# 6.730 Physics for Solid State Applications

## Lecture 4: Vibrations in Solids

# <u>Outline</u>

- Review Lecture 3
- Sommerfeld Theory of Metals
- 1-D Elastic Continuum
- 1-D Lattice Waves
- 3-D Elastic Continuum
- 3-D Lattice Waves

### Microscopic Variables for Electrical Transport Drude Theory

Balance equation for forces on electrons:

$$m\frac{d\mathbf{v}(r,t)}{dt} = -\underbrace{m\frac{\mathbf{v}(r,t)}{\tau}}_{\mathsf{DRAG FORCE}} \underbrace{\frac{-e\left[\mathbf{E}(\mathbf{r},\mathbf{t}) + \mathbf{v}(\mathbf{r},\mathbf{t}) \times \mathbf{B}(\mathbf{r},\mathbf{t})\right]}_{\mathsf{LORENTZ FORCE}}$$

In steady-state when **B=0**:

$$\mathbf{v} = -\frac{e\tau}{m} \mathbf{E}_{\mathsf{DC}}$$

$$\mathbf{J} = -ne\mathbf{v} = \frac{ne^2\tau}{m} \mathbf{E}_{\mathsf{DC}}$$

$${
m J}=\sigma {
m E}_{
m DC}$$
 and  $\sigma={{
m ne}^2 au\over {
m m}}$ 



$$n = \frac{N}{V} = \int_{-\infty}^{\infty} \frac{1}{1 + e^{(E_{\mathbf{k}} - \mu)/k_B T}} 2\frac{d^3 \mathbf{k}}{(2\pi)^3}$$

$$n = \int_{-\infty}^{\infty} g(E)f(E-\mu)dE = \int_{-\infty}^{\infty} g(E)\frac{1}{1+e^{(E-\mu)/k_BT}}dE$$

### **Microscopic Variables for Electrical Transport**

Balance equation for energy of electrons:

$$\frac{dE}{dt} = -\frac{\Delta E}{\tau} + IV$$

In steady-state:

$$\Delta E = \tau I V$$

In the continuum models, we assume that electron scattering is sufficiently fast that all the energy pumped into the electrons is randomized; all additional energy heats the electrons

How do we relate  $\Delta E$  and T?

## **Specific Heat and Heat Capacity**

Again assume that the heat and change in internal energy are the same:

$$c_V = \left(\frac{dQ}{dT}\right)_V = \left(\frac{dE_{\text{total}}}{dT}\right)_V$$
 (heat capacity)

Take constant volume since this ensures none of the extra energy is going into *work* (think ideal gas)

$$C_V = \frac{1}{V} \frac{d}{dT} \left(\frac{3}{2} N k_B T\right) = \frac{3}{2} n k_B \qquad \text{(specific heat)}$$

$$C_v = 2 \times 10^6 \frac{\text{erg}}{\text{cm}^3 - \text{K}} = 11 \frac{\text{Joule}}{\text{mole-K}}$$

Specific heat is independent of temperature...Law of Dulong and Petit

## **Specific Heat Measurements**

(hyperphysics.phy-astr.gsu.edu)

### Specific heat is independent of temperature...NOT TRUE !

To get this correct we will need to (a) quantize electron energy levels, (b) introduce discreteness of lattice and (c) the heat capacity of lattice

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### Low Temperature Specific Heat of the Free Electron Gas Sommerfeld Approximation



Conductivity of the Free Electron Gas Sommerfeld Approximation

$$\begin{aligned} \mathbf{v}_{d} &= (-\mathbf{e}\tau/\mathbf{m})\mathbf{E}_{\mathsf{DC}} \\ \mathbf{v} &= \mathbf{v}_{\mathsf{F}} - \frac{\mathbf{e}\tau}{\mathbf{m}}\mathbf{E}_{\mathsf{DC}} \\ E &= \frac{1}{2}mv^{2} \approx \frac{1}{2}mv_{F}^{2} + e\tau\mathbf{v}\cdot\mathbf{E}_{\mathsf{DC}} \\ \Delta E &= e\tau v_{F}|\mathbf{E}_{\mathsf{DC}}| \end{aligned}$$



$$J = -e(\delta n)v_F$$

 $\delta n \approx g(E_F) \Delta E$ 

Only electrons near  $E_F$  contribute to current !

Conductivity of the Free Electron Gas Sommerfeld Approximation





Sommerfeld recovers the phenomenological results !

# Sommerfeld Expansion

$$f(E-\mu) = \lim_{T \to 0} \frac{1}{1 + e^{(E-\mu)/k_B T}} = 1 - u(E-\mu)$$
$$f'(E-\mu) = -\delta(E - E_{Fo})$$

$$\int_{-\infty}^{\infty} f(E-\mu)H(E)dE = \int_{-\infty}^{\mu} H(E)dE + \frac{\pi^2}{6}(k_BT)^2 H'(\mu) + O\left(\frac{k_BT}{E_{F0}}\right)^4$$
$$\int_{-\infty}^{\mu} H(E)dE = \int_{-\infty}^{E_{F0}} H(E)dE + (\mu - E_{F0})H(E_{F0}) + O\left(\frac{k_BT}{E_{F0}}\right)^4$$

## Sommerfeld Expansion for Electron Density

$$n = \underbrace{\int_{0}^{E_{F0}} g(E)dE}_{\approx n} + \underbrace{\left[(\mu - E_{F0})g(E_{F0}) + \frac{\pi^{2}}{6}(k_{B}T)^{2}g'(E_{F0})\right]}_{0}$$

$$\mu = E_{F0} \left\{ 1 - \frac{\pi^2}{6} \left( \frac{(k_B T)^2}{E_{F0}} \right) \frac{g'(E_{F0})}{g(E_{F0})} \right\}$$

$$\mu = E_{F0} \left\{ 1 - \frac{1}{3} \left( \frac{\pi k_B T}{2 E_{F0}} \right)^2 \right\}$$

# Sommerfeld Expansion for Electron Energy

$$\frac{E}{\nabla} = \int_{-\infty}^{\infty} Eg(E)f(E-\mu)dE$$
  
=  $\int_{0}^{E_{F0}} Eg(E)dE + E_{F0} \underbrace{\left[(\mu - E_{F0})g(E_{F0}) + \frac{\pi^{2}}{6}(k_{B}T)^{2}g'(E_{F0})\right]}_{0}$   
+  $\frac{\pi^{2}}{6}(k_{B}T)^{2}g(E_{F0}) + O(T^{4})$ 

$$\frac{E}{V} = \int_0^{E_{F0}} Eg(E)dE + \frac{\pi^2}{6} (k_B T)^2 g(E_{F0})$$

$$=\frac{3}{5}E_{F}n+\frac{\pi^{2}}{6}(k_{B}T)^{2}g(E_{F}0)$$

$$C_V = \frac{\partial \left( (E/V) \right)}{\partial T} \bigg|_{V,N} = \frac{\pi^2}{3} k_B^2 T g(E_{F0}) = \gamma T$$

## **Specific Heat Measurements**

(hyperphysics.phy-astr.gsu.edu)

To get this correct we will need to (a) quantize electron energy levels, (b) introduce discreteness of lattice and (c) the heat capacity of lattice

## Density of States is the Central Character in this Story

Goal: Calculate electrical properties (eg. resistance) for solids

### Approach:

In the end calculating resistance boils down to calculating the electronic energy levels and wavefunctions; to knowing the *bandstructure* 

You will be able to relate a bandstructure to macroscopic parameters for the solid

$$\sigma = e^2 v_F^2 \tau g(E_F)$$

$$C_V = \frac{\partial \left( (E/V) \right)}{\partial T} \bigg|_{V,N} = \frac{\pi^2}{3} k_B^2 T g(E_{F0}) = \gamma T$$

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### 1-D Elastic Continuum Stress and Strain

uniaxial loading



### Stress:

$$T_{xx} = \frac{F_x}{A} \left[ N/m^2 \right]$$

Strain:  $\delta(dx) = u_x(x + dx) - u_x(x)$ Normal strain:  $E_{xx} = \frac{\delta(dx)}{dx} = \frac{\partial u_x}{\partial x}$ 

If  $u_x$  is uniform there is no strain, just rigid body motion.

# **1-D Elastic Continuum**

Young's Modulus

 $T_{xx} = E_Y E_{xx}$ 

### Young's Modulus For Various Materials (GPa) from Christina Ortiz

#### **CERAMICS GLASSES AND SEMICONDUCTORS**

Diamond (C)	1000
Tungsten Carbide (WC)	450 -650
Silicon Carbide (SiC)	450
Aluminum Oxide $(Al_2O_3)$	390
Berylium Oxide (BeO)	380
Magnesium Oxide (MgO)	250
Zirconium Oxide (ZrO)	160 - 241
Mullite $(Al_6Si_2O_{13})$	145
Silicon (Si)	107
Silica glass $(SiO_2)$	94
Soda-lime glass ( $Na_2O - SiO_2$ )	69

### **METALS :**

Tungsten (W)	406
Chromium (Cr)	289
Berylium (Be)	200 - 289
Nickel (Ni)	214
Iron (Fe)	196
Low Alloy Steels	200 - 207
Stainless Steels	190 - 200
Cast Irons	170 - 190
Copper (Cu)	124
Titanium (Ti)	116
Brasses and Bronzes	103 - 124
Aluminum (Al)	69

#### PINE WOOD (along grain): 10

### **POLYMERS :**

Polyimides	3 - 5
Polyesters	1 - 5
Nylon	2 - 4
Polystryene	3 - 3.4
Polyethylene	0.2 -0.7
Rubbers / Biological	
Tissues	0.01-0.1



Net force on incremental volume element:

$$f_x = [T_{xx}(x + dx) - T_{xx}(x)] \, dy \, dz$$
$$m \frac{\partial^2 u_x}{\partial t^2} = [T_{xx}(x + dx) - T_{xx}(x)] \, dy \, dz$$

$$\rho \frac{\partial^2 u_x}{\partial t^2} dx \, dy \, dz = [T_{xx}(x+dx) - T_{xx}(x)] \, dy \, dz$$

$$\rho \frac{\partial^2 u_x}{\partial t^2} = \frac{\partial T_{xx}}{\partial x}$$

### Dynamics of 1-D Continuum 1-D Wave Equation



Velocity of sound, c, is proportional to stiffness and inverse prop. to inertia

Dynamics of 1-D Continuum 1-D Wave Equation Solutions

$$\frac{\partial^2 u_x}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 u_x}{\partial t^2}$$

### **Clamped Bar: Standing Waves**

$$u_x(x,t) = A_{\pm} \sin(kx) \exp(i\omega t)$$
  $\omega = ck$ 

$$u_{x,m,\pm}(x,t) = A_{m,\pm} \sin\left(\frac{m\pi x}{L}\right) \exp\left(\pm i\frac{m\pi c}{L}t\right)$$
 $m\pi$ 

$$k = \frac{m\pi}{L}$$
 for  $m = 1, 2, ...$ 

Dynamics of 1-D Continuum 1-D Wave Equation Solutions

$$\frac{\partial^2 u_x}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 u_x}{\partial t^2}$$

### Periodic Boundary Conditions: Traveling Waves

$$u_x(x,t) = A_{\pm} \exp(ikx) \exp(i\omega t)$$
  $\omega = ck$ 

$$u_{x,n,\pm}(x,t) = B_{n,\pm} \exp\left(\pm i \frac{2n\pi x}{L}(x\pm ct)\right)$$

$$k = \frac{2n\pi}{L}$$
 for  $n = \pm 1, \pm 2, \dots$ 

### 3-D Elastic Continuum Volume Dilatation



$$e = \frac{\delta V}{V} = \frac{dx(1 + E_{xx})dy(1 + E_{yy})dz(1 + E_{zz}) - dxdydz}{dxdydz}$$

 $e = E_{xx} + E_{yy} + E_{zz}$ 

Volume change is sum of all three normal strains

### 3-D Elastic Continuum Poisson's Ratio

$$E_{xx} = \frac{\partial u_x}{\partial x}$$
  $E_{yy} = \frac{\partial u_y}{\partial y}$   $E_{zz} = \frac{\partial u_z}{\partial z}$ 

$$e = E_{xx} + E_{yy} + E_{zz} = \nabla \cdot \mathbf{u}(\mathbf{r})$$

v is Poisson's Ratio – ratio of lateral strain to axial strain

$$E_{yy} = E_{zz} = -\nu E_{xx}$$
$$e = E_{xx}(1 - 2\nu)$$

Poisson's ratio can not exceed 0.5, typically 0.3

3-D Elastic Continuum Poisson's Ratio Example

Aluminum:  $E_{\gamma}$ =68.9 GPa,  $\nu$  = 0.35



### 3-D Elastic Continuum Poisson's Ratio Example

Aluminum:  $E_{\gamma}$ =68.9 GPa,  $\nu$  = 0.35



$$\Delta l = -0.0173 \text{mm}$$

## 3-D Elastic Continuum Poisson's Ratio Example

Aluminum:  $E_{\gamma}$ =68.9 GPa,  $\nu$  = 0.35

$$T_{xx} = \frac{F_x}{A} = \frac{5 \times 10^3}{\pi (10 \times 10^{-3})^2} = -15.9 \text{MPa}$$

$$F_{xx} = \frac{T_{xx}}{E_Y} = \frac{-15.9 \times 10^6}{68.9 \times 10^9} = -0.231 \times 10^{-3}$$

$$E_{xx} = \frac{\Delta l}{l} = -0.231 \times 10^{-3}$$

$$\Delta l = -0.0173 \text{mm}$$

$$E_{trns} = -\nu E_{xx} = -0.35 E_{xx} = 0.081 \times 10^{-3}$$
$$E_{trns} = \frac{\Delta d}{d} \qquad \qquad \Delta d = +0.001617 \text{mm}$$

### 3-D Elastic Continuum Shear Strain



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

For most general isotropic medium,

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

Initially we had three elastic constants:  $E_{\gamma}$ , 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



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

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



Net force on incremental volume element:

$$\mathbf{F} = \int_{\mathbf{V}} \mathbf{f} \mathbf{d} \mathbf{x} \mathbf{d} \mathbf{y} \mathbf{d} \mathbf{z}$$

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

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

Total force is the sum of the forces on all the surfaces



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

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

### Dynamics of 3-D Continuum 3-D Wave Equation

$$F_{x} = \int \int \int \left[ \frac{\partial T_{xx}}{\partial x} + \frac{\partial T_{xy}}{\partial y} + \frac{\partial T_{xz}}{\partial z} \right] dx dy dz \qquad T_{ij} = \lambda e \,\delta_{ij} + 2\mu E_{ij}$$
$$F_{x} = \int_{v} \rho \frac{\partial^{2} \mathbf{u}}{\partial t^{2}} dx dy dz = \int \int \int \int \underbrace{\left[ (\mu + \lambda) \frac{\partial}{\partial x} (\nabla \cdot \mathbf{u}) + \mu \nabla^{2} \mathbf{u}_{\mathbf{x}} \right]}_{\mathbf{f}_{x}} dx dy dz$$

Finally, 3-D wave equation....

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

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

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

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

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

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

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....

$$\rho\omega^{2}\begin{bmatrix}\mathbf{U}_{1}\\\mathbf{U}_{2}\\\mathbf{U}_{3}\end{bmatrix} = \begin{bmatrix}\mu q^{2} + (\lambda + \mu)q_{1}^{2} & (\lambda + \mu)q_{1}q_{2} & (\lambda + \mu)q_{1}q_{3}\\ (\lambda + \mu)q_{2}q_{1} & \mu q^{2} + (\lambda + \mu)q_{2}^{2} & (\lambda + \mu)q_{2}q_{3}\\ (\lambda + \mu)q_{3}q_{1} & (\lambda + \mu)q_{3}q_{2} & \mu q^{2} + (\lambda + \mu)q_{3}^{2}\end{bmatrix}\begin{bmatrix}\mathbf{U}_{1}\\\mathbf{U}_{2}\\\mathbf{U}_{3}\end{bmatrix}$$

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

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

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:

 $\mathbf{q} \cdot \mathbf{U}(\mathbf{q}, \omega) = \mathbf{q}\mathbf{U}$   $\rho \omega^2 U = (\lambda + 2\mu)q^2 U$  $\omega = c_L |\mathbf{q}|$  where

for longitudinal waves

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

### 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  $\omega = c_i |\mathbf{q}|$

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

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

$$\frac{c_L}{c_T} = \left(\frac{\lambda + 2\mu}{\mu}\right)^{1/2} = \left(1 + \frac{1}{1 - 2\nu}\right)^{1/2}$$