NOTES 4: MASS IN MOTION: ELASTIC WAVES

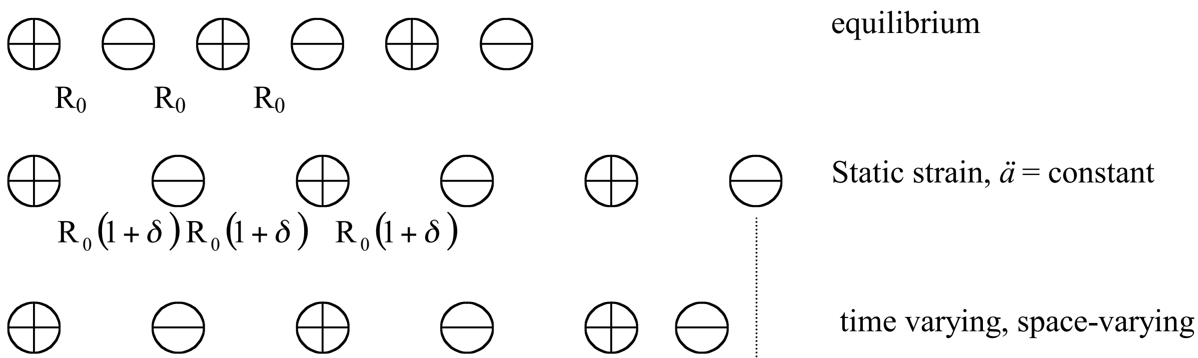
Solid with Time-Varying Pressure (Sound)

The previous Notes developed a powerful formalism – elasticity theory – which allows the mathematical description of the static response of a solid to an external force. The formalism works well provided the solid returns to its original form after the external force is removed (Hooke's law). But because the atoms are bound in potential "wells" whether by ionic, covalent, or metallic bonds, one might expect the bonds will "oscillate" about the equilibrium position if the force is applied or released suddenly. Stated in mechanical terms, the bond is equivalent to great extent to a mass-spring combination – a mechanical resonator. As in all resonators, there are two forms of energy and the oscillation entails the back-and-forth motion relative to the equilibrium point. This relatively simple concept is the basis for the entire field of solid-state acoustics.

To get a good image of how acoustics works in solids, we start with a simple one-dimensional model, which will also helps clarify the connection between acoustics and elasticity theory. The model pertains to an ionic-bond, but an identical analysis could be made for a covalent bond. Also, like the static elasticity formalism, the acoustic analysis does not care whether the solid is amorphous, crystalline, or something in between. But as we shall see in future notes on lattice waves and phonons, the analysis gets more elegant and some new effects occur (e.g., "optical" lattice waves) occur when the solid is crystalline.

One-Dimensional Analysis

One immediate benefit of being in one dimension is that the strain reduces from a 3x3 matrix (or 6-element column vector) to a scalar, which we call δ. We shall evaluate a small set of neighboring atoms with nearly identical bonds and equilibrium bond length, R_0 (again, this does not require a perfect crystal).



For static strain we had $P_m = \sum C_{mn} e_n$ which in 1D becomes $F = +K\delta$ (Hooke's Law)

In static case, a spatially-independent force exists (i.e., δ is independent of position)

But if $\delta = \delta(x)$ a spatial variation of the force will exist which can be calculated simply if slowly varying enough:

Define: $\Delta F \equiv F_2 - F_1$ (difference in force across a given length)

$$F_2 = F_1 + \left.\frac{\partial F}{\partial x}\right|_{r_2} (\Delta x) \quad \text{(starting from static)}$$

(F_1 ↑ static)

$$\Delta F = F_2 - F_1 = \left.\frac{\partial F}{\partial x}\right|_{r_2} \Delta x$$

but $F = +K\delta$

↑ A constant that depends only on R_0

so
$$\left.\frac{\partial F}{\partial x}\right|_{r_2} = +K\left.\frac{d\delta}{dx}\right|_{r_2}$$

Also we defined stress in such a way that in 1D, $\delta \equiv \frac{d\Delta r}{dx}$

so
$$\Delta F = +K\Delta x \left.\frac{d^2\Delta r}{dx^2}\right|_{r_2}$$

according to Newton's laws, any net force must correspond to an acceleration of a limit of mass.

m → mass of ion

a → acceleration $= \left.\frac{d^2\Delta r}{dt^2}\right|_{r_2}$

so we have $m\left.\frac{d^2\Delta r}{dt^2}\right|_{r_2} = K\Delta x\left.\frac{d^2\Delta r}{dx^2}\right|_{r_2}$ or $\frac{d^2\Delta r}{dt^2} - \frac{K}{\rho}\frac{d^2\Delta r}{dx^2} = 0$

Where $\frac{m}{\Delta x} \equiv \rho$ (linear density)

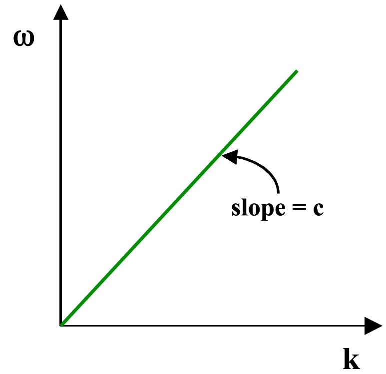
In HW#3 you will find general solutions: $f = f_1(ct - x) + f_2(ct + x)$ (due to Euler)

Where f_1 and f_2 arbitrary functions and $K/\rho = c^2$ where c is the wave velocity

The simplest solutions (and the only ones used in this course) are the sinusoids:

$$\Delta r = Ae^{j(kx-\omega t)} + Be^{j(kx+\omega t)}$$

yields: $\omega^2 = k^2c^2$ as expected: the dispersion curve for the plane wave.



Generalize to three-dimensions

The generalization to the realistic case of a 3D solid is facilitated by:

$$P_M = \sum_{N=1}^{6} C_{MN}\eta_N$$

stress stiffness strain

This assumed that η_M was uniform throughout solid for all M.
When η_M is non-uniform, we have the possibility of a net force acting along certain dimensions of a unit cube (see illustration below)
For example, the net force along x direction is:

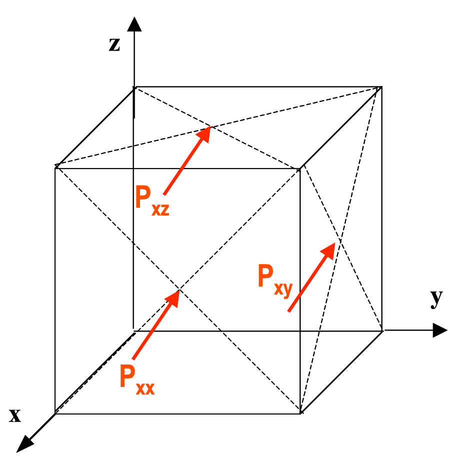
$$\Delta F_x = F_x' - F_{x0} = \frac{\partial P_{xx}}{\partial x}\Delta x \cdot \Delta A_x + \frac{\partial P_{xy}}{\partial y}\Delta y \cdot \Delta A_y + \frac{\partial P_{xz}}{\partial z}\Delta z \cdot \Delta A_z$$

where the facets A_x , A_y, and A_z are defined perpendicular to the respective axes.
But for small changes,

$$\Delta A_x = \Delta y \Delta z ; \Delta A_y = \Delta x \Delta z ; \Delta A_z = \Delta x \Delta y$$

and $\Delta V = \Delta x \Delta y \Delta z$

So
$$\Delta F_x = \left(\frac{\partial P_{xx}}{\partial x} + \frac{\partial P_{xy}}{\partial y} + \frac{\partial P_{xz}}{\partial z} \right) \Delta V$$



Similarly:

$$\Delta F_y = \left(\frac{\partial P_{yx}}{\partial x} + \frac{\partial P_{yy}}{\partial y} + \frac{\partial P_{yz}}{\partial z} \right) \Delta V$$

$$\Delta F_z = \left(\frac{\partial P_{zx}}{\partial x} + \frac{\partial P_{zy}}{\partial y} + \frac{\partial P_{zz}}{\partial z} \right) \Delta V$$

And just as in the 1D case, the nonzero ΔF must create an acceleration of mass (Newton's Law)

$$\Delta \vec{F} = \Delta F_x \hat{x} + \Delta F_y \hat{y} + \Delta F_z \hat{z} = m \frac{\partial^2 \Delta \vec{r}}{\partial t^2}$$

At this point the easiest action is the same decomposition of the stress as in the elasticity formalism: into six unique terms:

$$P_{xx} \equiv P_1 \qquad P_{yy} \equiv P_2 \qquad P_{zz} \equiv P_3$$

$$P_{yz} = P_{zy} \equiv P_4 \qquad P_{xz} = P_{zx} \equiv P_5 \qquad P_{xy} = P_{yx} \equiv P_6$$

and utilize the matrix relationship $P_M = \sum_{N=1}^{6} C_{MN} \eta_N$ so that wave equation becomes

$$\frac{m}{\Delta V} \frac{d^2 \Delta r}{dt^2} = \left(\frac{\partial P_1}{\partial x} + \frac{\partial P_6}{\partial y} + \frac{\partial P_5}{\partial z} \right) \hat{x} + \left(\frac{\partial P_6}{\partial x} + \frac{\partial P_2}{\partial y} + \frac{\partial P_4}{\partial z} \right) \hat{y} + \left(\frac{\partial P_5}{\partial x} + \frac{\partial P_4}{\partial y} + \frac{\partial P_3}{\partial z} \right) \hat{z}$$

At this point we take one of two paths:

1. analytic: look at each term on RHS using $P_M = \sum_{N=1}^{6} C_{MN} \eta_N$ and utilize zero C_{MN} elements to eliminate many terms.
2. numeric: expand all $\frac{\partial P}{\partial x}, \frac{\partial P}{\partial y}, \frac{\partial P}{\partial z}$ in terms of $\frac{\partial \eta}{\partial x}, \frac{\partial \eta}{\partial y}, \frac{\partial \eta}{\partial z}$ and compute by brute force

- for this course, we follow path (1) only. As we would need powerful (matrix-based) code like Matlab for path 2
- for path (1) it's good to keep the elements of C matrix close by for reference (look at Kittel (50) in Chapter 3).

For example, the x components in an isotropic solid or one with cubic symmetry:

$$\frac{\partial P_1}{\partial x} = \sum_{N=1}^{6} C_{1N} \frac{\partial \eta_N}{\partial x} = C_{11} \frac{\partial \eta_1}{\partial x} + C_{12} \frac{\partial \eta_2}{\partial x} + C_{12} \frac{\partial \eta_3}{\partial x}$$

$$\frac{\partial P_6}{\partial y} = \sum_{N=1}^{6} C_{6N} \frac{\partial \eta_N}{\partial y} = C_{44} \frac{\partial \eta_6}{\partial y}$$

$$\frac{\partial P_5}{\partial z} = \sum_{N=1}^{6} C_{5N} \frac{\partial \eta_N}{\partial z} = C_{44} \frac{\partial \eta_5}{\partial z}$$

$$\frac{\partial P_4}{\partial z} = \sum_{N=1}^{6} C_{4N} \frac{\partial \eta_N}{\partial z} = C_{44} \frac{\partial \eta_4}{\partial z}$$

but recall definition of strain components (for all η_N slowly varying in space)

$$\eta_1 \equiv \eta_{xx} = \varepsilon_{xx} = \frac{d\Delta r_x}{dx}$$

$$\eta_2 \equiv \eta_{yy} = \varepsilon_{yy} = \frac{d\Delta r_y}{dy}$$

$$\eta_3 \equiv \eta_{zz} = \varepsilon_{zz} = \frac{d\Delta r_z}{dz}$$

$$\eta_4 \equiv \eta_{yz} = \varepsilon_{yz} + \varepsilon_{zy} = \frac{d\Delta r_y}{dz} + \frac{d\Delta r_z}{dy}$$

$$\eta_5 \equiv \eta_{zx} = \varepsilon_{zx} + \varepsilon_{xz} = \frac{d\Delta r_z}{dx} + \frac{d\Delta r_x}{dz}$$

$$\eta_6 \equiv \eta_{xy} = \varepsilon_{xy} + \varepsilon_{yx} = \frac{d\Delta r_x}{dy} + \frac{d\Delta r_y}{dx}$$

Hence, the wave equation for the x component Δr_x becomes

$$\frac{m}{\Delta V}\frac{d^2\Delta r_x}{dt^2} = \Delta F_x = C_{11}\frac{\partial^2 \Delta r_x}{\partial x^2} + C_{12}\frac{\partial^2 \Delta r_y}{\partial x \partial y} + C_{12}\frac{\partial^2 \Delta r_z}{\partial x \partial z} + C_{44}\left(\frac{\partial^2 \Delta r_x}{\partial y^2} + \frac{\partial^2 \Delta r_y}{\partial x \partial y}\right) + C_{44}\left(\frac{\partial^2 \Delta r_z}{\partial x \partial z} + \frac{\partial^2 \Delta r_x}{\partial z^2}\right)$$

$$= C_{11}\frac{\partial^2 \Delta r_x}{\partial x^2} + C_{44}\left(\frac{\partial^2 \Delta r_x}{\partial y^2} + \frac{\partial^2 \Delta r_x}{\partial z^2}\right) + \left(C_{12} + C_{44}\right)\left(\frac{\partial^2 \Delta r_y}{\partial x \partial y} + \frac{\partial^2 \Delta r_z}{\partial x \partial z}\right)$$

similar analysis for Δr_y and Δr_z components yields

$$\frac{m}{\Delta V}\frac{d^2\Delta r_y}{dt^2} = C_{11}\frac{\partial^2 \Delta r_y}{\partial y^2} + C_{44}\left(\frac{\partial^2 \Delta r_y}{\partial x^2} + \frac{\partial^2 \Delta r_y}{\partial z^2}\right) + \left(C_{12} + C_{44}\right)\left(\frac{\partial^2 \Delta r_x}{\partial y \partial x} + \frac{\partial^2 \Delta r_z}{\partial y \partial z}\right)$$

$$\frac{m}{\Delta V}\frac{d^2\Delta r_z}{dt^2} = C_{11}\frac{\partial^2 \Delta r_z}{\partial z^2} + C_{44}\left(\frac{\partial^2 \Delta r_z}{\partial x^2} + \frac{\partial^2 \Delta r_z}{\partial y^2}\right) + \left(C_{12} + C_{44}\right)\left(\frac{\partial^2 \Delta r_x}{\partial z \partial x} + \frac{\partial^2 \Delta r_y}{\partial z \partial y}\right)$$

Note the similar form of these equations

<u>Very important observation:</u>

- each component equation couples Δr_x, Δr_y, and Δr_z through time and space derivatives. Thus if we look for *plane-wave* solutions $e^{j(k\cdot r-\omega t)}$, we will find for Δr_x

$\Delta r_x = \Delta r_{x_0} e^{j(k_x x-\omega t)}$ → propagation along x axis

$\Delta r_x = \Delta r_{x_0} e^{j(k_y y-\omega t)}$ → propagation along y axis

$\Delta r_x = \Delta r_{x_0} e^{j(k_z z-\omega t)}$ → propagation along z axis

and similarly for Δr_y and Δr_z. So there are two types of plane waves:

1) component of Δr along propagation direction → compressional wave
2) component of Δr perpendicular to propagation direction → shear wave

For example: plane wave in x direction of isotropic solid or one with cubic symmetry:

→ $\Delta r_x = \Delta r_{x_0} e^{j(k_x x-\omega t)}$ (compressional)

$\Delta r_y = \Delta r_{y_0} e^{j(k_x x-\omega t)}$ (shear)

$\Delta r_z = \Delta r_{z_0} e^{j(k_x x-\omega t)}$ (shear)

or general solution $\Delta r = \left(\Delta r_{x_0}\hat{x} + \Delta r_{y_0}\hat{y} + \Delta r_{z_0}\hat{z}\right)e^{j(kx-\omega t)}$

Substitution into coupled wave equations yields (x component)

$$\frac{m}{\Delta V}\frac{d^2\Delta r_x}{dt^2} = -C_{11}\Delta r_{x_0} k^2 e^{j(kx-\omega t)}$$ or by taking time derivative

or $$\rho\omega^2 = \frac{m}{\Delta V}\omega^2 = C_{11}k^2;\ v_p \equiv \frac{\omega}{k} = \sqrt{\frac{C_{11}}{\rho}}$$ phase velocity

Second equation (y component)

$$\rho\frac{d^2\Delta r_y}{dt^2} = -C_{44}\Delta r_{y_0} k^2 e^{j(ky-\omega t)}$$

or $$\rho\omega^2 = C_{44}k^2;\ v_p = \sqrt{\frac{C_{44}}{\rho}}$$ phase velocity

Third equation (z component)

$$\rho\frac{d^2\Delta r_z}{dt^2} = -C_{44}\Delta r_{z_0} k^2 e^{i(kz-\omega t)}$$

or $$\rho\omega^2 = C_{44}k^2;\ v_p = \sqrt{\frac{C_{44}}{\rho}}$$ phase velocity

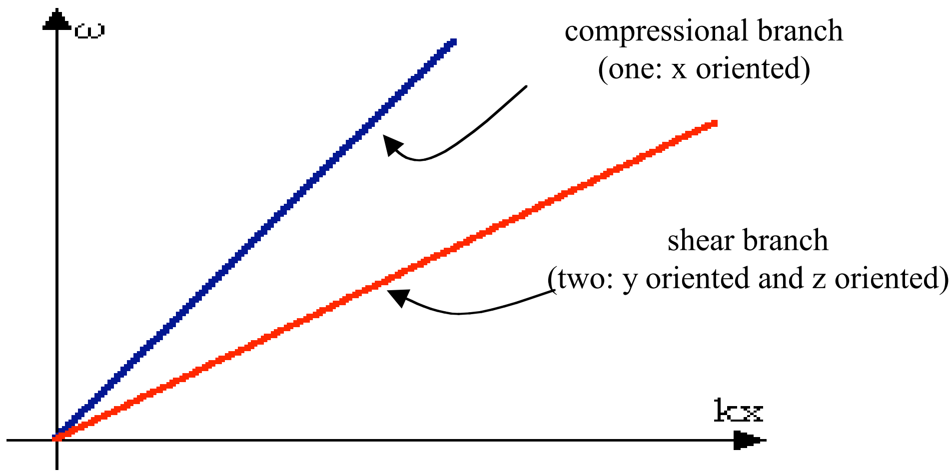
• note: in all common isotropic solids or ones with cubic symmetry $C_{11} > C_{44}$

1) e.g. Cubic silicon $C_{11} = 1.66\times10^{11}\ N/m^2;\ C_{44} = 0.796\times10^{11}\ N/m^2\quad \rho = 2330\ kg/m^3$

→ $$v = \sqrt{\frac{C_{11}}{\rho}} = 8441\ m/s$$ (compressional)

$$v = \sqrt{\frac{C_{44}}{\rho}} = 5845\ m/s$$ (shear)

General trend: v(compressional)> v(shear)



• note: since C coefficients measure stiffness, stiffer materials display higher sound velocities. Stiffness is closely related to hardness: both reflect the curvature of potential energy valley in the microscopic bonds !

Perspective on sound velocity in solids vs gases and liquids:

- velocity of sound in water $= 1481\, m/s = \sqrt{\dfrac{B}{\rho}}$ B→ Bulk modulus of water, $\rho \equiv 1000\, \mathrm{KG/m^3}$

(1 atm, 298 K)

- velocity of sound in air $= v \approx \sqrt{\dfrac{P}{\rho}} \approx 331\, m/s$

using $P = 1\, atm = 10^5\, N/m^2$

$$\text{so } \frac{v_{solid}}{v_{gas}} \approx \sqrt{\underset{0.5\times 10^6}{\frac{C}{P}}\ \underset{\sim 10^{-3}}{\frac{\rho_{gas}}{\rho_{solid}}}} \approx \sqrt{500}$$

• So it's the hardness, or large spring constants of solids that makes sound velocity higher than in fluids !
• Higher density causes sound velocity to go down!