HW 8 ECE 65600 by Peide Ye

Due on November 19 Tuesday Lecture Time

1) What is the proper, near-equilibrium current equation when the temperature varies slowly with position?

   a) $J_{nx} = \sigma_n \frac{d(F_n/q)}{dx}$

   b) $J_{nx} = \sigma_n \frac{d(F_n/q)}{dx} - S_n \frac{dT}{dx}$

   c) $\boldsymbol{J_{nx} = \sigma_n \frac{d(F_n/q)}{dx} - S_n \sigma_n \frac{dT}{dx}}$

   d) $J_{nx} = \sigma_n \frac{d(F_n/q)}{dx} - \pi_n \frac{dT}{dx}$

   e) $J_{nx} = \sigma_n \frac{d(F_n/q)}{dx} - \kappa_n \sigma_n \frac{dT}{dx}$

Answer: c)

The near-equilibrium current equation combines the effect of both electrochemical potential gradients F_n/q and temperature gradients dT. The term $\sigma_n \frac{d(F_n/q)}{dx}$ accounts for the current driven by the electrochemical potential gradient and $-S_n \sigma_n \frac{dT}{dx}$ represents the thermoelectric contribution to the current, where S_n is the Seebeck coefficient.

2) What is the strongest factor that determines the magnitude of the Seeback coefficient?

   a) The location of the Fermi level with respect to the band edge.
   b) The shape of the density of states.
   c) The energy dependence of the mean-free-path for backscattering.
   d) The dimensionality of the semiconductor.
   e) All of the above-listed factors are equally important.

Answer: a)

The Seebeck coefficient measures the voltage generated in response to a temperature gradient and depends primarily on the location of the Fermi level. The closer the Fermi level is to the band edge, the more asymmetric the carrier transport, leading to a higher Seebeck coefficient. While factors like the density of states and mean-free path also contribute, their influence is secondary compared to the Fermi level's position relative to the band edge.

3) What are the two most general driving forces for current?

   a) Gradients in the electrostatic potential and temperature.
   b) Gradients in the carrier concentration and temperature.
   c) Gradients in the electrochemical potential and temperature.
   d) Gradients in the electrostatic potential and carrier concentration.
   e) Gradients in the electron density and electrostatic potential.

Answer: c)

The electrochemical potential gradient is the primary driving force for electrical current, as it combines both the electric potential and the chemical potential (carrier concentration gradient). The temperature gradient drives thermoelectric currents (Seebeck effect). Together, these two gradients form the most general driving forces for current.

4) For a non-degenerate, n-type semiconductor, the current typically flows at an energy Δ_s above the bottom of the conduction band. What is a typical value for Δ_s?

   a) Much less than $k_B T$.
   b) Much greater than $k_B T$.
   c) On the order of $k_B T$.
   d) Approximately $E_F - E_C$.
   e) Approximately $E_C - E_F$.

Answer: c)

In a non-degenerate n-type semiconductor, most electrons occupy states within a few $k_B T$ (thermal energy) above the conduction band edge E_C, as their distribution follows the Boltzmann statistics.

5) For a degenerate, n-type semiconductor, the current typically flows at an energy Δ_s above the bottom of the conduction band. What is a typical value for Δ_s?

   a) Much less than $k_B T$.
   b) Much greater than $k_B T$.
   c) On the order of $k_B T$.
   d) Approximately $E_F - E_C$.
   e) Approximately $E_C - E_F$.

Answer: d)

In a degenerate semiconductor, the Fermi level (E_F) lies within or close to the conduction band. This means most carriers contributing to the current occupy states near the Fermi level. The energy difference corresponds to the position of the Fermi level relative to the conduction band edge $E_F - E_C$.

6) What is the relation between the Peltier coefficient and the Seebeck coefficient called?

   a) The Wiedemann-Franz law.
   b) The Lorenz relation.
   c) Mathiessen's rule.
   d) The Kelvin relation.
   e) Dulong and Petit law.

Answer: d)

The Kelvin relation links the Peltier coefficient π and the Seebeck coefficient S through the equation $\pi = TS$, where T is the absolute temperature. The Wiedemann-Franz law relates electrical and thermal conductivities, and the Lorenz relation deals with the proportionality between the thermal and electrical conductivities at constant temperature. Mathiessen's rule addresses the total scattering rate in a material. The Dulong and Petit law pertains to heat capacities in classical thermodynamics.

7) What are the coefficients k_0 and k_e?

   a) k_0 is the thermal conductivity due to phonons and k_e is the same quantity due to electrons.
   b) k_0 is the thermal conductivity due to electrons and k_e is the same quantity due to phonons.
   c) k_0 is the open-circuit thermal conductivity due to electrons and k_e is the short-circuit thermal conductivity due to electrons.

d) **k_0 is the short-circuit thermal conductivity due to electrons and k_e is the open-circuit thermal conductivity due to electrons.**
e) k_0 and k_e are two names for the same quantity, the thermal conductivity due to electrons.

Answer: d)

k_0 and k_e are thermal conductivity coefficients related to the transport of electrons under different circuit conditions:

- k_0 (short-circuit thermal conductivity) refers to the heat transported by electrons when no electrical current flows (short-circuit condition).
- k_e (open-circuit thermal conductivity) refers to the heat transported when there is no net electrical potential difference across the material (open-circuit condition).

These definitions are specific to thermoelectric materials, where the interplay of electrical and thermal transport phenomena is critical.

8) When we write the current equation in this form: $J_{nx} = L_{11}(\frac{d(F_n/q)}{dx}) + L_{12}\frac{dT_L}{dx}$
What is the coefficient L_{12} called?

a) The Seebeck coefficient.
b) **The Soret coefficient.**
c) The Peltier coefficient.
d) The electronic thermal conductivity, κ_e.
f) The electronic thermal conductivity, κ.

Answer: b)

The term $L_{12}\frac{dT_L}{dx}$ represents the coupling between a temperature gradient (dT_L) and the current density (J_{nx}). This coupling describes how a temperature gradient drives a flux of charge carriers. This phenomenon is known as the Soret effect, which describes how a temperature gradient induces particle movement or electrical effects.

9) When we write the current equation in this form: $\frac{d(F_n/q)}{dx} = L_{11}J_{nx} + L_{12}\frac{dT_L}{dx}$
What is the coefficient L_{12} called?

a) **The Seebeck coefficient.**
b) The Soret coefficient.
c) The Peltier coefficient.
d) The electronic thermal conductivity, κ_e.
e) The electronic thermal conductivity, κ.

Answer: a)

Here, L_{12} appears in a term related to the electric field ($\frac{d(F_n/q)}{dx}$) generated by a temperature gradient ($\frac{dT_L}{dx}$). This effect is described by the Seebeck coefficient, which quantifies the relationship between a temperature gradient and the resulting voltage (or electric field).

10) The current in an n-type conductor flows at an energy Δ_s above the bottom of the conduction band. What determines the value of Δ_s?

a) The location of the Fermi level.

b) The shape of the band structure.
c) The energy dependence of the mean-free-path.
d) All of the above.
e) None of the above.

Answer: d)

The value of Δ_s, the characteristic energy at which current flows, depends on multiple factors: (a) The location of the Fermi level determines the energy range where carriers are most populated. (b) The band structure influences the density of states and carrier dynamics. (c) The energy dependence of the mean-free path impacts how easily carriers at specific energies can transport.

11) What is the "power factor"?

a) S_σ.
b) $S^2\sigma$.
c) $S^2\sigma T$.
d) $k_e + k_p$.
e) k_0/k_L.

Answer: b)

The power factor, defined as $S^2\sigma$, measures the thermoelectric efficiency of a material. It combines the Seebeck coefficient (S) and electrical conductivity (σ), which are critical for generating electrical power from heat.

12) Where should the Fermi level be placed to maximize the power factor in an n-type semiconductor?

a) Well below the conduction band edge, E_C.
b) Well above the conduction band edge, E_C.
c) Very close to the conduction band edge, E_C.
d) Very close to the valence band edge, E_V.
e) Well below the valence band edge, E_V.

Answer: c)

For n-type semiconductors, the power factor is maximized when the Fermi level is placed near the conduction band edge. This ensures an optimal balance between high carrier concentration (for high conductivity) and sufficient asymmetry in carrier distribution (for a large Seebeck coefficient)

13) Which of the following is true about the location of the Fermi level to maximize the power factor in an n-type semiconductor?

a) It is higher in 1D than in 2D and higher in 2D than in 3D.
b) It is lower in 1D than in 2D and lower in 2D than in 3D.
c) It is the same in 1D, 2D, and 3D.
d) It is the same in 1D and 2D, but higher in 3D.
e) It is the same in 2D and 3D, but lower in 1D.

Answer: b)

The Fermi level for maximizing the power factor depends on the dimensionality of the semiconductor. In lower dimensions (1D and 2D), the density of states (DOS) increases more sharply near the band edge compared to 3D systems. This means the optimal Fermi level can be positioned closer to the band edge in 1D and 2D, resulting in a lower Fermi level in these dimensions. In 3D, the DOS rises more gradually with energy, requiring the Fermi level to be slightly higher to maintain the balance between conductivity and the Seebeck coefficient.

14) The best thermoelectric materials all have one thing in common. What is it?

a) A very high mobility.
b) A very high conductivity.
c) A very high Seebeck coefficient.
d) A very low lattice thermal conductivity.
e) A very low Peltier coefficient.

Answer: d)

For high thermoelectric efficiency, the material must have a high figure of merit (ZT), which depends on the power factor ($S^2\sigma$) and low thermal conductivity (κ). A low lattice thermal conductivity minimizes heat leakage, ensuring a larger temperature gradient to drive the thermoelectric effect.

15) For a general (possibly anisotropic) material, we write:

$$E_i = \rho_{ij}J_j - S_{ij}\partial_j T$$

Assume that J_x is non-zero and all other components are zero, and that the temperature is uniform. What is E_y?

a) $E_y = \rho_{yy}J_x$.
b) $E_y = \rho_{xy}J_x$.
c) $E_y = \rho_{yx}J_x$.
d) $E_y = \rho_{yy}J_y$.
e) $E_y = \rho_{yx}J_y$.

Answer: c)

Since the temperature gradient ($\partial_j T$) is zero, the equation simplifies to: $E_i = \rho_{ij}J_j$. For E_y, the equation becomes: $E_y = \rho_{yy}J_y + \rho_{yx}J_x$. However, by assumption: $J_y = 0$ (no current flows in the y-direction). This reduces the equation further to: $E_y = \rho_{yx}J_x$. Note that ρ_{yx}x describes the off-diagonal resistivity component, which captures how the current in the x-direction can induce an electric field in the y-direction due to anisotropy in the material.

16) For practical thermoelectric (TE) devices, the semiconductor is doped so that $E_F \approx E_C$. Work out the four thermoelectric transport coefficients for n-type Ge doped at $N_D = 10^{19}$cm^{-3}. You may assume that T = 300 K, that the dopants are fully ionized, and that the mean-free path for backscattering, λ_0, is independent of energy.

Use the following material parameters:

T = 300 K
N_C = 1.04 × 10^{19} cm^{-3}
μ_n = 330 cm^2/V-s
m^* = 0.12 m_0

You may assume **non-degenerate carrier statistics** (but realize that this assumption may not be well-justified for $E_F \approx E_C$, which is the case here, so we will only obtain estimates). Work out approximate, numerical values for λ_0, ρ, S, π, and κ_e

Answer:

Compute the thermal velocity, which represents the average velocity of charge carriers due to thermal motion and is derived from the kinetic energy equation:

$$v_T = \sqrt{\frac{2k_B T}{m^*}}$$

m^* = 0.12 m_0, where m_0 is the electron mass. Substituting the values, we get:

$$v_T = 1.55 \times 10^7 \text{cm/s}$$

Compute the Diffusion Coefficient, D_n to determine the mean free path:

$$D_n = \frac{v_T \lambda_0}{2}$$

$$D_n = \frac{k_B T \mu_n}{q} = \frac{(1.38 \times 10^{-23})(300)(330)}{1.6 \times 10^{-19}} = 8.6 \text{ cm}^2/\text{s}$$

$$\lambda_0 = \frac{2D_n}{v_T} = \frac{2(8.6)}{(1.55 \times 10^7)} = 11.1 \times 10^{-7} \text{cm}$$

Compute the resistivity, ρ:

$$\rho = \frac{1}{n_0 q \mu_n} = \frac{1}{(10^{19})(1.6 \times 10^{-19})(330)} = 0.0019\, \Omega - \text{cm}$$

Compute the Seebeck Coefficient, S:

$$S = -\frac{k_B}{q} \{\frac{(E_C - E_F)}{k_B T} + \delta_n\}$$

By using the given approximations $\frac{(E_C - E_F)}{k_B T} \approx \ln\left(\frac{N_C}{n_0}\right)$ and $\delta_n \approx 2$

$$\frac{(E_C - E_F)}{k_B T} \approx \ln\left(\frac{N_C}{n_0}\right) = \ln\left(\frac{1.04 \times 10^{19}}{10^{19}}\right) = 3.9 \times 10^{-2}$$

$$S = -\frac{k_B}{q}\left\{\frac{(E_C - E_F)}{k_B T} + \delta_n\right\} = -8.6\ \mu\text{V/K} \times \{3.9 \times 10^{-2} + 2\} = -175\ \mu\text{V/K}$$

Compute the Peltier Coefficient, π proportional to the Seebeck coefficient:

$$\pi = TS = (300 \text{ K}) \times \left(-175 \frac{\mu\text{V}}{\text{K}}\right) \approx -0.05 \text{ V}$$

Compute the Electronic Thermal Conductivity, κ_e. Thermal conductivity due to electrons is related to electrical conductivity (σ =1/ρ) and the Lorenz number L. Assuming $L = 2(k_B T)^2$ non-degenerate carriers:

$$\kappa_e = T\sigma L = \frac{TL}{\rho} = \frac{T \times 2(k_B T)^2}{\rho} = 0.24 \text{ W/m} - \text{K}$$