

Homework Assignment 1

Due Wednesday, February 20, 2 pm, by electronic upload

Go through the details of the derivations of the transition rates, relaxation rates, and momentum relaxation rates for all the scattering mechanisms covered in the ECE 745 class.

Problem 1. a) Calculate and plot the relevant scattering rates and momentum relaxation rates for electrons in GaAs at room temperature (300 K):

- ❖ acoustic phonon scattering (absorption and emission together, within the elastic and equipartition approximations);
- ❖ polar optical phonon scattering (absorption and emission separately) for electrons in the Γ valley;
- ❖ intervalley scattering ($\Gamma \rightarrow L$ and $L \rightarrow \Gamma$, together in one graph; $\Gamma \rightarrow X$ and $X \rightarrow \Gamma$ together, $X \rightarrow L$ and $L \rightarrow X$ together, $L \rightarrow L$, $X \rightarrow X$)
- ❖ ionized impurity scattering at doping densities of 10^{17} and 10^{19} cm^{-3} .

The electron energy range should be 0 to 2 eV. Use the data from the table provided. Intervalley spacing is $\Delta E_{L\Gamma} = 0.29 \text{ eV}$, $\Delta E_{X\Gamma} = 0.48 \text{ eV}$. Assume $m^* = 0.067m_0$ for electrons in the Γ valley (not 0.063 as the table suggests). A good repository of data on various semiconductors is the Ioffe institute page <http://www.ioffe.ru/SVA/NSM/Semicond/index.html>

b) Calculate and plot the relaxation rates and momentum relaxation rates for POP and ionized impurity scattering in the same energy range. (Note how different they are.)

Hint: You have done this problem already when you took ECE 745. The point is to find your old scattering rate data in preparation for the Monte Carlo simulation project.

Problem 2. (Lundstrom, problem 3.8) Derive the Boltzmann transport equation for a semiconductor with a slowly varying (in space) effective mass. (Hint: First derive an expression for $d\vec{p}/dt$).

Problem 3. a) Prove that the relaxation time approximation (RTA) can be employed only for elastic and isotropic scattering processes. Which relaxation time should be used as the characteristic relaxation time τ_f in the RTA for isotropic, and which for elastic processes?

b) Dominant scattering mechanisms in bulk Si are acoustic phonon scattering, ionized impurity scattering, and equivalent intervalley scattering. For which ones among them can we employ the RTA?

c) Dominant scattering mechanisms in bulk GaAs at low fields are acoustic phonon scattering, ionized impurity scattering, and the most efficient one is the polar-optical-phonon scattering (at higher electric fields, nonequivalent intervalley scattering starts to be appreciable). For which ones among these scattering mechanisms can we employ the RTA?

Problem 4.

- For a uniform sample of GaAs doped n -type to 10^{17} cm^{-3} and kept at room temperature (300 K), calculate the position of the Fermi level with respect to the conduction band.
- For the same sample, using the relaxation-time approximation, calculate the mobility limited only by acoustic phonon scattering, then only by ionized impurity scattering, and finally only by polar-optical-phonon scattering. (For some of these mechanisms the RTA is technically not justified, but is still widely used to produce order-of-magnitude estimates).
- Use Matthiessen's rule to calculate the mobility and from it the conductivity of this sample. How does it compare to the experimentally measured value or your Rode's method calculation from ECE 745?
- Do not use Matthiessen's rule, but rather sum up the momentum relaxation rates for every given energy, then invert the sum to get the total momentum relaxation rate, and then find the average of that time, $\langle\tau_m\rangle$. With it, calculate the mobility and conductivity. How does it compare to that obtained using Matthiessen's rule? How does it compare to experiment/your calculation using Rode's method?

Problem 5. (*Lundstrom, problem 3.14*)

In metals, we often assume that $\partial f_s / \partial t \approx -\delta(\varepsilon - \varepsilon_F)$.

- Explain and justify the approximation (e.g., why can it be used in metals, and not in semiconductors)
- Derive an expression for the mobility of electrons in a metal and compare the result to Eq. (3.61).

Problem 6. (*Lundstrom, problem 3.10*)

Use the principle of detailed balance in equilibrium [i.e., that $\partial f_0 / \partial t = 0$], and answer the following questions:

- Establish the following relation between the equilibrium transition rate and its inverse:

$$\frac{S_0(\vec{p}', \vec{p})}{S_0(\vec{p}, \vec{p}')} = \exp\left(\frac{\varepsilon(\vec{p}') - \varepsilon(\vec{p})}{k_B T_L}\right)$$

(This relation is often true away from equilibrium, because S are determined by the scattering potentials and are relatively insensitive to the applied fields.)

- Use physical arguments to explain why transitions to higher energy states are less probable than transitions to lower energy states.

(THERE IS MORE...)

Lundstrom's book, problems 4.1 through 4.4.

Problems

- 4.1** Verify the results eqs. (4.37d), (4.37e), and (4.37f) for the tensors, B_{ij} , p_{ij} , and K_{ij} .
- 4.2** The integrand in the numerator of the expression for $\langle\langle\tau\rangle\rangle$, eq. (4.36), is of the form

$$\int_0^\infty e^{-p^2/2m^*k_B T_L} \tau_0 \left(\frac{p^2}{2m^*k_B T_L} \right)^s p^4 dp.$$

Assume that τ_0 is a constant, change variables to integrate over energy, and show that the integrand peaks at

$$\hat{E} = (s + 3/2)k_B T_L.$$

For ionized impurity scattering, τ_0 varies with energy, but the variation is slow so it can be moved outside the integral and evaluated at $E = \hat{E}$ when computing $\langle\langle\tau\rangle\rangle$. This technique is used to evaluate the Brooks–Herring mobility, eq. (4.128).

- 4.3** For a thermal average electron, show that $|\nabla_c f_S| \gg |\nabla_c f_A|$. Assume n -type silicon with $\mathcal{E} = 100 \text{ V/cm}$.
- 4.4** Show that eq. (4.30a) reduces to the conventional drift–diffusion equation under isothermal conditions.

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Table 2.1. Transport parameters for silicon and gallium arsenide

Parameter	Symbol	Value in Si	Value in GaAs
Mass density (g/cm ³)	ρ	2.329	5.36
Lattice constant (Angstroms)	a_0	5.43	5.462
Low frequency dielectric constant	κ_0	11.7	12.90
High frequency dielectric constant	κ_∞	—	10.92
Piezoelectric constant (C/m ²)	e_{pq}	—	0.160
Longitudinal acoustic velocity ($\times 10^5$ cm/s)	v_l or v_s	9.04	5.24
Transverse acoustic velocity ($\times 10^5$ cm/s)	v_t	5.34	3.0
Longitudinal optical phonon energy (eV)	$\hbar\omega_0$	0.063	0.03536
Electron effective mass ratio (lowest valley)	m^* (m_l/m_l^*)	— (0.916, 0.19)	0.067
Electron effective mass ratio (upper valley)	m^* α	— —	0.22 (L) 0.58 (X)
Non-parabolicity parameter parameter (eV ⁻¹)	α	1.59, 0.12 0.5	0.610 (Γ) 0.461 (L) 0.204 (X)
Electron acoustic deformation potential (eV)	D_A	9.5	7.01 (Γ) 9.2 (L) 9.0 (X)
Electron optical deformation potential ($\times 10^8$ eV/cm)	D_o	—	3.0 (L)
Optical phonon energy (eV)	ω_0	—	0.0343 (L)
Hole acoustic deformation potential (eV)	D_A	5.0	3.5
Hole optical deformation potential (eV/cm)	D_o	6.00	6.48
Intervalley parameters g -type (X-X)	D_{if}, E_{in}	0.5, 0.012 (TA) 0.8, 0.019 (LA) ($\times 10^8$ eV/cm)(eV)	—
Intervalley parameters f -type (X-X)	D_{if}, E_{in}	11.0, 0.062 (LO) 0.3 0.019 (TA) 2.0 0.047 (LA) ($\times 10^8$ eV/cm)(eV)	—
Intervalley parameters (X-L)	D_{if}, E_{in}	2.0 0.059 (TO) 2.0 0.058 2.0 0.055 ($\times 10^8$ eV/cm)(eV)	—
		2.0 0.041 2.0 0.017	

Table 2.1. (continued)

Parameter	Symbol	Value in Si	Value in GaAs
Intervalley deformation potential ($\times 10^8$ eV/cm)	$D_{\Gamma L}, D_{\Gamma X}$ D_{LL}, D_{LX} D_{XX}	—	10, 10. 10, 5.0 7.0
Intervalley phonon energy (eV)	$E_{\Gamma L}, E_{\Gamma X}$ E_{LL}, E_{LX} E_{XX}	—	0.0278, 0.0299 0.0290, 0.0293 0.0299
Energy separation between valleys (eV)	$\Delta E_{L\Gamma}$ $\Delta E_{X\Gamma}$	—	0.29