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

Specific Heat Measurements

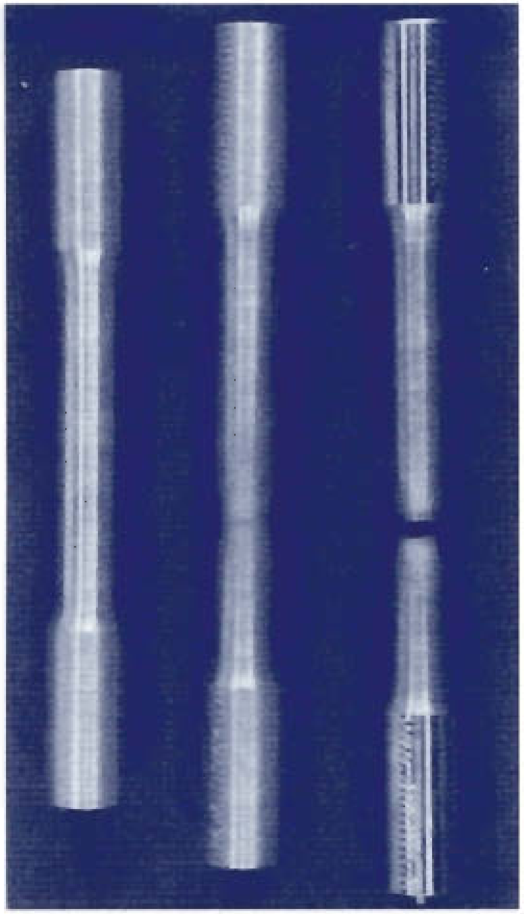
(hyperphysics.phy-astr.gsu.edu)

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

3-D Elastic Continuum

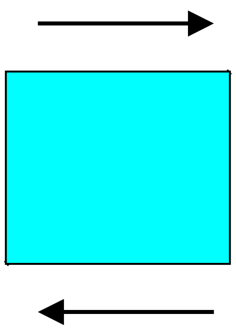
Poisson's Ratio Example

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?

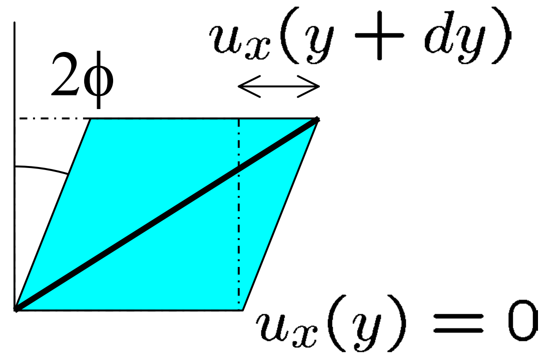


3-D Elastic Continuum
Shear Strain

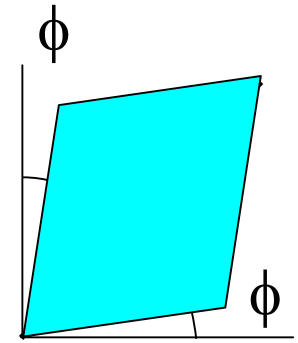
Shear loading



Shear plus rotation



Pure shear



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

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

$$T_{xy} = G\,2\phi = 2GE_{xy}$$

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,

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

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

Now reduced to only two: λ, μ

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

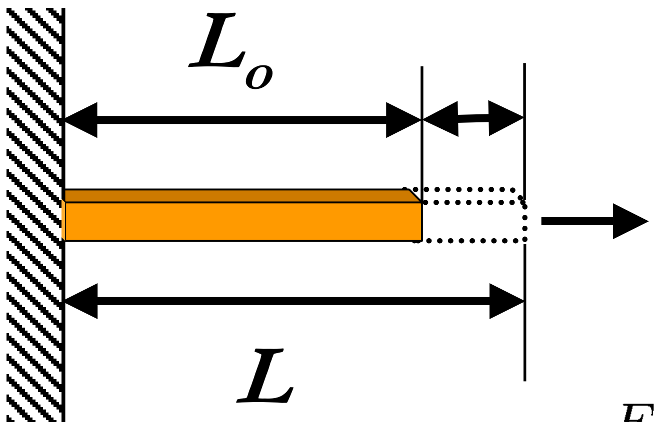
$$\sum_{k=1}^{3} T_{kk} = 3\lambda e + 2\mu e$$

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

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



$T_{11} \neq 0$

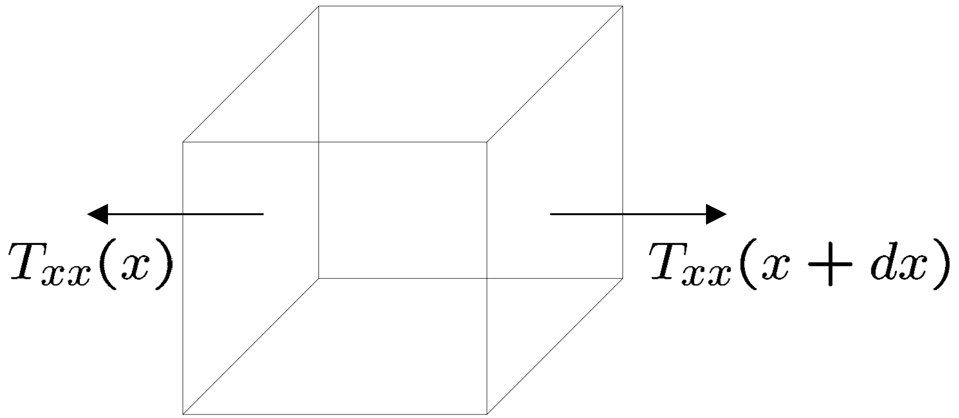
$$E_{ij} = \frac{1}{2\mu}\left[T_{ij} - \frac{\lambda}{3\lambda + 2\mu}\left(\sum_k T_{kk}\right)\delta_{ij}\right]$$

$$E_{11} = \underbrace{\frac{\lambda + \mu}{\mu(3\lambda + 2\mu)}}_{E_Y} T_{11}$$

$$E_{22} = E_{33} = -\underbrace{\frac{\lambda}{2(\lambda + \mu)}}_{\nu} E_{11}$$

Dynamics of 3-D Continuum

3-D Wave Equation



Net force on incremental volume element:

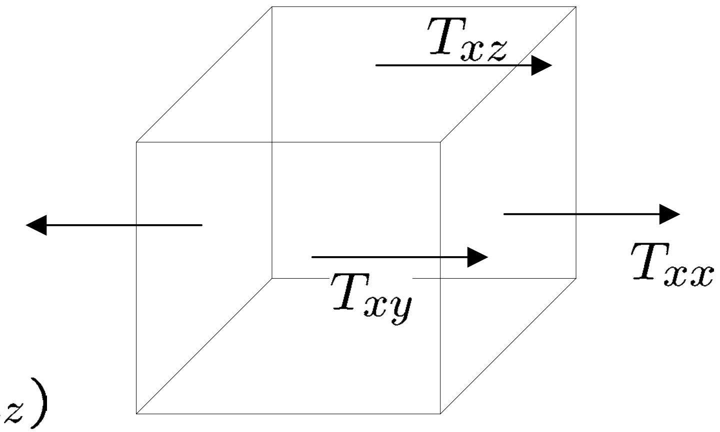
$$\mathbf{F} = \int_{\mathbf{V}} \mathbf{f} \mathbf{dxdydz}$$

$$\mathbf{F} = \int_{\mathbf{v}} \rho \frac{\partial^2 \mathbf{u}}{\partial \mathbf{t}^2} \mathbf{dxdydz}$$

$$\mathbf{f} = \rho \frac{\partial^2 \mathbf{u}}{\partial \mathbf{t}^2}$$

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:

$$F_x = \sum_{\text{surfaces}} \left(T_{xx}\, dA_x + T_{xy}\, dA_y + T_{xz}\, dA_z \right)$$

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

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

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

Dynamics of 3-D Continuum

3-D Wave Equation

$$F_x = \int\int\int \left[\frac{\partial T_{xx}}{\partial x} + \frac{\partial T_{xy}}{\partial y} + \frac{\partial T_{xz}}{\partial z} \right] dx\, dy\, dz \qquad T_{ij} = \lambda e\, \delta_{ij} + 2\mu E_{ij}$$

$$F_x = \int_v \rho \frac{\partial^2 \mathbf{u}}{\partial t^2} dx dy dz = \int\int\int \underbrace{\left[(\mu + \lambda) \frac{\partial}{\partial x} (\nabla \cdot \mathbf{u}) + \mu \nabla^2 \mathbf{u_x} \right]}_{\mathbf{f}_x} dx\, dy\, dz$$

Finally, 3-D wave equation….

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

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

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

Express the system of equations as a matrix….

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

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:

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

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

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

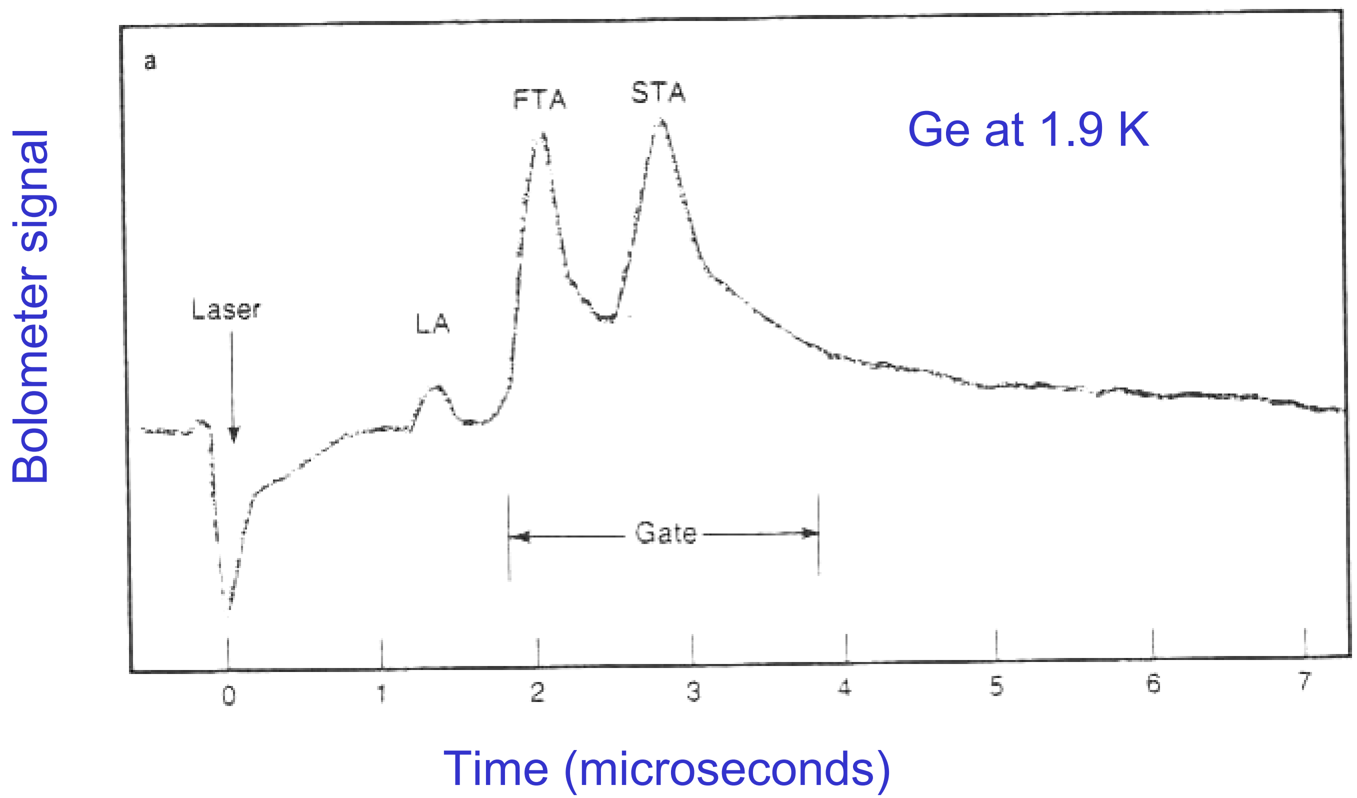
Longitudinal polarization waves:

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

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

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

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

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

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:

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

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

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

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

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

number of states in $d\omega$:

$$\boxed{g_\sigma(\omega) = \frac{\omega^2}{2\pi^2 c_\sigma^3}}$$

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 $d\omega$: $$g_\sigma(\omega) = \frac{\omega^2}{2\pi^2 c_\sigma^3}$$

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

Specific Heat of a Crystal Lattice

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

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

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

$$\boxed{C_V = \frac{\partial (E/V)}{\partial T} = A T^3}$$

$$A = \frac{2\pi^2}{5} \frac{k_B^4}{\hbar^3 v_s^3}$$

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

Specific Heat Measurements

(hyperphysics.phy-astr.gsu.edu)

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

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 :

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