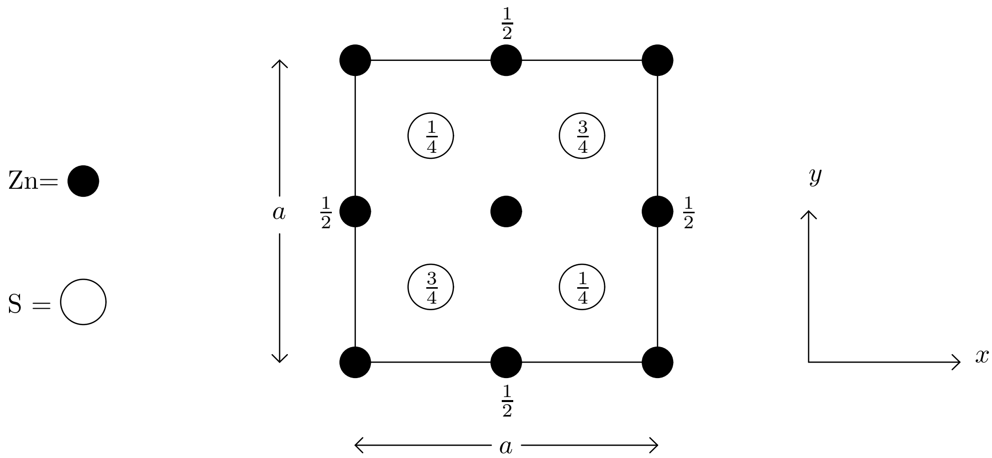
Problem Set 3

Crystal Structure, Reciprocal Lattice, and Scattering

3.1. **Crystal Structure**



The diagram above shows a plan view of a structure of cubic ZnS (zinc blende) looking down the z axis. The numbers attached to some atoms represent the heights of the atoms above the $z = 0$ plane expressed as a fraction of the cube edge a. Unlabeled atoms are at $z = 0$ and $z = a$.

(a) What is the Bravais lattice type

(b) Describe the basis

(c) Given that $a = 0.541$ nm, calculate the nearest-neighbor Zn-Zn, Zn-S, and S-S distances.

(d) Copy the drawing above, and show the [210] direction and the set of (210) planes.

(e) Calculate the spacing between adjacent (210) planes.

3.2. **Directions and Spacings of Crystal Planes**

▷ Explain briefly what is meant by the terms "Crystal Planes" and "Miller Indices."

▷ Show that the general direction $[hkl]$ in a cubic crystal is normal to the planes with Miller indices (hkl).

▷ Is the same true in general for an orthorhombic crystal?

▷ Show that the spacing d of the (hkl) set of planes in a cubic crystal with lattice parameter a is

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

▷ What is the generalization of this formula for an orthorhombic crystal?

3.3. ‡**Reciprocal Lattice**

(a) Define the term Reciprocal Lattice.

(b) Show that if a lattice in 3d has primitive lattice vectors $\mathbf{a_1}$, $\mathbf{a_2}$ and $\mathbf{a_3}$ then primitive lattice vectors for the reciprocal lattice can be taken as

$$\mathbf{b_1} = 2\pi \frac{\mathbf{a_2} \times \mathbf{a_3}}{\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})} \tag{1}$$

$$\mathbf{b_2} = 2\pi \frac{\mathbf{a_3} \times \mathbf{a_1}}{\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})} \tag{2}$$

$$\mathbf{b_3} = 2\pi \frac{\mathbf{a_1} \times \mathbf{a_2}}{\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})} \tag{3}$$

What is the proper formula in 2d?

(c) Define tetragonal and orthorhombic lattices. For an orthorhombic lattice, show that $|\mathbf{b_j}| = 2\pi/|\mathbf{a_j}|$. Hence, show that the length of the reciprocal lattice vector $\mathbf{G} = h\mathbf{b_1} + k\mathbf{b_2} + l\mathbf{b_3}$ is equal to $2\pi/d$, where d is the spacing of the (hkl) planes (see question 3.2.)

3.4. **Reciprocal Lattice and X-ray Scattering**

A two-dimensional rectangular crystal has a unit cell with sides $a_1 = 0.468$ nm and $a_2 = 0.342$ nm. A collimated beam of monochromatic X-rays with wavelength 0.166 nm is used to examine the crystal.

(a) Draw to scale a diagram of the reciprocal lattice.

▷ Label the reciprocal lattice points for indices in the range $0 \le h \le 3$ and $0 \le k \le 3$.

(b) Calculate the magnitude of the wavevectors $\mathbf{k}$ and $\mathbf{k}'$ of the incident and reflected X-ray beams, and hence construct on your drawing the "scattering triangle" corresponding to the Laue condition $\Delta\mathbf{k} = \mathbf{G}$ for diffraction from the (210) planes. (the scattering triangle includes $\mathbf{k}$, $\mathbf{k}'$ and $\Delta\mathbf{k}$).

(c) Draw the first and second Brillouin zones using the Wigner-Seitz construction.

3.5. ‡ **X-ray scattering II**

$BaTiO_3$ has a primitive cubic lattice and a basis with atoms having fractional coordinates

Ba	[0,0,0]		
Ti	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$		
O	$[\frac{1}{2}, \frac{1}{2}, 0]$,	$[\frac{1}{2}, 0, \frac{1}{2}]$,	$[0, \frac{1}{2}, \frac{1}{2}]$

▷ Sketch the unit cell.

▷ Show that the X-ray structure factor for the $(00l)$ Bragg reflections is given by

$$S_{hkl} = f_{Ba} + (-1)^l f_{Ti} + \left[1 + 2(-1)^l\right] f_O \tag{4}$$

where f_{Ba} is the atomic form factor for Ba, etc.

▷ Calculate the ratio I_{002}/I_{001}, where I_{hkl} is the intensity of the X-ray diffraction from the (hkl) planes. You may assume that the atomic form factor is proportional to atomic number (Z), and neglect its dependence on the scattering vector. [$Z_{\mathrm{Ba}} = 56$, $Z_{\mathrm{Ti}} = 22$, $Z_{\mathrm{O}} = 8$]

3.6. ‡ **X-ray scattering and Systematic Absences**

(a) Explain what is meant by "Lattice Constant" for a cubic crystal structure.

(b) Explain why X-ray diffraction may be observed in first order from the (110) planes of a crystal with a body-centred cubic lattice, but not from the (110) planes of a crystal with a face-centred cubic lattice.

▷ Derive the general selection rules for which planes are observed in bcc and fcc lattices.

(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) A collimated beam of monochromatic X-rays of wavelength 0.162 nm is incident upon a powdered sample of the cubic metal palladium. Peaks in the scattered X-ray pattern are observed at angles of 42.3°, 49.2°, 72.2°, 87.4° and 92.3° from the direction of the incident beam.

▷ Identify the lattice type

▷ Calculate the lattice constant.

▷ If you assume there is only a single atom in the basis, how well does this lattice constant agree with the known data that the density of palladium is 12023 kg m^{-3}? [Atomic mass of palladium = 106.4].

(e) How could you improve the precision with which the lattice constant is determined.

3.7. ‡ **Neutron Scattering**

(a) X-ray diffraction from sodium hydride (NaH) established that the Na atoms are arranged on a face-centred cubic lattice.

▷ Why is it difficult to locate the positions of the H atoms using X-rays?

The H atoms were thought to be displaced from the Na atoms either by $[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$ or by $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$, to form the ZnS (zincblende) structure or NaCl (sodium chloride) structure, respectively. To distinguish these models a neutron powder diffraction measurement was performed. The intensity of the Bragg peak indexed as (111) was found to be much larger than the intensity of the peak indexed as (200).

▷ Write down expressions for the structure factors S_{hkl} for neutron diffraction assuming NaH has

(i) the sodium chloride (NaCl) structure

(ii) the zinc blende (ZnS) structure.

▷ Hence, deduce which of the two structure models is correct for NaH. [Nuclear scattering length of Na $= 0.363 \times 10^{-5}$nm; nuclear scattering length of H $= -0.374 \times 10^{-5}$ nm]

(b) How does one produce monochromatic neutrons for use in neutron diffraction experiments?

▷ What are the main differences between neutrons and X-rays?

▷ Explain why (inelastic) neutron scattering is well suited for observing phonons, but x-rays are not.