

Quiz 4 XRD 020207

- 1) **What** is the unit cell for NaCl (B1)?
What atoms are in a single lattice position for NaCl?
Give the direction vectors of atoms in a single lattice position for NaCl.
Give the direction vectors in the unit cell for all lattice positions.

- 2) For Cu,
sketch the unit cell
and **give** the real space vectors locating atom positions in the unit cell.
Explain why a (100) reflection is not observed in diffraction from Cu using the atom positions you listed above.

- 3) **What** is the transverse direction in a $\langle 111 \rangle \{100\}$ standard projection cubic pole figure?
(Use the equation for a zone axis/plane and the idea that the dot product of two perpendicular directions is zero, i.e. for [100] and [010], $1*0+0*1+0*0=0$.)

Answers: **Quiz 4 XRD 020207**

1) The unit cell is FCC for NaCl with two atoms per lattice position, Na at [000] and Cl at [1/2 0 0]. The unit cell has lattice positions at [000], [1/2 1/2 0], [0 1/2 1/2], and [1/2 0 1/2].

2) Cu is FCC with atoms at [000], [1/2 1/2 0], [0 1/2 1/2], and [1/2 0 1/2]. A (100) reflection isn't seen since a wave from the atom at [000] is completely out of phase with a wave from the atom at [1/2 1/2 0] and a wave from the atom at [0 1/2 1/2] is completely out of phase with a wave from the atom at [1/2 0 1/2] for (100) reflections. The phase angle is $2\pi(hu + kv + lw)$ where $(hkl) = (100)$.

3) The transverse direction, [uvw], must fulfill the following two equations:

$$[111] \cdot [uvw] = 0 \text{ so } u+v+w=0$$

and

$$[100] \cdot [uvw] = 0 \text{ so } \mathbf{u=0}$$

Then $\mathbf{v = -w}$ and the transverse direction is of the type $\langle \mathbf{0 \ 1 \ 1} \rangle$.