MSE 5460/ECE 5570, Spring Semester 2016
Compound Semiconductors Materials Science

Debdeep Jena (`djena@cornell.edu`), Depts. of ECE and MSE, Cornell University

Assignment 5 (+ Prelims)

Policy on assignments: Please turn in this assignment by 5pm, **Friday, May 20th, 2016**.

General notes: Present your solutions *neatly.* Do not turn in rough unreadable worksheets - learn to **take pride in your presentation**. Show the relevant steps, so that partial points can be awarded. $\boxed{\text{BOX}}$ your final answers where applicable. Draw figures wherever necessary. Please print out this question sheet and staple to the top of your homework. Write your name and email address on the cover. The problems in red count as your prelims.

Problem 5.1) Crystal Anharmonicity and Thermal Conductivity

In class, we discussed the thermal conductivities of various semiconductors. In particular, we discussed the high lattice thermal conductivity of diamond, BN, AlN, GaN, Silicon, and other semiconductors and discussed the microscopic physics responsible for this phenomena. A large role was played by the anharmonicity of the crystal lattice.

a) I stated that if the interatomic interaction potential is purely parabolic, the lattice will not expand or contract with heat. Show that if the interatomic potential is $\mathcal{U}(x) = c_2x^2 - c_3x^3 - c_4x^4$, then the thermodynamic average amplitude of vibrations is $\langle x \rangle \approx \frac{3c_3k_BT}{4c_2^2+3c_4k_BT}$. In other words, if $c_3 = 0$, there is no thermal expansion! Neglecting the fourth power term, show that the coefficient of thermal expansion is $\frac{\partial\langle x \rangle}{\partial T} = \frac{3c_3k_B}{4c_2^2}$. The Grüneisen parameter γ may be derived from these anharmonicities, but I am not asking you to do so.

b) The total heat flux due to various phonon modes q of energy $\hbar\omega_q$ is $\mathbf{J}_{\text{heat}} = \sum_q N_q\hbar\omega_q\mathbf{v}_q$, where $\mathbf{v}_q$ is the group velocity of the phonon mode q and N_q is the number of phonons in that mode. Under thermal equilibrium, N_q^0 is the Bose-Einstein distribution. In analogy to electrical current, for diffusive flow of heat (phonons), we can write $\mathbf{J}_{\text{heat}} = -\kappa_L\nabla T$, where T is the temperature and κ_L is the lattice thermal conductivity. Use the steady state solution of the Boltzmann equation for phonons $\frac{N_q-N_q^0}{\tau_q} = -(\mathbf{v}_q\cdot\nabla T)\frac{\partial N_q^0}{\partial T}$ where τ_q^{-1} is the phonon scattering rate, and Debye approximations to show that the lattice thermal conductivity can be written[1] as $\kappa_L = \frac{k_B}{2\pi^2v_s}(\frac{k_BT}{\hbar})^3\int_0^{\theta_D/T}dx\frac{x^4e^x}{\tau_q^{-1}(x)(e^x-1)^2}$, where $x = \hbar\omega/k_BT$, and θ_D is the Debye temperature.

c) The above expression for the thermal conductivity can be reduced at high temperatures ($T \sim \theta_D$ and especially close to room temperature) to the form $\kappa_L \approx A\frac{\overline{M}\theta^3\delta}{\gamma^2Tn^{\frac{2}{3}}}$ as claimed in the Morelli and Slack article. Explain the terms that appear in the expression, and evaluate it to find the room temperature thermal conductivity of a few semiconductors such as Si, GaAs, GaN, AlN, SiC, BN, and Diamond. Use the parameters provided in the in the Morelli and Slack article.

d) Explain how one may expect the thermal conductivity of compound semiconductor alloys or superlattices to behave when compared to the thermal conductivity of the the binary constituents. How do isotopes affect the thermal conductivity of semiconductors? Which sorts of devices require high thermal conductivity, and how might one exploit low thermal conductivities?

Contd...

---

[1] This is the same expression that appears in the posted article by Morelli and Slack.

Problem 5.2) Compound Semiconductor Growth

a) Solve Rockett Problem 10.14 #1, Page 499.
b) Solve Rockett Problem 10.14 #2, Page 499.

Problem 5.3) MBE growth, Epitaxy, and Devices

a) Show, starting from the kinetic theory of gases, that the flux of gas particles impinging on a flat surface is $f = \frac{p}{\sqrt{2\pi m k_B T}}$, where all symbols have their usual meanings.

At 5 pm I check the growth chamber of my compound semiconductor GaN MBE system in Duffield Hall. It is sitting at a background pressure of $p_1 \approx 10^{-10}$ Torr with only N_2 molecules in the chamber. A wafer of n-type GaN with doping $N_D \sim 10^{17}/\text{cm}^3$ is sitting at room temperature in this vacuum. I leave for the night, planning to grow the next morning.

b) Find the number of Nitrogen molecules impinging on the GaN surface per unit area per second. Is there any growth?

A storm caused a power failure in Duffield Hall exactly at 6:50 am. The vacuum pump shut off to prevent damage, and the growth chamber developed a minor Oxygen leak. When I rush to the lab at 7:00 am, I find the pressure has gone up to $p_2 \approx 10^{-9}$ Torr entirely due to the leaked Oxygen.

c) If I assume the leak was instantaneous, and the sticking coefficient of Oxygen to GaN at room temperature is $s \sim 0.05$, find the area density of Oxygen incorporated on the GaN surface. For this problem, assume the oxygen is atomic. Assume all of the Oxygen atoms replace Nitrogen atoms and are shallow donors.

d) I am able to restart the pump and get rid of the Oxygen in the chamber, and am ready to grow my device. I decide to grow a thick layer of exactly the same n-typed doped GaN with $N_D \sim 10^{17}/\text{cm}^3$ as the underlying layer. Find the height of the energy barrier for hole transport that results due to the unwanted oxygen incorporation due to the power failure.

Problem 5.4) Surface Morphology and Growth Kinetics

Refer to Tsao's discussion on thermodynamic evolution of surface morphology in Chapter 6.

a) Reproduce Figure 6.2 for the phase transition between the rough and the phase-separated by smooth surfaces.

b) Reproduce Figure 6.6 of the free energy for the formation of steps on the surface.

c) How will you design an experiment to experimentally probe these predictions in an MBE growth system?

Problem 5.5) The Last Problem

This is *probably* the hardest problem in this course. Design a problem for the final exam of future versions of this class, and provide the solution. Your problem should test the learning of several (not necessarily all!) topics covered in this class. Remember a good problem is not one that is necessarily difficult, but one that a) tests concepts, b) is clearly stated, and c) not trivial to solve. Please write the solution nicely.