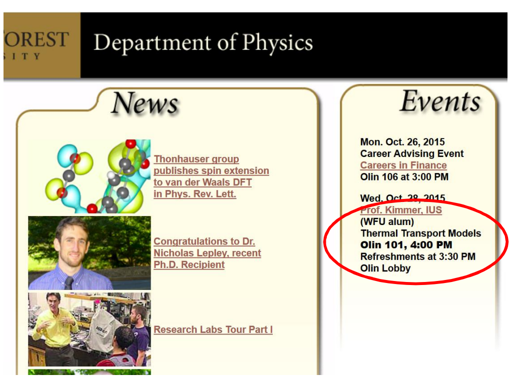
PHY 752 Solid State Physics
11-11:50 AM MWF Olin 103

Plan for Lecture 25:

- **Optical and transport properties of metals (Chap. 11 in GGGPP)**
  - **Boltzmann treatment of electrical transport in metals**
  - **Thermal transport**

12	Mon, 9/21/2015	Chap. 4	One electron approximations to the many electron problem	#11
13	Wed, 9/23/2015	Chap. 4	Density functional theory	#12
14	Fri, 9/25/2015	Chap. 5	Implementation of density functional theory	#13
15	Mon, 9/28/2015	Chap. 5	Implementation of density functional theory	#14
16	Wed, 9/30/2015	Chap. 5	First principles pseudopotential methods	#15
17	Fri, 10/02/2015	Chap. 6	Example electronic structures	#16
18	Mon, 10/05/2015	Chap. 6	Ionic and covalent crystals	#17
19	Wed, 10/07/2015	Chap. 6	More examples of electronic structures	#18
20	Fri, 10/09/2015	Chap. 1-6	Review	Start exam
	Mon, 10/12/2015		No class	Take-home exam
	Wed, 10/14/2015		No class	Exam due before 10/19/2015
	Fri, 10/16/2015		Fall break -- no class	
21	Mon, 10/19/2015	Chap. 10	X-ray and neutron diffraction	#19
22	Wed, 10/21/2015	Chap. 10	Scattering of particles by crystals	#20
23	Fri, 10/23/2015	Chap. 11	Optical and transport properties of metals	#21
24	Mon, 10/26/2015	Chap. 11	Optical and transport properties of metals	#22
25	Wed, 10/28/2015	Chap. 11	Transport in metals	#23
	Wed, 12/02/2015		Student presentations I	
	Fri, 12/04/2015		Student presentations II	
	Mon, 12/07/2015		Begin Take-home final	



WFU Physics Colloquium

TITLE: Effect of interfacial adhesive layers on thermal transport in model systems

SPEAKER: Christopher J. Kimmer, (WFU alum)

School of Natural Sciences,
Indiana University Southeast

TIME: Wednesday October 28, 2015 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge. All interested persons are cordially invited to attend.

ABSTRACT

The thermal properties of nanoscale systems often critically depend on phonon scattering at internal interfaces. The Kapitza conductance of an interface provides an overall measure of this scattering, and the ability to design systems with a prescribed or maximal conductance requires a deeper understanding of how interfacial properties effect this quantity. Experimental challenges with measurements of thermal properties at the nanoscale along with the need for predictive models to aid in systems design invites computer simulation to play a prominent role in the study of phonon-mediated thermal transport in these systems. One proposed approach to enhancing thermal transport across an interface is to include so-called adhesive layers with vibrational properties intermediate to those on either side of the interface. We focus on the effects of adhesion layers by considering model bicrystalline systems on diamond lattices interacting via the Stillinger-Weber interatomic potential. We vary the thickness, atomic mass, and interfacial bonding to conduct a study of the effect of these parameters on the interfacial conductance. The systems are characterized using the "direct method", a non-equilibrium molecular dynamics approach. We find the strongest enhancement in transport at weak interfacial bonding and discuss the implications of this result.

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Boltzmann distribution function:
f(**r**,**k**,*t*)

Number of electrons per phase space volume at the phase space point **r**, **k**, and time *t*

Equilibrium distribution: $f_0(\mathbf{k}) = \dfrac{1}{e^{(E(\mathbf{k})-\mu)/k_BT}+1}$.

Assumed isothermal conditions at temperature *T.*

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Two-body collision in Boltzmann equation

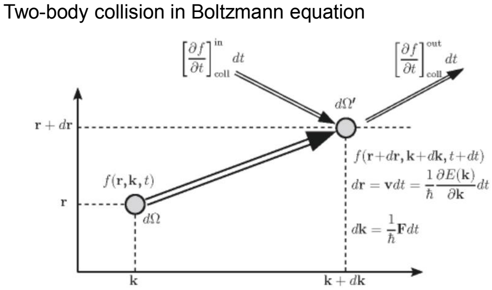

Figure 11.8 Schematic representation of the conservation of the number of electrons moving in the space phase $\mathbf{r}$, $\mathbf{k}$. The region $d\Omega$ around $\mathbf{r}$, $\mathbf{k}$ at time t evolves into a new region $d\Omega'$, whose volume is the same as $d\Omega$ (Liouville theorem). The distribution function $f(\mathbf{r}+d\mathbf{r}, \mathbf{k}+d\mathbf{k}, t+dt)$ equals $f(\mathbf{r}, \mathbf{k}, t)$ supplemented by the net change $[\partial f/\partial t]_{\rm coll}\, dt = [\partial f/\partial t]_{\rm coll}^{\rm in}\, dt - [\partial f/\partial t]_{\rm coll}^{\rm out}\, dt$ of the number of electrons forced in and ejected out because of collision processes.

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Determining physical quantities in terms from the distribution function

Current charge density:

$$\mathbf{J} = \frac{1}{4\pi^3}\int (-e)\,\mathbf{v}\,f\,d\mathbf{k},$$

Energy density:

$$\mathbf{U} = \frac{1}{4\pi^3}\int E\,\mathbf{v}\,f\,d\mathbf{k},$$

$$f\left(\mathbf{r}+\mathbf{v}\,dt, \mathbf{k}+\frac{\mathbf{F}}{\hbar}dt, t+dt\right) \equiv f(\mathbf{r},\mathbf{k},t) + \left[\frac{\partial f}{\partial t}\right]_{\text{coll}} dt.$$

with: $\mathbf{v}_{\mathbf{k}} = \frac{1}{\hbar}\frac{\partial E(\mathbf{k})}{\partial \mathbf{k}}, \qquad \frac{d(\hbar\mathbf{k})}{dt} = \mathbf{F},$

Equilibrium distribution: $f_0(\mathbf{k}) = \frac{1}{e^{(E(\mathbf{k})-\mu)/k_B T}+1},$

Boltzmann equation:

$$\boxed{\frac{\partial f}{\partial \mathbf{r}}\cdot\mathbf{v} + \frac{\partial f}{\partial \mathbf{k}}\cdot\frac{\mathbf{F}}{\hbar} + \frac{\partial f}{\partial t} = \left[\frac{\partial f}{\partial t}\right]_{\text{coll}}}$$

Evaluating the collision term:

$$\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} = I_{\text{coll}}[f(\mathbf{r},\mathbf{k},t)]$$

$$I_{\text{coll}}[f(\mathbf{r},\mathbf{k},t)] = \frac{1}{(2\pi)^3}\int \left[P_{\mathbf{k}\leftarrow\mathbf{k}'} f_{\mathbf{k}'}(1-f_{\mathbf{k}}) - P_{\mathbf{k}'\leftarrow\mathbf{k}} f_{\mathbf{k}}(1-f_{\mathbf{k}'})\right] d\mathbf{k}'.$$

Relaxation time approximation:

$$\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} = -\frac{f-f_0}{\tau}.$$

Solution of the Boltzmann equation in the relaxation time approximation:

$$\frac{\partial f}{\partial \mathbf{r}} \cdot \mathbf{v} + \frac{1}{\hbar}\frac{\partial f}{\partial \mathbf{k}} \cdot \mathbf{F} + \frac{\partial f}{\partial t} = -\frac{f - f_0}{\tau}.$$

For **F**=0 and $\frac{\partial f}{\partial \mathbf{r}}$=0: $f(\mathbf{k}, t) = f_0 + [f(\mathbf{k}, t=0) - f_0]e^{-t/\tau}$.

Static conductivity for uniform material

Bolzmann equation

$$\frac{\partial f}{\partial \mathbf{r}} \cdot \mathbf{v} + \frac{1}{\hbar}\frac{\partial f}{\partial \mathbf{k}} \cdot \mathbf{F} + \frac{\partial f}{\partial t} = -\frac{f - f_0}{\tau}.$$

assumed 0 | *-eE* | assumed 0

$$\frac{1}{\hbar}\frac{\partial f}{\partial \mathbf{k}} \cdot (-e)\mathbf{E} = -\frac{f - f_0}{\tau}$$

$$f = f_0 + \frac{e\tau}{\hbar}\frac{\partial f_0}{\partial \mathbf{k}} \cdot \mathbf{E}.$$

$$= f_0 + \frac{e\tau}{\hbar}\frac{\partial f_0}{\partial E}\frac{\partial E(\mathbf{k})}{\partial \mathbf{k}} \cdot \mathbf{E} = f_0 + e\tau\frac{\partial f_0}{\partial E}\mathbf{v} \cdot \mathbf{E}$$

Static conductivity for uniform material – continued:

$$\mathbf{J} = \frac{e^2}{4\pi^3}\int \tau\left(-\frac{\partial f_0}{\partial E}\right)\mathbf{v}(\mathbf{v}\cdot\mathbf{E})\,d\mathbf{k} \implies J_\alpha = \sum_\beta \sigma_{\alpha\beta}E_\beta$$

For isotropic case (**J** parallel to **E**)

$$\sigma_0 = \frac{e^2}{4\pi^3}\int \tau(\hat{\mathbf{e}}\cdot\mathbf{v})^2\left(-\frac{\partial f_0}{\partial E}\right)d\mathbf{k}$$ $\hat{\mathbf{e}}$ denotes direction of **E**.

$$-\frac{\partial f_0}{\partial E} \approx \delta\left(E(\mathbf{k}) - E_F\right)$$

For $E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m^*}$: $\sigma_0 = \frac{ne^2}{m^*}\tau_F$

Mean free path

For the parabolic band:

$$v_F = \frac{\hbar k_F}{m^*} \qquad k_F = \left(3\pi^2 n\right)^{1/3}$$

Complex mean free path:

$$\Lambda(\omega) = \frac{v_F \tau}{1 - i\omega\tau}$$

Frequency and wavevector dependent conductivity of a uniform material -- linear approximation

$$\frac{\partial f}{\partial \mathbf{r}} \cdot \mathbf{v} + \frac{1}{\hbar}\frac{\partial f}{\partial \mathbf{k}} \cdot (-e)\mathbf{E} + \frac{\partial f}{\partial t} = -\frac{f - f_0}{\tau}. \qquad f = f_0 + f_1$$

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 e^{i(\mathbf{q}\cdot\mathbf{r} - \omega t)}, \quad \mathbf{E}_0 \perp \mathbf{q}.$$

$$\frac{\partial f_1}{\partial \mathbf{r}} \cdot \mathbf{v} + \frac{1}{\hbar}\frac{\partial f_0}{\partial \mathbf{k}} \cdot (-e)\mathbf{E} + \frac{\partial f_1}{\partial t} = -\frac{f_1}{\tau}.$$

assume: $f_1(\mathbf{r}, \mathbf{k}, t) = \Phi(\mathbf{k}) e^{i(\mathbf{q}\cdot\mathbf{r} - \omega t)}$

$$i\mathbf{q} \cdot \mathbf{v}\Phi(\mathbf{k}) + \frac{1}{\hbar}\frac{\partial f_0}{\partial \mathbf{k}}(-e) \cdot \mathbf{E}_0 - i\omega\Phi(\mathbf{k}) = -\frac{\Phi(\mathbf{k})}{\tau}.$$

Frequency and wavevector dependent conductivity of a uniform material -- linear approximation -- continued

$$\Phi(\mathbf{k}) = \frac{e\tau \mathbf{v} \cdot \mathbf{E}_0}{1 - i\tau(\omega - \mathbf{q} \cdot \mathbf{v})} \frac{\partial f_0}{\partial E}.$$

$$\mathbf{J} = \frac{1}{4\pi^3} \int (-e)\mathbf{v} f_1 d\mathbf{k} = \frac{e^2}{4\pi^3} \int \tau \left(-\frac{\partial f_0}{\partial E}\right) \mathbf{v} \frac{\mathbf{v} \cdot \mathbf{E}}{1 - i\tau(\omega - \mathbf{q} \cdot \mathbf{v})} d\mathbf{k}$$

$$\boxed{\sigma(\mathbf{q}, \omega) = \frac{e^2}{4\pi^3} \int \frac{\tau(\widehat{\mathbf{e}} \cdot \mathbf{v})^2}{1 - i\tau(\omega - \mathbf{q} \cdot \mathbf{v})} \left(-\frac{\partial f_0}{\partial E}\right) d\mathbf{k}} \; .$$

Frequency and wavevector dependent conductivity of a uniform material -- linear approximation -- continued

$$\sigma(\mathbf{q},\omega) = \frac{e^2}{4\pi^3}\int \frac{\tau(\hat{\mathbf{e}}\cdot\mathbf{v})^2}{1-i\tau(\omega-\mathbf{q}\cdot\mathbf{v})}\left(-\frac{\partial f_0}{\partial E}\right)d\mathbf{k}\ .$$

Assume: $\hat{\mathbf{e}} = \hat{\mathbf{x}} \qquad \mathbf{q} = q\hat{\mathbf{z}}$

$$\sigma(q,\omega) = \frac{e^2}{4\pi^3}\int \frac{\tau v_x^2}{1-i\tau(\omega-qv_z)}\left(-\frac{\partial f_0}{\partial E}\right)d\mathbf{k}\ .$$

After some algebra:

$$\sigma(q,\omega) = \frac{3}{4}\frac{\sigma_0}{1-i\omega\tau}\left[\frac{2}{s^2}+\frac{s^2-1}{s^3}\ln\frac{1+s}{1-s}\right] \quad \text{with} \quad s = \frac{iqv_F\tau}{1-i\omega\tau}$$

Note that $s = iq\ \Lambda(\omega)$

$$\sigma(q,\omega) = \frac{3}{4}\frac{\sigma_0}{1-i\omega\tau}\left[\frac{2}{s^2}+\frac{s^2-1}{s^3}\ln\frac{1+s}{1-s}\right] \quad \text{with} \quad s = \frac{iqv_F\tau}{1-i\omega\tau}$$

For $|s| << 1 \qquad \sigma(q,\omega) = \dfrac{\sigma_0}{1-i\omega\tau}$

For $|s| >> 1 \qquad \sigma(q,\omega) = \dfrac{3\pi\sigma_0}{4qv_F\tau}$

Transport in presence of spatially varying temperature ***T*(r)**

In a crystal kept at non-uniform temperature, it is convenient to define the local equilibrium distribution function $f_0(\mathbf{k},\mathbf{r})$ as

$$f_0(\mathbf{k},\mathbf{r}) = \frac{1}{\exp[(E(\mathbf{k})-\mu(\mathbf{r}))/k_BT(\mathbf{r})]+1}; \qquad (11.45)$$

Spatially varying temperature

Spatially varying chemical potential

$$\frac{\partial f_0}{\partial \mathbf{r}} = \frac{\partial f_0}{\partial E}k_BT\frac{\partial}{\partial \mathbf{r}}\frac{E(\mathbf{k})-\mu}{k_BT} = \frac{\partial f_0}{\partial E}\left[-\frac{\partial \mu}{\partial \mathbf{r}} - \frac{E(\mathbf{k})-\mu}{T}\frac{\partial T}{\partial \mathbf{r}}\right]$$

$$\frac{1}{\hbar}\frac{\partial f_0}{\partial \mathbf{k}} = \frac{1}{\hbar}\frac{\partial f_0}{\partial E}\frac{\partial E(\mathbf{k})}{\partial \mathbf{k}} = \frac{\partial f_0}{\partial E}\mathbf{v}(\mathbf{k})\ .$$

$$\frac{\partial f}{\partial \mathbf{r}}\cdot\mathbf{v}+\frac{1}{\hbar}\frac{\partial f}{\partial \mathbf{k}}\cdot(-e)\mathbf{E} = -\frac{f-f_0}{\tau} = -\frac{f_1}{\tau}$$

First order solution: $f_1 = -\tau\frac{\partial f_0}{\partial \mathbf{r}}\cdot\mathbf{v} - \frac{\tau}{\hbar}\frac{\partial f_0}{\partial \mathbf{k}}\cdot(-e)\mathbf{E}$

$$f_1 = \left(-\frac{\partial f_0}{\partial E}\right)\tau\left[-e\,\mathbf{E} - \nabla\mu - \frac{E-\mu}{T}\nabla T\right]\cdot\mathbf{v},$$

$$\mathbf{J} = \frac{1}{4\pi^3}\int(-e)\,\mathbf{v}\,f_1\,d\mathbf{k}; \qquad \mathbf{U} = \frac{1}{4\pi^3}\int(E-\mu)\,\mathbf{v}\,f_1\,d\mathbf{k} - \frac{\mu}{e}\mathbf{J}.$$

Evaluation of integrals for the isotropic case:

$$f_1 = \left(-\frac{\partial f_0}{\partial E}\right)\tau\left[-e\,\mathbf{E} - \nabla\mu - \frac{E-\mu}{T}\nabla T\right]\cdot\mathbf{v},$$

$$\mathbf{J} = \frac{1}{4\pi^3}\int(-e)\,\mathbf{v}\,f_1\,d\mathbf{k}; \qquad \mathbf{U} = \frac{1}{4\pi^3}\int(E-\mu)\,\mathbf{v}\,f_1\,d\mathbf{k} - \frac{\mu}{e}\mathbf{J}.$$

$$\mathbf{J} = e\,K_0\left[e\,\mathbf{E}+\nabla\mu\right] + e\,\frac{K_1}{T}\nabla T,$$

$$\mathbf{U} = -K_1\left[e\,\mathbf{E}+\nabla\mu\right] - \frac{K_2}{T}\nabla T - \frac{\mu}{e}\mathbf{J}$$

where

Electric field direction

$$K_n = \frac{1}{4\pi^3}\int\tau\,(\hat{\mathbf{e}}\cdot\mathbf{v})^2\,(E-\mu)^n\left(-\frac{\partial f_0}{\partial E}\right)d\mathbf{k}, \quad n = 0, 1, 2,$$

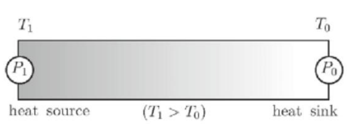


Figure 11.11 Schematic representation of a bar of homogeneous material, whose ends are kept at different temperatures.

Regrouping terms:

$$\mathbf{J} = e^2 K_0\left[\mathbf{E} + \frac{1}{e}\nabla\mu - S(T)\nabla T\right] \quad \text{with} \quad S(T) = -\frac{1}{e\,T}\frac{K_1}{K_0}$$

$e^2 K_0 = \sigma_0$: $\sigma_0\,\mathbf{E},$

Seebeck coefficient

Expression for the power dissipated

$$\mathcal{P} = \mathbf{E}\cdot\mathbf{J} = \frac{J^2}{\sigma_0} - \frac{1}{e}\nabla\mu\cdot\mathbf{J} + S(T)\nabla T\cdot\mathbf{J}$$

Energy flux

$$\boxed{\mathbf{U} = \left[-\frac{K_1}{e\,K_0} - \frac{\mu}{e}\right]\mathbf{J} - k_e\,\nabla T} \quad \text{with} \quad \boxed{k_e = \frac{1}{T}\left(K_2 - \frac{K_1^2}{K_0}\right)}$$

Electron thermal conductivity

Evaluation of expression for various configurations

Isothermal conditions $\nabla T = 0$

$$\mathbf{J} = \sigma_0\left[\mathbf{E} + \frac{1}{e}\nabla\mu\right]$$

$$\sigma_0 = n e^2\tau/m^*, \quad \mu = (\hbar^2/2m^*)(3\pi^2 n)^{2/3}$$

$$\nabla\mu/\mu = (2/3)\nabla n/n.$$

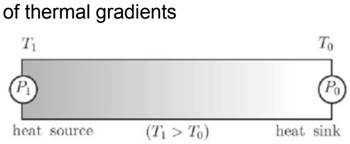
$$\boxed{\mathbf{J} = n\,e\,\mu_e\mathbf{E} + e\,D\,\nabla n},$$

where $\mu_e = e\tau/m^*$ is the *electron mobility*, and D is the *diffusion coefficient*

$$\boxed{D = \frac{2}{3}\frac{E_F}{e}\mu_e},$$

(here $E_F=\mu$)

Effects of thermal gradients



Assume open circuit conditions J=0

$$\mathbf{E} = -\frac{1}{e}\nabla\mu + S(T)\nabla T.$$

The potential difference between the end points P_0 and P_1, at temperatures T_0 and T_1, is

$$\phi_1 - \phi_0 = -\int_{P_0}^{P_1}\mathbf{E}\cdot d\mathbf{l} = \frac{1}{e}(\mu_1 - \mu_0) - \int_{T_0}^{T_1} S(T)\,dT. \qquad (11.57)$$

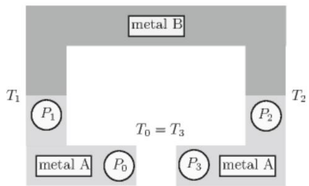


Figure 11.12 Standard bimetallic circuit to measure the thermoelectric effect. The two junctions between the metals are kept at different temperatures ($T_1 \neq T_2$); a voltage appears between points P_0 and P_3.

$$\phi_{3A} - \phi_{0A} = -\int_{T_0}^{T_1} S_A(T)\,dT - \int_{T_1}^{T_2} S_B(T)\,dT - \int_{T_2}^{T_0} S_A(T)\,dT\,.$$

$$\boxed{\phi_{3A} - \phi_{0A} = \int_{T_1}^{T_2} S_A(T)\,dT - \int_{T_1}^{T_2} S_B(T)\,dT}$$