Project List

1. Compute the phonon dispersion curves for a real material (solid Argon) including deformation gradient effects. This will involve changing the potential in your phonon program and then computing the dispersion curves along standard wave vector directions (directions in the reciprocal lattice space). The Lennard-Jones interatomic potential may be used for obtaining the dispersion curves. The following two references might be useful: (i) Fujii Y., et. al., Phys. Rev. B. **10**, 8, 3647-3659 (1974) (ii) Goldman. V., et. al., J.Phys. C: Solid State Phys. 3, L33 (1970). The first reference has experimental results and the second reference uses a model for the potential to reproduce the experimental results.

2. Find the phonon density of states function via brute force computation for an ideal 2D lattice with and without basis atoms. This is a classic technique that involves binning the possible values and computing the distribution functions. The first Brillouin zone of a crystal lattice and the high symmetry $\mathbf{k}$ points need to be understood. References: Born and Huang, *Dynamical Theory of Crystal Lattices*, p71, 1954 (2002 printing). M. Blackman, *Proc. Roy. Soc. (London) A*, v159, p416, 1937, Ziman, *Electrons and Phonons*, p526, 1960 (for further Blackman references). See also the website http://cst-www.nrl.navy.mil/users/mehl/phonons/sc/ for information on k-space points.

3. Find the phonon density of states via velocity auto correlation in a simple 2D setting using molecular dynamics. LAMMPS, a molecular dynamics software, may be used to obtain velocities at different times.

   See the website http://cmt.dur.ac.uk/sjc/thesis/thesis/node38.html

4. Reproduce the computations in Chopra and Zettl *Solid State Communications* **105**, 297-300 (1998).

5. Report on the detail balance argument in the Saha ionization theory to show that even though the expectation value of the separation of two atoms in a molecule is infinite, it is unlikely to occur if they start in a "bonded" configuration and the temperatures are modest.

6. Report on the computation of heat capacity in crystals using phonon frequencies and the Debye and Einstein approximations to the density of states. See Ashcroft and Mermin, Solid State Physics text book; Charles Kittles, Solid State Physics.

7. Presentation and discussion of the paper of Flory, Hoeve, and Ciferri, J.Poly.Sci, **34**, 337-347 (1959) with special attention given to a discussion of internal energy contributions with data analysis from this and other papers. See e.g. Shen and Blatz, J.Appl.Phys, **39**, 4937-4943 (1968).

8. Report on the effects of nearest neighbor interactions for dihedral bond potentials in linear polymers. See Chapter 5 of P.J. Flory *Statistical Mechanics of Chain Molecules* with particular emphasis on reproducing the results found in §5.4.

9. Report on the Worm-Like Chain (WLC) model. Here a polymer chain is treated like flexible continuous rod. Instead of $\boldsymbol{R} = \sum_i \boldsymbol{a}_i$, one now has an expression like $\boldsymbol{R} = \int_0^L \boldsymbol{t}(s)ds$, where $\boldsymbol{t}(s) = d\boldsymbol{r}(s)/ds$ is the tangent vector to the rod with $\boldsymbol{r}(s)$ being the position vector to a point along the rod. Such a model is popular for stiff polymers and is well-known in the DNA modeling literature. Possible potential energies can come from bending (bond angle like effects) and torsion (dihedral like effects). Some articles to get you started: *J. Chem. Phys*, **58**, 1564-1568 (1973). *Macromolecules*, **15**, 537-541 (1982). *Biophysical Journal*, **76**, 409-413 (1999). *J Chem. Phys.*, **80**, 930-935, (1984). [N.B. Notation varies from paper to paper so you have to read carefully.]