6.730 PHYSICS FOR SOLID STATE APPLICATIONS

Department of Electrical Engineering and Computer Science
Massachusetts Institute of Technology

"REAL" SEMICONDUCTOR PROJECT

Introduction

This is an extensive group project intended to introduce you to something approximating the real world of solid state calculations. Because this is a "real" problem, you are encouraged to collaborate with classmates and work as a team. Your group may turn in your report as a typed written document or as a Web site or as a combination. Only one report per group is required.

Each team will be assigned a different semiconductor material to use throughout the project. The project consists of the following three parts: First, you will be asked to describe fully a material's crystal structure, and to determine x-ray diffraction patterns for it. The second section of the project involves development of a model for the material's vibrational properties (phonon dispersion relationships, elastic constants, specific heat, etc.). In the final part of the project, you will use an empirical tight-binding model to calculate the material's electronic band structure (energy gap, whether the material is direct or indirect, effective densities of states for the valence and conduction bands, etc.). Throughout the project you are expected to check how good/bad your calculations are on the basis of real experimental and theoretical results. In general, your calculations should yield reasonable (within 20-30%) answers, so these experimental checks are a good way to ensure that you're on the right track.

This project does involve both library research and significant matlab coding. Much of the information you need can be found in the books that are on reserve. All literature sources, whether print or electronic, must be documented appropriately. All `matlab` code must be sent by email to `orlando@mit.edu`, as well as included, with comments, as an appendix to the project. Also email all eltronic source that you found useful and they will be put on the 6.730 Web page, under Links.

PART 1: CRYSTAL STRUCTURE

Issued: 2-16-99 Due: 3-3-99, at the beginning of class.

This part of the project is relatively simple, but does lay important ground work for parts II and III of the project. When you do the research for this part, be sure to make copies of any information you find on your material—it will come in handy for parts II and III.

Do appropriate research to answer the following questions about your material:

1. What is the crystal structure?
2. What is the lattice constant?
3. What is the basis?
4. What are the primitive lattice vectors?
5. What is the structure of the reciprocal lattice?
6. What are the primitive reciprocal lattice vectors?
7. what are the atomic form factors for your material?

The following can be done by hand, or by using `Matlab` when appropriate:

1. Provide pictures of the crystal and of the reciprocal lattice in the [100], [110], and [111] planes. Indicate the vertical positions of atoms with respect to the plane. (See for example, Kittel, p. 19.) Note that $[hkl]$ are *Miller indices* with respect to a simple cubic basis (see Aschroft and Merim, pp. 89—93).
2. Calculate the structure factor for all the reciprocal lattice vectors $\mathbf{K}_\ell < 16(2\pi/a)^2$. It will be convenient to choose a simple cubic basis with 8 atoms per unit cell. Then $\mathbf{K} = p(h\mathbf{i}_x + k\mathbf{i}_y + l\mathbf{i}_z)$ where p is the lattice constant for the cubic cell and $[hkl]$ are the Miller indices.
3. Describe qualitatively an experimental set-up you could use to determine the crystal structure of your material by x-ray diffraction. Provide some sketches. Specify what wavelength(s) of x-ray is(are) necessary in your set-up. What centrally shared facilities in the Center for Materials Science and Engineering would be good for your material if it were in bulk form. (See http://web.mit.edu/afs/athena.mit.edu/org/c/cmse/www/ for a start.)
4. Calculate the ratio of the intensities expected for the following lines of the diffraction pattern with respect to the [111] line: [100], [200], [220] [311] and [400].
5. What are the ratios if the material were Si? How could you use this information to distinguish Si from your material by x-ray diffraction?
6. Compare your calculations of the x-ray ratios with experimental data for your material. Comment on the comparison.