6.730 PHYSICS FOR SOLID STATE APPLICATIONS

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PROJECT PART II. PHONONS

Issued: 3-5-99 Due: 3-16-99, at the beginning of class.

In this part of the project, you will be developing a simple model for the phonon spectra of your semiconductor. The game plan here is to develop a general model for the phonon dispersion relationship, in terms of some unknown force constants, and then to use experimental data to fit the force constants to the material. The model you will be using is a Born force constant model that incorporates bond bending and bond stretching, as we discussed in class.

A. Background Questions

For the Born force constant model, we can consider just nearest-neighbor interactions, or we can make the model more accurate (and more complicated) by including next-nearest neighbors, next-next nearest neighbors, etc. Before beginning on your calculation, answer the following general questions about the Born model:

1. How many force constants are required for each bond? Why?
2. What is the energy of a single bond in the Born model?
3. The model assumes that the bond is only slightly displaced from equilibrium. How would you modify the model to make the bond energy more realistically dependent on displacement from equilibrium–what order would the corrections be, and of what sign? Justify your answer physically; include sketches if appropriate.
4. If you use only nearest-neighbor couplings, how many force constants will your model require for your material? How large will the dynamical matrix be? What if you use nearest neighbor and next-nearest neighbor couplings?
5. How many independent elastic constants does your material possess? What are they (give numbers)? Why will a nearest-neighbor approach not provide the most general solution for a cubic material?

B. Construction of Dynamical Matrix

In fact, a nearest neighbor calculation that accounts for bond bending actually does a good job (within 20%), and is significantly more tractable than the next-nearest neighbors approach. We will therefore do the nearest neighbors approach.

1. Draw all the atoms in the basis and all their nearest neighbors. Label the atoms according to their lattice vector and basis vector.
2. Write a general expression for the potential energy of all the atoms in the crystal in terms of their displacement from equilibrium. Use a Born force model which considers only nearest neighbor interactions to simplify this expression (your expression should contain force constants and displacements at this point).
3. Use your simplified expression for the potential energy to determine the force on a given atom in the crystal in terms of its displacement and its neighbor's displacements. Check your answer by directly calculating the force from the spring constants and displacements.
4. Use your simplified expression for the potential energy to calculate the dynamical matrix. Is it Hermitian?
5. Write a matlab code to find the phonon spectra for general values of your force constants and atomic masses. Plot the phonon dispersion in appropriate units along the Γ—X, X—L, and Γ—L directions using force constants of $\alpha_{\text{BEND}} = 1$, $\alpha_\phi = 0.25$, and $M_1 = M_2 = 1$.
6. For these values of force constants and masses, determine the atomic displacements for all the modes at Γ, and for the highest optic and lowest acoustic modes at X and L. Provide drawings of the atomic motion of these modes. How many modes are there at Γ?

Model Optimization and Comparison to Macroscopic Properties

Look up experimental results for phonon dispersion in your material. Using whatever criteria you deem appropriate (sound velocities, elastic constants, zone edge frequencies, etc.), determine optimum values of your force constants to match measured results. Calculate sound velocities, zone edge frequencies, and elastic constants (C_{11}, C_{12}, and C_{44}) using your model and compare with values from the literature. Show all your calculations.

Using your model, do the following:

1. Plot a comparison of your calculated phonon dispersion with theoretical and/or experimental results along the Γ—X, X—L, and Γ—L directions.
2. Plot the total density of states (histogram method, include all modes) versus frequency.
3. Calculate the specific heat of your material versus temperature using (a) your calculated density of states, (b) a Debye model, and (c) a combined Debye-Einstein model (Debye for acoustic modes, Einstein for optical modes). Plot your results for temperatures between 0 K and $3\Theta_D$. comment on the strengths and weaknesses of your model.