PHYSICS 239.c : CONDENSED MATTER PHYSICS
HW ASSIGNMENT #2

(1) For each of the following structures, indicate whether or not it is a Bravais lattice. If it is, give the three primitive vectors. If not, describe it as a Bravais lattice with the smallest possible basis.

(a) Base-centered cubic (simple cubic with additional points in the centers of the two horizontal faces).

(b) Side-centered cubic (simple cubic with additional points in the centers of the four vertical faces).

(c) Edge-centered cubic (simple cubic with additional points at the midpoints of all nearest-neighbor links).

(2) Polycrystalline specimens of three different monatomic cubic crystals are analyzed with a Debye-Scherrer camera. It is known that one sample is fcc, one is bcc, and one has a diamond structure. The approximate angular position ϕ of the first four diffraction rings are found to be

$$\begin{aligned} \mathsf{A}:&\ 42.2^\circ, 49.2^\circ, 72.0^\circ, 87.3^\circ \\ \mathsf{B}:&\ 28.8^\circ, 41.0^\circ, 50.8^\circ, 59.6^\circ \\ \mathsf{C}:&\ 42.8^\circ, 73.2^\circ, 89.0^\circ, 115^\circ \end{aligned}$$

(a) Identify the crystal structures A, B, and C.

(b) If the wavelength of the incident X-ray is $\lambda = 1.5\text{Å}$, what is the length of the side of the cubic cell in each case?

(c) If the (monatomic) diamond structure were replaced by a (binary) zincblende structure, at what angles would the first four rings be observed?

(3) A monolayer of atoms is deposited on a surface. The atoms form a regular hexagonal lattice. This problem deals with the vibrations of these atoms.

(a) Suppose the surface is perfectly smooth. The atoms interact by a potential

$$\varPhi = \tfrac{1}{2} \sum_{\boldsymbol{R},\boldsymbol{R}'} v\big(|\boldsymbol{R} + \boldsymbol{u}_\perp(\boldsymbol{R}) - \boldsymbol{R}' - \boldsymbol{u}_\perp(\boldsymbol{R}')|\big) + \tfrac{1}{2} K_z \sum_{\boldsymbol{R}} u_z^2(\boldsymbol{R})$$

where $\boldsymbol{u}_\perp = u_x\,\hat{\boldsymbol{x}} + u_y\,\hat{\boldsymbol{y}}$ is the displacement along the surface (perpendicular to the surface normal $\hat{\boldsymbol{z}}$), $\boldsymbol{R}$ and $\boldsymbol{R}'$ denote sites of the hexagonal Bravais lattice, and the last term describes the binding of the atoms to the surface (u^z is the displacement along the surface normal). Show that the dynamical matrix for the lattice vibrations takes the form

$$\hat{\Phi}(\boldsymbol{k}) = \begin{pmatrix} \hat{\Phi}^{xx}(\boldsymbol{k}) & \hat{\Phi}^{xy}(\boldsymbol{k}) & 0 \\ \hat{\Phi}^{yx}(\boldsymbol{k}) & \hat{\Phi}^{yy}(\boldsymbol{k}) & 0 \\ 0 & 0 & \hat{\Phi}^{zz}(\boldsymbol{k}) \end{pmatrix}$$

where the upper left 2×2 block is given by

$$\Phi^{\alpha\beta}(\boldsymbol{k}) = 2 \sum_{\boldsymbol{R}} \sin^2(\tfrac{1}{2}\boldsymbol{k} \cdot \boldsymbol{R}) \left\{ (\delta^{\alpha\beta} - \hat{R}^\alpha \hat{R}^\beta) R^{-1} v'(R) + \hat{R}^\alpha \hat{R}^\beta v''(R) \right\}$$

with α, $\beta = 1$ or 2, and $\hat{\Phi}^{zz}(\boldsymbol{k}) = K_z$ independent of $\boldsymbol{k}$.

(b) Assuming that the above sum for $\hat{\Phi}^{\alpha\beta}(\boldsymbol{k})$ is dominated by the nearest neighbor terms, compute the phonon dispersions along the $(1,0)$ axis in reciprocal space. You should use M for the ionic mass, a for the lattice constant, and abbreviate $A \equiv a^{-1} v'(a)$ and $B \equiv v''(a)$.

(c) Sketch the phonon density of states. Find the normalized density of states at low frequencies. Make clear any assumptions.

(d) Find an expression for the low-temperature specific heat.

(e) Find an expression for the amplitude $e^{-2W(\boldsymbol{G})}$ of the Bragg peaks in a neutron scattering experiment (the Debye-Waller factor). Show that $W(\boldsymbol{G})$ diverges for any nonzero value of $\boldsymbol{G}$. Why does this happen? Suppose that the phonon dispersion is cut off at low frequencies at a scale $\omega_{\text{min}} \propto L^{-1}$, where L is the characteristic linear dimension of the system. Show that the Debye-Waller factor is then finite and evaluate its leading dependence on L in the limit $L \to \infty$.

We now allow for the "corrugation" of the surface through an additional term in the potential energy

$$\Delta\Phi = \tfrac{1}{2} K_\perp \sum_{\boldsymbol{R}} \boldsymbol{u}_\perp^2(\boldsymbol{R}) \, .$$

(f) Compute the new phonon frequencies for $\boldsymbol{k} \approx 0$.

(g) What is the temperature dependence of the density of states?

(h) Show that the Debye-Waller factor is now finite even in the $L \to \infty$ limit.

(4) Find the longitudinal and transverse phonon speeds for a cubic crystal with mass density ρ and nonzero elastic moduli C_{11}, C_{12}, and C_{44} for the following cases: (a) $\boldsymbol{k} \parallel (1,0,0)$, (b) $\boldsymbol{k} \parallel (1,1,0)$, and (c) $\boldsymbol{k} \parallel (1,1,1)$.