. Plugging in these earlier results we get:

$$\rho\frac{\partial^2 u}{\partial t^2} = C_{11}\frac{\partial^2 u}{\partial x^2} + C_{12}\left(\frac{\partial^2 v}{\partial y\partial x} + \frac{\partial^2 w}{\partial z\partial x}\right) + C_{44}(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 v}{\partial y\partial x} + \frac{\partial^2 u}{\partial z^2} + \frac{\partial^2 w}{\partial x\partial z})$$

Now collect terms which have common derivative terms

$$\rho\frac{\partial^2 u}{\partial t^2} = C_{11}\frac{\partial^2 u}{\partial x^2} + C_{44}\left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) + (C_{12} + C_{44})\left(\frac{\partial^2 v}{\partial y\partial x} + \frac{\partial^2 w}{\partial z\partial x}\right)$$

This is the wave equation very close to its familiar form, $\frac{\partial^2 u}{\partial t^2} = \frac{k}{\rho}\frac{\partial^2 u}{\partial x^2}$, in that one side has 2nd time derivatives, the other side has 2nd spatial derivatives, and the prefactor contains a spring constant (k) and a density. In the wave equation, people also define a propagation velocity, $c = \sqrt{\frac{k}{\rho}}$

By symmetry, the equations of motion for $\partial^2 v/\partial t^2$ and $\partial^2 w/\partial t^2$ are found in the same way, and they are written explicitly in your textbook.

Now we consider wave propagation in two specific directions in a cubic crystal

Waves in the [100] direction

Aside: what is the [100] direction?

- It is the direction **normal** to the (100) plane
- It is a vector pointing in the x direction only: $\boldsymbol{r} = \hat{\boldsymbol{x}}$

One solution to the wave equation that we have written is a longitudinal wave:

$$u = u_0 e^{i(Kx - \omega t)}$$

Longitudinal means that both the wavevector (K, the direction that the wave propagates in) and the direction of particles' motion is along the x direction.

We substitute this solution into the wave equation to solve for wavevector K in terms of variables we already have:

$$\omega^2 \rho = C_{11} K^2$$

The velocity of a longitudinal wave is given by angular frequency divided by wavevector ($v_s = \omega/K$) which is also related to the density and elastic constants:

$$v_s = \sqrt{\frac{C_{11}}{\rho}}$$

Now we consider a **transverse** or **shear** wave, where the wave propagates along the x axis, but displacements are along the y axis (for this example; they can in principle be along the z axis too)

Another solution to the wave equation above is:

$$v = v_0 e^{i(Kx - \omega t)}$$

When we substitute this into the wave equation we get:

$$\omega^2 \rho = C_{44} K^2$$

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

There are actually two shear waves, because we could have used the solution

$$w = w_0 e^{i(Kx - \omega t)}$$

For propagation in the [100] direction in a cubic system, both the shear waves have the same velocity.

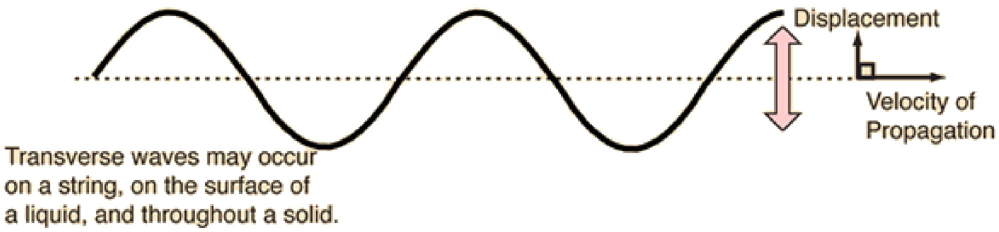
Important example of transverse/shear waves: S-waves in an earthquake (S is for shear). These waves propagate through the volume of the earth, rather than on the surface. And they involve a propagating ripple.

Q: is it better to be on denser, stiffer rock close to the earthquake epicenter or on less dense, more compliant rock further away?

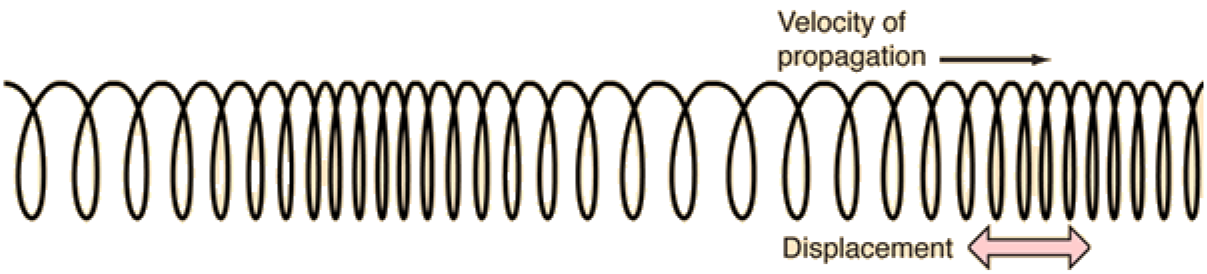
A: the propagation velocity has density in the denominator and an elastic constant in its numerator. The wave will move slower in a less dense rock, which isn't obviously good or bad by itself. But if the less-dense rock is also more compliant (smaller C) is means that the same force will produce a larger displacement. A larger displacement is generally bad if it happens inhomogenously to half of your house and not the other half.

Examples of longitudinal and transverse waves

Transverse: volume element moves in direction orthogonal to propagation direction



Longitudinal: volume element moves in same direction as propagation direction



Are the following types of waves transverse or longitudinal?

- Sound
- Ripples when you drop a rock into a tub of water

Waves in the [110] direction in cubic crystal

These waves propagate in the direction specified by the vector $\boldsymbol{r} = \hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}$

First, consider a shear wave which propagates in the xy plane with particle displacement w in the z direction

$$w = w_0 e^{i(K_x x + K_y y - \omega t)}$$

Plug this into the wave equation to get

$$\omega^2 \rho = C_{44}(K_x^2 + K_y^2) \equiv C_{44} K^2$$

We get the same propagation velocity for the transverse/shear wave as we did before

Now we consider a longitudinal wave: propagation in the xy plane and particle motion in the xy plane

We get two solutions:

$$u = u_0 e^{i(K_x x + K_y y - \omega t)}$$

$$v = v_0 e^{i(K_x x + K_y y - \omega t)}$$

When we plug this into the wave equation, we get two equations

$$0 = \left(C_{11}K_x^2 + C_{44}K_y^2 - \omega^2\rho\right)u + (C_{12} + C_{44})K_xK_yv$$

$$0 = \left(C_{11}K_y^2 + C_{44}K_x^2 - \omega^2\rho\right)v + (C_{12} + C_{44})K_xK_yu$$

In the [110] direction, we have an additional constraint that $K_x = K_y = K/\sqrt{2}$

The equation above can be expressed as a matrix equation of the form

$$0 = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \binom{u}{v}$$

And a nontrivial solution of this can be found by setting the determinant of the matrix to zero and finding the roots of that equation. Doing this, we get:

$\omega^2\rho = \frac{1}{2}(C_{11} + C_{12} + 2C_{44})K^2$ (longitudinal)

$\omega^2\rho = \frac{1}{2}(C_{11} - C_{12})K^2$ (transverse)

How do we know that these longitudinal or shear/transverse waves?

Substitute the first one into $0 = \left(C_{11}K_x^2 + C_{44}K_y^2 - \omega^2\rho\right)u + (C_{12} + C_{44})K_xK_yv$

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

When we set u=v, the equality is preserved, which means that the first equation describes a longitudinal wave.

Substitute the second root into the same equation:

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

This equality holds if we set u=-v, which implies particle displacement along the [1-10] direction, which is perpendicular to the [110] direction

Summary:

- In [100] (and equivalent) directions, there are two transverse (with the same velocity) and one longitudinal wave with different propagation velocities
- In [110] (and equivalent) directions, there are 2 transverse (with different propagation velocities) and one longitudinal (with different propagation velocity from the transverse) waves

Next lecture: microscopic derivation of waves in solids, starting with interatomic interactions.