6.730 Physics for Solid State Applications

Lecture 5: Specific Heat of Lattice Waves

Outline

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

February 13, 2004

3-D Elastic Continuum

Stress and Strain Tensors

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

$$\rightarrow \quad E_{xx} = \frac{\partial u_x}{\partial x}$$

$$\rightarrow \quad E_{xy} = \frac{1}{2}\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)$$

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

For *most* general isotropic medium,

$$\mathbf{T} = \lambda \mathbf{e}\mathbf{I} + 2\mu\mathbf{E}$$

Initially we had three elastic constants: E_Y, G, e

Now reduced to only two: λ, μ

Dynamics of 3-D Continuum
Fourier Transform of 3-D Wave Equation

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

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

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

$$\rho\omega^2\mathbf{U}(\mathbf{q},\omega) = (\lambda+\mu)\mathbf{q}\left[\mathbf{q}\cdot\mathbf{U}(\mathbf{q},\omega)\right] + \mu\mathbf{q}^2\mathbf{U}(\mathbf{q},\omega)$$

Three coupled equations for U_x, U_y, and U_z….

Dynamics of 3-D Continuum
Dynamical Matrix

$$\rho\omega^2\mathbf{U}_\mathbf{i}(\mathbf{q},\omega) = (\lambda+\mu)\mathbf{q}_\mathbf{i}\left[\mathbf{q}\cdot\mathbf{U}(\mathbf{q},\omega)\right]+\mu\mathbf{q}^2\mathbf{U}_\mathbf{i}(\mathbf{q},\omega)$$

Express the system of equations as a matrix….

$$\rho\omega^2\begin{bmatrix}\mathbf{U}_1\\ \mathbf{U}_2\\ \mathbf{U}_3\end{bmatrix} = \begin{bmatrix}\mu q^2+(\lambda+\mu)q_1^2 & (\lambda+\mu)q_1q_2 & (\lambda+\mu)q_1q_3\\ (\lambda+\mu)q_2q_1 & \mu q^2+(\lambda+\mu)q_2^2 & (\lambda+\mu)q_2q_3\\ (\lambda+\mu)q_3q_1 & (\lambda+\mu)q_3q_2 & \mu q^2+(\lambda+\mu)q_3^2\end{bmatrix}\begin{bmatrix}\mathbf{U}_1\\ \mathbf{U}_2\\ \mathbf{U}_3\end{bmatrix}$$

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

$$\rho\omega^2\mathbf{U} = \mathbf{D}\,\mathbf{U}$$

Dynamics of 3-D Continuum

Solutions to 3-D Wave Equation

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

Transverse polarization waves:

$$\mathbf{q}\cdot\mathbf{U}(\mathbf{q},\omega) = \mathbf{0}$$

$$\rho\omega^2 = \mu q^2 \qquad \text{for transverse waves}$$

$$\omega = c_T|\mathbf{q}| \qquad \text{where} \qquad c_T = \sqrt{\frac{\mu}{\rho}}$$

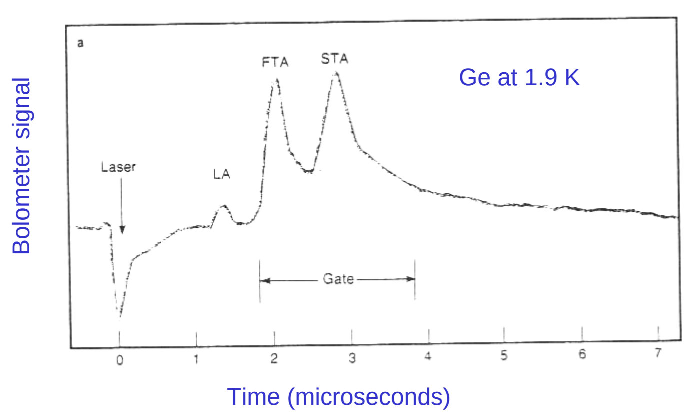
Longitudinal polarization waves:

$$\mathbf{q}\cdot\mathbf{U}(\mathbf{q},\omega) = \mathbf{qU}$$

$$\rho\omega^2 U = (\lambda+2\mu)q^2 U \qquad \text{for longitudinal waves}$$

$$\omega = c_L|\mathbf{q}| \qquad \text{where} \qquad c_L = \sqrt{\frac{\lambda+2\mu}{\rho}}$$

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

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

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

3. The dispersion relations are linear $\omega = c_i|\mathbf{q}|$

$$c_T = \sqrt{\frac{\mu}{\rho}} \qquad c_L = \sqrt{\frac{\lambda+2\mu}{\rho}}$$

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:

$$\mathbf{u}_{\mathbf{k}}(\mathbf{r},t) = \exp\left[i(\mathbf{k}\cdot\mathbf{r} \pm \omega \mathbf{t})\right]\vec{\epsilon}_{\mathbf{k},\omega}$$

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

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

$$\frac{d^3\mathbf{k}}{(2\pi/L)^3} = L^3 g_\sigma(\omega)\,d\omega$$

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

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:

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

$n_{\mathbf{k},\sigma}$ is the quantum number associated with harmonic

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

lattice waves	electromagnetic waves
acoustic cavity (solid)	optical cavity (metal box)
quanta observed by light scattering	quanta observed by photoelectric effect
bosons ?	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…

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

Bose-Einstein distribution

$$\langle n_{\mathbf{k},\sigma} \rangle = \frac{1}{e^{\hbar\omega_{\mathbf{k},\sigma}/k_B T} - 1}$$

Total Energy of a Lattice in Thermal Equilibrium

$$E = \sum_{\mathbf{k},\sigma} \frac{\hbar\omega_{\mathbf{k},\sigma}}{e^{\hbar\omega_{\mathbf{k},\sigma}/k_B T} - 1}$$

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

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

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

Specific Heat of a Crystal Lattice

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

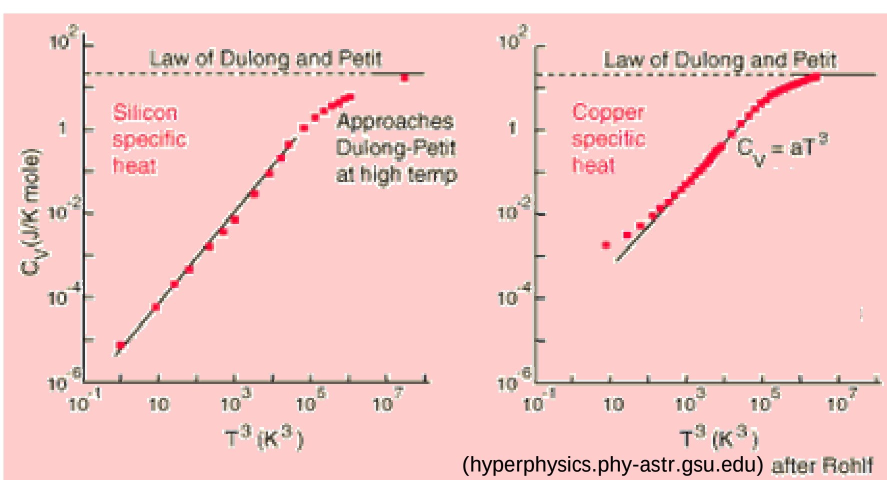
$$\frac{E}{V} = \sum_\sigma \frac{(k_B T)^4}{2\pi^2 c_\sigma^3 \hbar^3} \underbrace{\int_0^\infty \frac{x^3 dx}{e^x - 1}}_{\pi^4/15} \qquad x = \hbar\omega/k_B T$$

$$\boxed{\frac{E}{V} = \sum_\sigma \frac{\pi^2 k_B^4 T^4}{30 c_\sigma^3 \hbar^3}}$$

$$\boxed{C_V = \frac{\partial(E/V)}{\partial T} = AT^3} \qquad A = \frac{2\pi^2}{5} \frac{k_B^4}{\hbar^3 v_s^3}$$

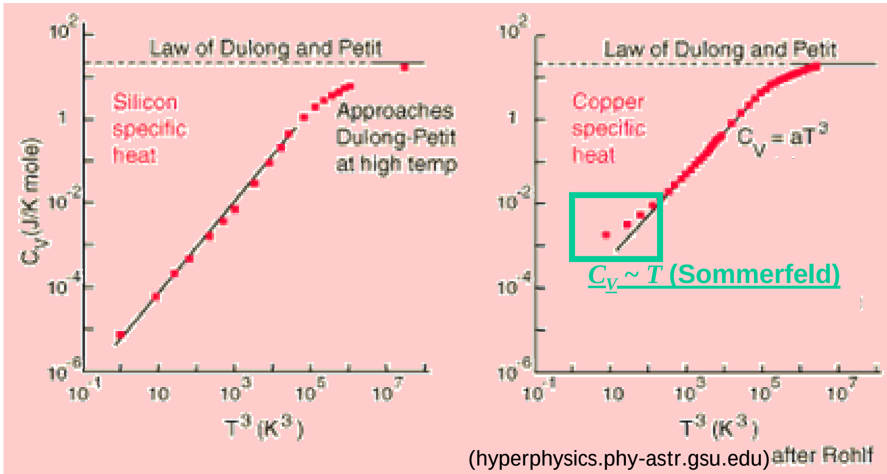
$$v_s^{-3} = 3(c_L^{-3} + 2c_T^{-3})$$

Specific Heat Measurements



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

Specific Heat Measurements



$$\frac{\Delta E}{V} \approx \underbrace{[g(E_{Fo})k_B T]}_{\text{excited states}} \qquad \underbrace{k_B T}_{\text{increase in energy}}$$

Aside: Thermal Energy of Photons

Energy density of blackbody:

$$\frac{E}{V} = \int_0^\infty \frac{\hbar\omega^3}{\pi^2 c_\sigma^3 (e^{\hbar\omega/k_B T} - 1)} d\omega$$

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

Specific heat :

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