

Physics 555 Fall 2011 Problem set # 2 due Friday Sept. 16

1. X-ray scattering Aluminum has the fcc crystal structure. Silicon has the diamond crystal structure [fcc lattice, basis = atoms at + and $-(a/8)(1,1,1)$]. AlP (aluminum phosphide) has the zincblende crystal structure [same as diamond or silicon, except one of the silicon atoms is replaced by Al, and the other by P.] The lattice constants are $a = (4.05\text{\AA}, 5.43\text{\AA}, 5.46\text{\AA})$ for (Al, Si, and AlP) respectively. Consider x-ray diffraction from (111) planes.

- Sketch the geometry of these planes. Show that they are evenly spaced in Al, but in Si and AlP, there are additional plane spacings of $1/4$ and $3/4$ of the primary spacing.
- What is the primary plane spacing in Al, Si, and AlP? [answer $a/\sqrt{3}$]
- Suppose your monochromatic x-rays are Mo ($K\alpha$) with wavelength 0.711\AA . At what angles (2θ) are the first, second, third, and fourth-order diffraction peaks seen in Al (sketch the geometry.)
- Explain why the second order diffraction peak is missing in diamond structure. What other peaks in this (111) series are missing?
- Will the second-order [or (222)] peak be seen in AlP? If so, explain its intensity.

2. Kittel p.44 problem 2

Hexagonal space lattice. The primitive translation vectors of the hexagonal space lattice may be taken as

$$\mathbf{a}_1 = (3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}} \quad ; \quad \mathbf{a}_2 = -(3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}} \quad ; \quad \mathbf{a}_3 = c\hat{\mathbf{z}} \quad .$$

- Show that the volume of the primitive cell is $(3^{1/2}/2)a^2c$.
- Show that the primitive translations of the reciprocal lattice are

$$\mathbf{b}_1 = (2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}} \quad ; \quad \mathbf{b}_2 = -(2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}} \quad ; \quad \mathbf{b}_3 = (2\pi/c)\hat{\mathbf{z}} \quad ,$$

so that the lattice is its own reciprocal, but with a rotation of axes.

- Describe and sketch the first Brillouin zone of the hexagonal space lattice.

3. This is Ibach and Lüth, p. 71, problem 3.8, perhaps a bit clarified using Kittel, p.44 problem 4. We start with a 1-d finite lattice with M sites.

Width of diffraction maximum. We suppose that in a linear crystal there are identical point scattering centers at every lattice point $\mathbf{r}_m = m\mathbf{a}$, where m is an integer. By analogy with (20), the total scattered radiation amplitude will be proportional to $F = \sum \exp[-im\mathbf{a} \cdot \Delta\mathbf{k}]$. The sum over M lattice points is

$$F = \frac{1 - \exp[-iM(\mathbf{a} \cdot \Delta\mathbf{k})]}{1 - \exp[-i(\mathbf{a} \cdot \Delta\mathbf{k})]} \quad ,$$

Show that the width of the diffraction peak is proportional to $1/M$ and find the coefficient. Now proceed with Ibach and Lüth problem 3.8.

4. Ibach and Lüth, problem 3.6 (EXAFS) – but here I try to clarify. EXAFS stands for “extended x-ray absorption fine structure.” You use x-ray photons with $h\nu$ above the threshold for continuum absorption (leaving a core hole behind.) The measured absorption has characteristic structure as a function of $h\nu$. Suppose $|i\rangle$ is an initial core-level p state, localized on atom X in a disordered condensed phase material with other atoms Y, Z. We are hoping to learn something about the local structure near atom X. Let $|f\rangle$ be an outgoing spherical wave of s symmetry. The outgoing wave $|f\rangle$ scatters elastically from neighboring atoms Y, Z, emitting secondary spherical out-going waves, that alter the matrix element $\sim \langle f | \vec{p} \cdot \vec{A} | i \rangle \approx \langle f | x | i \rangle$. How does the x-ray absorption depend on energy $h\nu$ above threshold? How can this be used to measure the distance distribution of nearest neighbors in an amorphous material?