Solid State Physics
Homework 4: Diffraction Applications (25 pts)

1. Alternating Chain (15 points)

Calculate the intensity as a function of $\Delta \vec{k}$ for an alternating chain of atoms. Run through the solution twice, using these assumptions:

(a) Assume the scattering density of the atoms can be treated as $\delta$ functions.

$$n(\vec{r}) = \sum_{j=0}^{1000} 3\delta(x - j\vec{a}_1) + 2\delta(x - j\vec{a}_1 - \frac{1}{2}\vec{a}_1)$$

(b) Assume the scattering density can be treated as spherical gaussians with the following local functions about each atom:

Atom 1: $n_1(\vec{r}) = 2e^{-|\vec{r}|^2}$

Atom 2: $n_2(\vec{r}) = e^{-|\vec{r}|^2}$

Here, a structure factor approach may be simpler than going through the full Fourier transform. Extra points for doing both.

2. Structure Factor. (10 pts)

Assume X-rays for incident radiation.

(a) Consider a primitive tetragonal crystal with a basis of (0,0,0) and (0,0,$\frac{1}{4}$). Solve for the structure factor and determine rules for when destructive interference occurs.

(b) Translating the origin leads to a structure with a basis of (0,0,$\frac{1}{8}$) and (0,0,$\frac{7}{8}$). Sketch the two different cells, then solve for the structure factor and determine rules for destructive interference occurs.

(c) Pick a non-primitive cell for this same structure and re-solve for the structure factor. Compare the locations of peaks in reciprocal space between these approaches.

3. Thin film diffraction (20 pts)

(a) Let’s begin with a (111) wafer of silicon. After cleaning the surface, you have a hexagonal pattern of Si, with each Si atom terminated w/ a hydrogen. Using Vesta, determine the dimensions of the hexagonal net on this surface and provide a sketch.

(b) If you tried to grow epitaxial wurtzite ZnS (from last homework) on this surface, what orientation would you expect and what is the lattice mismatch?

(c) After completing your first growth, you take your ZnS/Si sample to a thin film diffractometer. Think like an experimentalist: what do you want to know, how would you test it, and what quantitative results do you expect? This should be an extensive answer.

(d) Great news, the first sample met your expectations and it’s a beautiful epitaxial film. Take a break and enjoy life.

(e) While you were off enjoying life, your pesky lab mate fiddled with the growth chamber. The next sample you grew gave the pattern shown in Figure 1 when you ran a $\theta - 2\theta$ scan. What can you say about your second film based on this information? What is still unknown?
4. Diffraction on Detritus. (10 pts) On a trip to the beach, you pick up a shell and put in in your pocket. On a late Saturday night in the lab, you think to yourself, “I know, let’s see what this shell does in the diffractometer!”.

(a) Read about the structure of nacre on Wikipedia. Then open the structure in Vesta. Which growth directions are similar and which are distinct from a crystal chemistry perspective?

(b) What do you expect to see when you run a \( \theta - 2\theta \) scan?

(c) Do you expect to see if you run a \( \omega \) rocking curve on a peak normal to the sample surface?

(d) What do you expect to see if you run a \( \phi \) scan on an off-axis peak?

Figure 1: \( \theta - 2\theta \) scan of the second growth of ZnS film on Si.

Figure 2: Scanning electron microscopy image of nacre.