Outline

- Review Lecture 4
- 3-D Elastic Continuum
- 3-D Lattice Waves
- Lattice Density of Modes
- Specific Heat of Lattice
Specific Heat Measurements

\[ \frac{\Delta E}{V} \approx \left[ g(E_{F_0})k_B T \right] \]

excited states  \[ k_B T \]

increase in energy
3-D Elastic Continuum
Poisson’s Ratio Example

A prismatic bar with length $L = 200$ mm and a circular cross section with a diameter $D = 10$ mm is subjected to a tensile load $P = 16$ kN. The length and diameter of the deformed bar are measured and determined to be $L' = 200.60$ mm and $D' = 9.99$ mm. What are the modulus of elasticity and the Poisson’s ratio for the bar?
3-D Elastic Continuum
Shear Strain

Shear loading

Shear plus rotation

Pure shear

Shear loading

Shear plus rotation

Pure shear

\[ \frac{u_x(y + dy)}{L_y} = \tan(2\phi) \approx 2\phi \]

Pure shear strain

\[ \phi = E_{xy} = \frac{1}{2} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \]

Shear stress

\[ T_{xy} = G \ 2\phi = 2GE_{xy} \quad G \ is \ shear \ modulus \]
3-D Elastic Continuum
Stress and Strain Tensors

\[ E_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]

\[ E_{xx} = \frac{\partial u_x}{\partial x} \]

\[ E_{xy} = \frac{1}{2} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \]

\[ e = \sum_{k=1}^{3} E_{kk} \]

For *most* general isotropic medium,

\[ T = \lambda eI + 2\mu E \]

Initially we had three elastic constants: \( E_Y, G, e \)

Now reduced to only two: \( \lambda, \mu \)
3-D Elastic Continuum
Stress and Strain Tensors

\[ T_{ij} = \lambda e \delta_{ij} + 2\mu E_{ij} \]

If we look at just the diagonal elements

\[ \sum_{k=1}^{3} T_{kk} = 3\lambda e + 2\mu e \]

\[ e = \frac{1}{3\lambda + 2\mu} \sum_{k=1}^{3} T_{kk} \]

Inversion of stress/strain relation:

\[ E_{ij} = \frac{1}{2\mu} \left[ T_{ij} - \frac{\lambda}{3\lambda + 2\mu} \left( \sum_{k} T_{kk} \right) \delta_{ij} \right] \]
3-D Elastic Continuum
Example of Uniaxial Stress

\[ \frac{L_o}{L} \]

\[ T_{11} \neq 0 \]

\[ E_{ij} = \frac{1}{2\mu} \left[ T_{ij} - \frac{\lambda}{3\lambda + 2\mu} \left( \sum_k T_{kk} \right) \delta_{ij} \right] \]

\[ E_{11} = \frac{\lambda + \mu}{\mu(3\lambda + 2\mu)} \frac{\lambda + \mu}{E_Y} T_{11} \]

\[ E_{22} = E_{33} = -\frac{\lambda}{2(\lambda + \mu)} E_{11} \]
Dynamics of 3-D Continuum

3-D Wave Equation

Net force on incremental volume element:

\[ F = \int_V f \, dx\, dy\, dz \]

\[ F = \int_V \rho \frac{\partial^2 u}{\partial t^2} \, dx\, dy\, dz \]

\[ f = \rho \frac{\partial^2 u}{\partial t^2} \]

Total force is the sum of the forces on all the surfaces
Dynamics of 3-D Continuum

3-D Wave Equation

Net force in the x-direction:

\[ F_x = \sum_{\text{surfaces}} (T_{xx} \, dA_x + T_{xy} \, dA_y + T_{xz} \, dA_z) \]

\[ \sum_{\text{surface}} T_{xx} \, dA_x = \frac{T_{xx}(x + dx) - T_{xx}(x)}{dx} \, dx \, dy \, dz \]

\[ \sum_{\text{surface}} T_{xx} \, dA_x = \frac{\partial T_{xx}}{\partial x} \, dx \, dy \, dz \]

\[ F_x = \int \int \int \left[ \frac{\partial T_{xx}}{\partial x} + \frac{\partial T_{xy}}{\partial y} + \frac{\partial T_{xz}}{\partial z} \right] \, dx \, dy \, dz \]
Dynamics of 3-D Continuum

3-D Wave Equation

\[ F_x = \int \int \int \left[ \frac{\partial T_{xx}}{\partial x} + \frac{\partial T_{xy}}{\partial y} + \frac{\partial T_{xz}}{\partial z} \right] \, dx \, dy \, dz \]

\[ T_{ij} = \lambda \delta_{ij} + 2\mu E_{ij} \]

\[ F_x = \int \int \int \left[ (\mu + \lambda) \frac{\partial}{\partial x} (\nabla \cdot \mathbf{u}) + \mu \nabla^2 \mathbf{u}_x \right] \, dx \, dy \, dz \]

Finally, 3-D wave equation....

\[ \rho \frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{r}, t) = (\mu + \lambda) \nabla [(\nabla \cdot \mathbf{u}(\mathbf{r}, t))] + \mu \nabla^2 \mathbf{u}(\mathbf{r}, t) \]
Dynamics of 3-D Continuum
Fourier Transform of 3-D Wave Equation

\[ \rho \frac{\partial^2 u}{\partial t^2}(r, t) = (\mu + \lambda) \nabla [(\nabla \cdot u(r, t)] + \mu \nabla^2 u(r, t) \]

Anticipating plane wave solutions, we Fourier Transform the equation….

\[ u(r, t) = \int \frac{d\omega}{2\pi} \int \frac{d^3q}{(2\pi)^3} U(q, \omega) e^{i(q \cdot r - \omega t)} \]

\[ \rho \omega^2 U(q, \omega) = (\lambda + \mu) q [q \cdot U(q, \omega)] + \mu q^2 U(q, \omega) \]

Three coupled equations for \( U_x, U_y, \) and \( U_z \)….
Dynamics of 3-D Continuum

Dynamical Matrix

\[ \rho \omega^2 U_i(q, \omega) = (\lambda + \mu) q_i [q \cdot U(q, \omega)] + \mu q^2 U_i(q, \omega) \]

Express the system of equations as a matrix….

\[ \rho \omega^2 \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix} = \begin{bmatrix} \mu q^2 + (\lambda + \mu) q_1^2 & (\lambda + \mu) q_1 q_2 & (\lambda + \mu) q_1 q_3 \\ (\lambda + \mu) q_2 q_1 & \mu q^2 + (\lambda + \mu) q_2^2 & (\lambda + \mu) q_2 q_3 \\ (\lambda + \mu) q_3 q_1 & (\lambda + \mu) q_3 q_2 & \mu q^2 + (\lambda + \mu) q_3^2 \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix} \]

Turns the problem into an eigenvalue problem for the polarizations of the modes (eigenvectors) and wavevectors \( q \) (eigenvalues)….

\[ \rho \omega^2 U = D U \]
Dynamics of 3-D Continuum
Solutions to 3-D Wave Equation

\[ \rho \omega^2 U_i(q, \omega) = (\lambda + \mu)q_i [q \cdot U(q, \omega)] + \mu q^2 U_i(q, \omega) \]

Transverse polarization waves:

\[ q \cdot U(q, \omega) = 0 \]

\[ \rho \omega^2 = \mu q^2 \quad \text{for transverse waves} \]

\[ \omega = c_T |q| \quad \text{where} \quad c_T = \sqrt{\frac{\mu}{\rho}} \]

Longitudinal polarization waves:

\[ q \cdot U(q, \omega) = q U \]

\[ \rho \omega^2 U = (\lambda + 2\mu)q^2 U \quad \text{for longitudinal waves} \]

\[ \omega = c_L |q| \quad \text{where} \quad c_L = \sqrt{\frac{\lambda + 2\mu}{\rho}} \]
Direct Measurements of Sound Velocity

LA phonons are faster, since real solids are not isotropic the TA phonons travel at different velocity
Dynamics of 3-D Continuum

Summary

1. Dynamical Equation can be solved by inspection

\[ \rho \omega^2 U(q, \omega) = (\lambda + \mu)q \cdot U(q, \omega) + \mu q^2 U(q, \omega) \]

2. There are 2 transverse and 1 longitudinal polarizations for each \( q \)

3. The dispersion relations are linear

\[ \omega = c_i |q| \]

\[ c_T = \sqrt{\frac{\mu}{\rho}} \quad c_L = \sqrt{\frac{\lambda + 2\mu}{\rho}} \]

4. The longitudinal sound velocity is always greater than the transverse sound velocity

\[ \frac{c_L}{c_T} = \left( \frac{\lambda + 2\mu}{\mu} \right)^{1/2} = \left( 1 + \frac{1}{1 - 2\nu} \right)^{1/2} \]
Counting Vibrational Modes
Solid as an Acoustic Cavity

For each of three polarizations:

\[ u_k(r, t) = \exp \left[ i(k \cdot r \pm \omega t) \right] \hat{\epsilon}_{k,\omega} \]

If the plane waves are constrained to the solid with dimension \( L \) and we use periodic boundary conditions:

\[ k = \left( \frac{2n_1\pi}{L}, \frac{2n_2\pi}{L}, \frac{2n_3\pi}{L} \right) \quad \text{with} \quad n_i = \pm 1, \pm 2, \pm 3 \ldots \]

\[ \frac{d^3k}{(2\pi/L)^3} = L^3 g_\sigma(\omega) \ d\omega \]

\[ \frac{4\pi k^2 \ dk}{(2\pi)^3} = g_\sigma(\omega) \ d\omega \]

number of states in \( d\omega \):

\[ g_\sigma(\omega) = \frac{\omega^2}{2\pi^2 c_\sigma^3} \]
Specific Heat of Solid
How much energy is in each mode?

Need to approximate the amount of energy in each mode at a given temperature…

If we assume equipartition, we will again Dulong-Petit which is not consistent with experiment for solids…

Approach:

• Quantize the amplitude of vibration for each mode
• Treat each quanta of vibrational excitation as a bosonic particle, the phonon
• Use Bose-Einstein statistics to determine the number of phonons in each mode
Lattice Waves as Harmonic Oscillator

Treat each mode and each polarization as an independent harmonic oscillator:

\[ E = \sum_{k,\sigma} \hbar \omega_{k,\sigma} \left[ n_{k,\sigma} + \frac{1}{2} \right] \]

\( n_{k,\sigma} \) is the quantum number associated with harmonic

Now, we think of each quantum of excitation as a particle…

lattice waves
acoustic cavity (solid)
quanta observed by light scattering
bosons ?
electromagnetic waves
optical cavity (metal box)
quanta observed by photoelectric effect
bosons (eg. laser)
Lattice Waves in Thermal Equilibrium

Lattice waves in thermal equilibrium don’t have a single well define amplitude of vibration…

For each mode, there is a distribution of amplitudes…

\[
E = \sum_{k,\sigma} \hbar \omega_{k,\sigma} \left[ \langle n_{k,\sigma} \rangle + \frac{1}{2} \right]
\]

Bose-Einstein distribution

\[
\langle n_{k,\sigma} \rangle = \frac{1}{e^{\hbar \omega_{k,\sigma}/k_B T} - 1}
\]
Total Energy of a Lattice in Thermal Equilibrium

\[ E = \sum_{k,\sigma} \frac{\hbar \omega_{k,\sigma}}{e^{\frac{\hbar \omega_{k,\sigma}}{k_B T}} - 1} \]

\[ \frac{E}{V} = \sum_{\sigma} \int \frac{\hbar \omega}{e^{\frac{\hbar \omega}{k_B T}} - 1} g_{\sigma}(\omega) \, d\omega \]

number of states in \( d\omega \):
\[ g_{\sigma}(\omega) = \frac{\omega^2}{2\pi^2 c_\sigma^3} \]

\[ \frac{E}{V} = \sum_{\sigma} \int \frac{\hbar \omega^3}{2\pi^2 c_\sigma^3 (e^{\frac{\hbar \omega}{k_B T}} - 1)} \, d\omega \]
Specific Heat of a Crystal Lattice

\[ \frac{E}{V} = \sum_{\sigma} \int \frac{\hbar \omega^3}{2\pi^2 c_\sigma^3 (e^{\hbar \omega/k_BT} - 1)} d\omega \]

\[ \frac{E}{V} = \sum_{\sigma} \frac{(k_BT)^4}{2\pi^2 c_\sigma^3 \hbar^3} \int_{0}^{\infty} \frac{x^3 dx}{e^x - 1} \]

\[ x = \hbar \omega/k_BT \]

\[ \frac{E}{V} = \sum_{\sigma} \frac{\pi^2 k^4_B T^4}{30 c_\sigma^3 \hbar^3} \]

\[ C_V = \frac{\partial (E/V)}{\partial T} = AT^3 \]

\[ A = \frac{2\pi^2}{5} \frac{k_b^4}{\hbar^3 v_s^3} \]

\[ v_s^{-3} = 3(c_L^{-3} + 2c_T^{-3}) \]
Specific Heat Measurements

\[ C_v = C_{el} + C_{phonon} = \gamma T + AT^3 \]

(hyperphysics.phy-astr.gsu.edu)
Aside: Thermal Energy of Photons

Energy density of blackbody:

\[
\frac{E}{V} = \int_0^\infty \frac{\hbar \omega^3}{\pi^2 c^3 \sigma \left( e^{\hbar \omega / k_B T} - 1 \right)} \, d\omega
\]

\[
\frac{E}{V} = \frac{\pi^2 k_B^4 T^4}{15 c \hbar^3}
\]

Specific heat:

\[
C_V = \frac{4 \pi^2 k_B^4 T^3}{15 c \hbar^3}
\]