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SCHOOL OF PHYSICS AND ASTRONOMY

Structure and Properties of Functional Materials

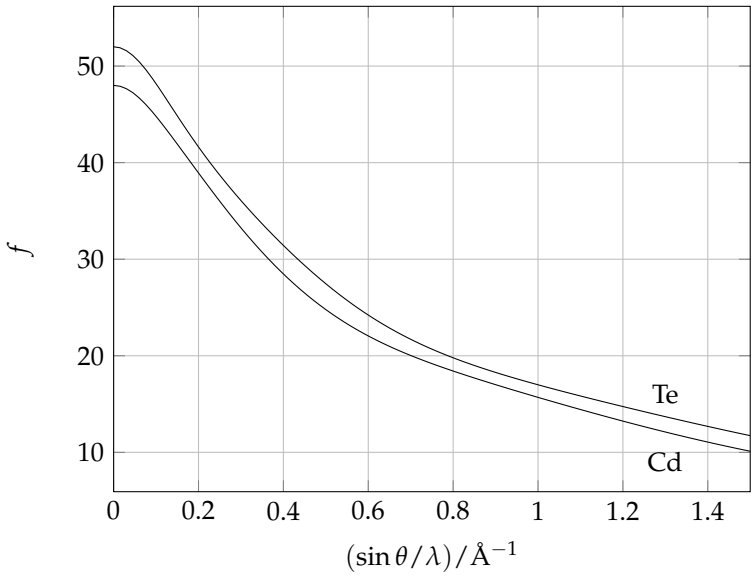
Exercise Set 2

Friday, 18 January, 2013

1. *For discussion:*
   (a) Explain why the simple cubic structure is rare, but the rock salt structure very common.
   (b) Explain why we say that the rock-salt structure is based on a face-centred cubic lattice, not a simple cubic lattice.

2. (a) Find the number of nearest neighbours and distance to these nearest neighbours (in terms of the cell parameter a) for an atom in each of the following structures: simple cubic, body-centred cubic, face-centred cubic, diamond.
   (b) Repeat the calculation, but this time for *second*-nearest neighbours.
   (c) Finally calculate the ratio between the second-nearest and nearest neighbour distances. For which structure is this ratio the lowest?

3. Cadmium telluride, CdTe, is an important material for photovoltaic manufacture. It has the cubic zinc blende structure. At room temperature, the lattice parameter is $a = 6.48\,\text{Å}$.
   (a) Calculate the X-ray structure factors $F(111)$, $F(200)$, and $F(733)$ and hence the intensities $|F|^2$ one would observe in experiment for each of these peaks. The X-ray form factors for Cd and Te are given below. Ignore the effects of thermal motion.
   (b) Why is $|F(733)|^2$ smaller than $|F(111)|^2$? Would $|F(733)|^2$ still be much smaller than $|F(111)|^2$ if neutron instead of X radiation were used? Why or why not?
   (c) Why is $|F(200)|^2$ smaller than $|F(111)|^2$? Would $|F(200)|^2$ still be much smaller than $|F(111)|^2$ if neutron instead of X radiation were used? Why or why not?
   (d) Why would it be difficult to investigate this structure using neutron diffraction?



4. The following lattices are, by convention, not used to describe crystal structures. In each case explain why not.
   (a) Body-centred triclinic
   (b) Base-centred cubic
   (c) Face-centred tetragonal