Homework: Week 2
Thermoelectricity from Atoms to Systems
Mark Lundstrom, nanoHUB-U Fall 2013

There are **seven HW questions** below. This homework will be graded in multiple choice format – no partial credit. Doing the homework before the solutions and tutorial are posted is a great way to test your understanding of the material covered. Some problems may be challenging, but give them a try, and review the tutorial and solutions later.

1) We have discussed the coupled current equations for 3D electrons:

$$\mathcal{E}_x = \rho J_x + S\frac{dT}{dx} \text{ V/m}$$

$$J_{Qx} = \pi J_x - \left(\kappa_e + \kappa_L\right)\frac{dT}{dx} \text{ W/m}^2$$

Consider a nanowire with 1D electrons. Instead of the current density, J_x, in A/m^2, we use the current, *I*, in A, and instead of the heat current density, J_{Qx}, in W/m^2, we use the heat current, I_Q, in W. Deduce the units of each of the four 1D transport coefficients.

The units of ρ_{1D}, S_{1D}, π_{1D}, and κ_{1D}^e, are:

a) Ω-m,V/K,V,W/$\left(\text{m-K}\right)$
b) Ω,V/K,V,W/K
c) Ω/m,V/K,V,W-m/K
d) Ω/m,V-K,V-K^2,W/$\left(\text{m-K}\right)$
e) Ω-m^2,V/K^2,V/K,W-K/m

2) The expression for the short circuit (electronic) thermal conductivity is:

$$\kappa_0 = \int_{-\infty}^{+\infty} \frac{\left(E - E_F\right)^2}{q^2 T}\sigma'\left(E\right)dE$$

where $\sigma'\left(E\right)$, the differential conductivity, is given by

$$\sigma'\left(E\right) = \frac{2q^2}{h}\lambda\left(E\right)\left(M\left(E\right)/A\right)\left(-\frac{\partial f_0}{\partial E}\right).$$

Homework: Week 2 Thermoelectric Materials and Devices (continued)

Evaluate this expression assuming that the Fermi level is located above the middle of the gap, so that only the conduction band need be considered. You may assume that the mean-free-path for backscattering is independent of energy, $\lambda(E) = \lambda_0$, and parabolic energy bands so that in 3D:

$$M(E)/A = \frac{m^*}{2\pi\hbar^2}(E - E_C)H(E - E_C),$$

where $H(E - E_C)$ is the Heaviside step function.

Your answer should be expressed in terms of Fermi-Dirac integrals. For a tutorial on Fermi-Dirac integrals see: "Notes on Fermi-Dirac Integrals, 3rd Ed." http://nanohub.org/resources/5475/

The expression for the short-circuit thermal conductivity of 3D electrons in a semiconductor with parabolic energy bands in terms of the normalized Fermi energy, $\eta_F = (E_F - E_C)/k_B T_L$ is:

a) $\kappa_0 = \left(-\frac{k_B}{q}\right)\{2 - \eta_F\}$

b) $\kappa_0 = \left(-\frac{k_B}{q}\right)\{2\mathcal{F}_1(\eta_F) - \eta_F\}$

c) $\kappa_0 = \left(-\frac{k_B}{q}\right)\left\{\frac{2\mathcal{F}_1(\eta_F)}{\mathcal{F}_0(\eta_F)} - \eta_F\right\}$

d) $\kappa_0 = \left[T\left(\frac{k_B}{q}\right)^2\left(\frac{2q^2}{h}\right)\lambda_0\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)\right] \times \left\{6\mathcal{F}_2(\eta_F) + \eta_F^2\mathcal{F}_0(\eta_F)\right\}$

e) $\kappa_0 = \left[T\left(\frac{k_B}{q}\right)^2\left(\frac{2q^2}{h}\right)\lambda_0\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)\right] \times \left\{6\mathcal{F}_2(\eta_F) - 4\eta_F\mathcal{F}_1(\eta_F) + \eta_F^2\mathcal{F}_0(\eta_F)\right\}$

3) In Lecture 2 we worked out the approximate values of the four thermoelectric transport coefficients for lightly doped n-type Ge. For practical TE devices, the material would be doped so that $E_F \approx E_C$. Work out the four thermoelectric transport coefficients for n-type Ge doped at $N_D = 10^{19}\ \text{cm}^{-3}$. 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.

Homework: Week 2 Thermoelectric Materials and Devices (continued)

Use the material parameters presented in Lecture 2, but use a mobility of $\mu_n = 330\,\mathrm{cm^2/V\text{-}s}$ (from http://www.ioffe.ru/SVA/NSM/Semicond/Ge/Figs/232.gif. You may assume non-degenerate carrier statistics (but realize that this assumption may not well-justified for $E_F \approx E_C$, which is the case here, so we will only obtain estimates).

The approximate values of λ_0, ρ, S, π, and κ_e, are:

a) 11 nm 0.0019 Ohm-cm, -1750 μV/K, -0.5 V, 0.0024 W/(m-K)
b) 11 nm 0.19 Ohm-cm, -175 μV/K, -0.05 V, 0.0024 W/(m-K)
c) 11 nm 0.0019 Ohm-cm, -175 μV/K, -0.05 V, 0.24 W/(m-K)
d) 33 nm 0.0019 Ohm-cm, -175 μV/K, -0.05 V, 0.24 W/(m-K)
e) 33 nm 0.0019 Ohm-cm, -175 μV/K, -0.05 V, 0.24 W/(m-K)

4) Perhaps we should use Fermi-Dirac statistics for thermoelectric calculations when $E_F \approx E_c$. Repeat problem 3), but this time use Fermi-Dirac statistics to determine the approximate values of λ_0, ρ, S, π, and κ_e. You might find it useful to know that

$$\sigma_{3D} = \frac{2q^2}{h}\lambda_0\left(\frac{g_V m^* k_B T}{2\pi\hbar^2}\right)\mathcal{F}_0(\eta_F) \text{ and } S = -\left(\frac{k_B}{q}\right)\left\{\frac{2\mathcal{F}_1(\eta_F)}{\mathcal{F}_1(\eta_F)} - \eta_F\right\}$$

a) 11 nm 0.0019 Ohm-cm, -1750 μV/K, -0.5 V, 0.0024 W/(m-K)
b) 11 nm 0.19 Ohm-cm, -175 μV/K, -0.05 V, 0.0024 W/(m-K)
c) 11 nm 0.0019 Ohm-cm, -175 μV/K, -0.05 V, 0.24 W/(m-K)
d) 13 nm 0.0019 Ohm-cm, -186 μV/K, -0.06 V, 0.40 W/(m-K)
e) 13 nm 0.19 Ohm-cm, -186 μV/K, -0.06 V, 0.24 W/(m-K)

5) We have discussed two different electronic thermal conductivities – one measured under short circuit conditions, κ_0, and one measured under open circuit conditions, κ_e. The two are related according to:

$$\kappa_e = \kappa_0 - T\sigma S^2$$

Using the estimated TE transport coefficients for Ge doped such that $E_F \approx E_C$ (from problem 4) deduce the ratio, κ_0/κ_e. For this example, the ratio, κ_0/κ_e, is closest to:

Homework: Week 2 Thermoelectric Materials and Devices (continued)

a) 0.2
b) 0.9
c) 1.3
d) 2.4
e) 5.5

6) Using the results of prob. 4), estimate the thermoelectric FOM, *ZT* for n-type Ge at *T* = 300 K. You may assume that $\kappa_L = 58 \text{ W/m-K}$.

a) ZT = 0.001
b) ZT = 0.01
c) ZT = 0.1
d) ZT = 1.0
e) ZT = 1.8

7) The expressions for conductance and Seebeck coefficient are:

$$G = \int G'(E)\,dE \qquad (1)$$

$$G'(E) = \frac{2q^2}{h}\frac{\lambda(E)}{L}M(E)\left(-\frac{\partial f_0}{\partial E}\right) \qquad (2)$$

$$S = \frac{-\int_{-\infty}^{+\infty}\frac{(E-E_F)}{qT}G'(E)\,dE}{\int G'(E)\,dE} \qquad (3)$$

Assuming 1D electrons, parabolic energy bands, and an energy-independent mean-free-path, $\lambda(E) = \lambda_0$, eqns. (1) – (3) can be evaluated to find (Lundstrom and Jeong, *Near-Equilibrium Transport*, Appendix, eqn. (A.25), World Scientific, 2013)

$$G_{1D} = \frac{2q^2}{h}\frac{\lambda_0}{L}\mathcal{F}_{-1}(\eta_F)$$

$$S_{1D} = \left(-\frac{k_B}{q}\right)\left(\frac{\mathcal{F}_0(\eta_F)}{\mathcal{F}_{-1}(\eta_F)} - \eta_F\right)$$

where

Homework: Week 2 Thermoelectric Materials and Devices (continued)

$$\eta_F = \left(E_F - E_C\right)/k_B T\ .$$

For energy independent scattering, the optimum location of the Fermi level for maximum power factor is $\hat{\eta}_F = -1.14$.

Assuming 3D electrons, parabolic energy bands, and an energy-independent mean-free-path, $\lambda\left(E\right) = \lambda_0$, eqns. (1) – (3) can be evaluated to find (Lundstrom and Jeong, *Near-Equilibrium Transport*, Appendix, eqn. (A.34), World Scientific, 2013)

$$G_{3D} = A\frac{2q^2}{h}\frac{\lambda_0}{L}\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)\mathcal{F}_0\left(\eta_F\right)$$

$$S_{3D} = \left(-\frac{k_B}{q}\right)\left(\frac{2\mathcal{F}_1\left(\eta_F\right)}{\mathcal{F}_0\left(\eta_F\right)} - \eta_F\right)$$

For energy independent scattering, the optimum location of the Fermi level for a 3D material is $\hat{\eta}_F = +0.668$.

Assuming $T = 300$ K, $m^* = m_0$, $\lambda_0 = 10$ nm, and L = 1 cm, compare the power factors in 1D and 3D for a 1 cm^2 cross-sectional area. Determine how many 1D nanowires would need to be placed in this 1 cm^2 area to equal the power factor of the 3D material.
The center-to center spacing of the nanowires is:

a) 0.1 nm
b) 1.5 nm
c) 2.4 nm
d) 5.7 nm
e) 10.3 nm

End of homework assignment. This assignment contains 7 questions.