6.730 PHYSICS FOR SOLID STATE APPLICATIONS

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PROBLEM SET 6 Part (A)

Issued: 3-13-96 Due: 3-20-96, at the beginning of class.

Readings:
Acoustic and Optical Phonons: 6.730 notes.
Tight Binding: Chapter 7.2 in the 6.730 notes, and Chapter 10 in Ashcroft and Mermin.

Problem 6.1 Ionic Crystal Phonon Project.

The elasticity, thermal property, and optical property of ionic crystals can be understood in terms of phonons. This multi-part mega-project will show us how to tie them up and relate all these properties to only several simple parameters of the crystal. You can see the power of physics in its simplicity in understanding and modeling the real world. Finally, you are required to compare your calculated results with the experimental data of the material.

As this is a quite comprehensive project, team work is encouraged. Each team will be assigned a different FCC ionic crystal by your TA, but the procedures to solve the problem are identical. Team members should collaborate freely on this project but everyone will be turning in his/her own project.

Independent library search is required. If you are able to find the answer to any part in the literature, that's fine; simply document your source the way you would if writing a technical paper.

Here is the project:

(a) What is the `simplest` spring-mass model which will correctly fit the elastic constants for your material? Specify numerical values for the springs, masses, and equilibrium positions. (You can use matlab, library, or hand to solve this part of the problem.)

(b) Use the results from (a), what effective charge must be assigned to the ions?

PROBLEM SET 6 Part (B)

(continuing Part (A))

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(c) Using the results from (a) and (b), write a matlab code which will plot the dispersion relation for all phonon branches and use it to plot the phonon modes for the following 2-D surfaces in **k**-space: (i) plane normal to [001], (ii) plane which includes both [110] and [111] directions, (iii) or some other selected plots which have the hope of being comparable to experiment.

(d) Using matlab to do the integral, what is the heat capacity of your material? Plot it out as a function of temperature.

(e) Plot the dielectric constant ϵ, in which the optical property of your material is contained, as a function of frequency ω. Then plot the reflection coefficient as a function of ω, and find the infrared `reststrahl` band for your material. Does it fit the Lyddane- Sachs-Teller relation?

(f) Try to find experimental data on the phonon spectrum for your material using the library reference shelves or on-line search engines in Athena, also the specific heat, the dielectric constant, and the infrared `reststrahl` band of your material. Document your effort, even if unsuccessful. If you do find data, compare with the results you calculate above, and comment on the discrepancies.

So far, how much can you convince yourself that this world is to some level made of simple things?

Problem 6.2 Tight-Binding for FCC Lattice with s-orbitals.

Do problem 1 in Chapter 10 of Ashcroft and Mermin. Also plot out each graph in part (a) using matlab. Assume that $E_s = 1.0$ eV, $\beta = 0.1\,\text{eV}$, $\gamma = 0.05\,\text{eV}$ for plots on matlab.