Solid State Physics
Homework 1: Diffraction
5% of final grade, divided into 50 pts

1. **Warm-up (10 pts)**

   (a) Write out the scattering amplitude derivation from start to finish (including Fourier expression for n(r)). Label all variables clearly in the beginning and final equations. All steps should be clear and any assumptions must be acknowledged and justified.

   (b) Spatial phase factor has historically led to confusion.

   (i) Plot the real and complex components of the source wave $e^{i(\vec{k}\cdot a\vec{R}-\omega t)}$ as a function of scalar a from zero to one (from source to sample) if $\vec{R}$ and $\vec{k}$ are parallel and time $t = 0$. In your drawing, use a wavelength that is 10 times smaller than $|\vec{R}|$. (Note, this is not realistic, λ is actually much smaller, but it is hard to draw 10^{10} oscillations.)

   (ii) Consider two points in the sample: $\vec{r}_1$ and $\vec{r}_2$. What is the difference in phase of the source wave at these two points in the sample? Recall $|\vec{k}| = 2\pi/\lambda$.

   (iii) By the time the two wavelets reach the detector at R', what is this the difference in phase?

   (c) What does $\vec{G}$ represent? Why is it important and where did it come from?

2. **Brain teasers. (10 pts)**

   (a) The 110 planes of a crystal with a body-centered cubic lattice will constructively interfere, leading to a 110 peak. However, the face-centered cubic lattice exhibits destructive interference for this reflection. By visual inspection of the crystals structure, can you rationalize this difference using the simple Bragg's law approach?

   (b) Derive the general selection rules for which reflections are observed in bcc and fcc structures (one atom basis of (0,0,0)). Double check the assertion in (a).

   (c) Show that these selection rules hold independent of what atoms are in the primitive unit cell, so long as the lattice is bcc or fcc respectively.

   (d) Using X-ray diffraction from sodium hydride (NaH), it was established that the Na atoms are arranged on a fcc lattice. Why was it difficult to locate the positions of the H atoms using X-rays?

3. **Diffraction Spectra. (10 pts)** As molten iron cools, it forms an allotrope with a body-centered cubic crystal structure. Cooling iron further causes the formation of a face-centered cubic allotrope. Figure 1 shows x-ray diffraction spectra of these iron allotropes with a Cu source at 1.54 Å.

   (a) Determine which spectrum (A or B) is bcc and which is fcc. Justify your response.

   (b) You're doing this measurement in-situ with a hot stage on the XRD. Sketch how the diffraction pattern will evolve with temperature as you cool from the liquid state to room temperature. For clarity, consider $100°$C steps from 1600 to $700°$C. Superimpose the patterns with off-sets to display this evolution and label the key features you expect to observe.
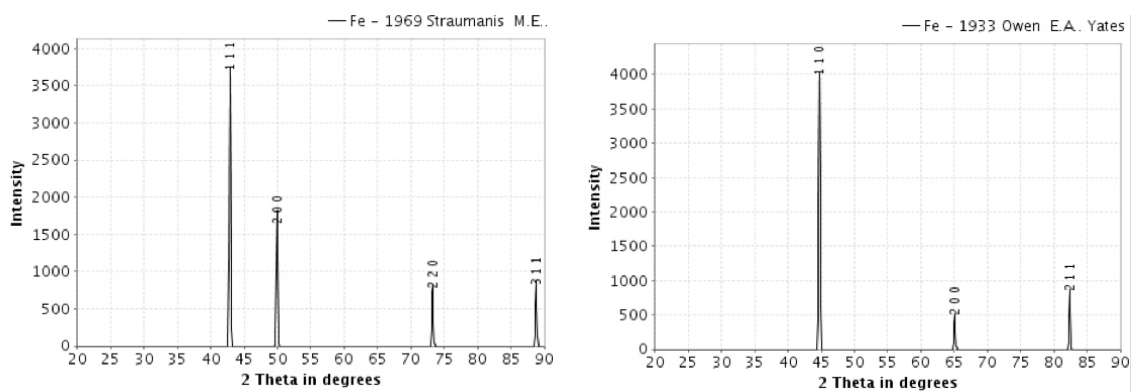
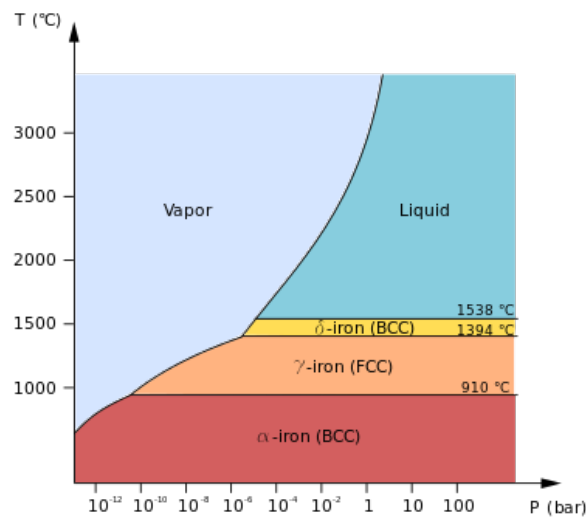(a) Diffraction pattern (A) (b) Diffraction pattern (B)

Figure 1: Two allotropes of iron and the associated phase diagram.

4. **Thin film diffraction (10 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. Note, only the atoms with dangling bonds should be counted as part of this net.

   (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 2 when you ran a $\theta - 2\theta$ scan. What can you say about your second film based on this information? What is still unknown?
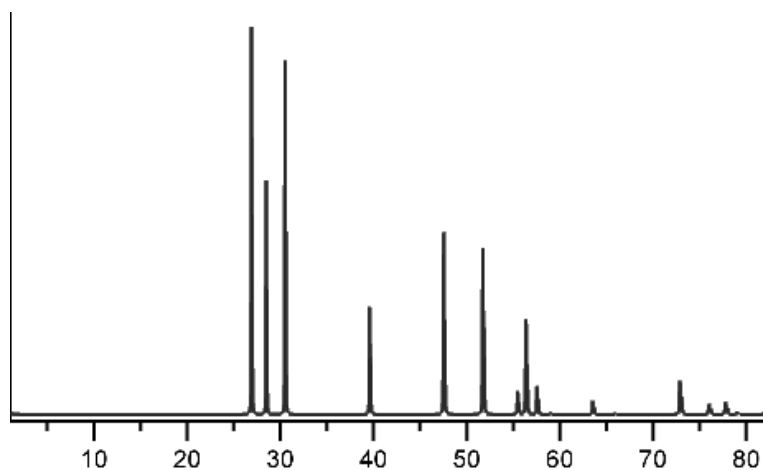

Figure 2: Cu K-alpha $\theta - 2\theta$ scan of the second growth of ZnS film on Si.

5. **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 ω rocking curve on a peak normal to the sample surface?

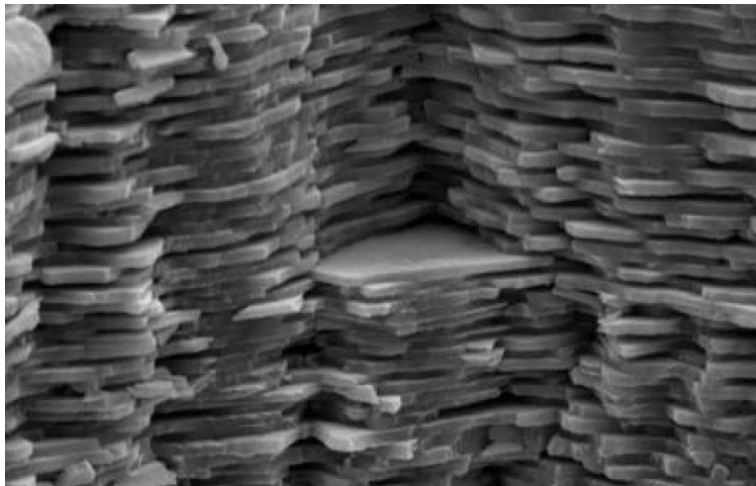   (d) What do you expect to see if you run a ϕ scan on an off-axis peak?

Figure 3: Scanning electron microscopy image of nacre.