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Structure and Properties of Functional Materials

Homework Set 2

Due Wednesday, 23 January, 2013 by 4 p.m.

Problem 1: Terms and definitions (8 marks)

Explain the following terms or concepts, giving an example of their significance in condensed matter physics:

(a) Time-of-flight diffractometer (4)

(b) Centred unit cell (4)

Problem 2: Allotropes of iron (16 marks)

Iron undergoes a phase transition at 912 °C from body-centred cubic (the room temperature α phase) to face-centred cubic (the γ phase). Just below the phase transition, the lattice parameter of the α phase is 2.90 Å. The atomic mass of Fe is $55.845\,\mathrm{g\,mol^{-1}}$, and Avogadro's number is $N_\mathrm{A} = 6.022 \times 10^{23}\,\mathrm{mol^{-1}}$.

(a) Calculate the density of α-iron just below the phase transition. (2)

(b) Estimate the radius of the atoms in metallic iron. (3)

(c) Hence estimate the lattice parameter and density of γ-iron just above the phase transition. (4)

(d) Calculate the intensity $|F|^2$ and angle θ of the (211) diffraction peak below and above the transition. Take $f = 26$ for Fe, ignore thermal motion, and assume Mo $K\alpha$ radiation, $\lambda = 0.709\,26$ Å, is used. (7)

Problem 3: Choice of radiation (8 marks)

In the following experiments, would you use neutron or X-ray diffraction? Explain your reasoning.

(a) Determination of the crystal structure of cadmium vanadate, CdV_2O_6. (2)

(b) Determination of the magnetic ordering in manganese(II) oxide, MnO. (2)

(c) Measurement of diffuse scattering from silica glass, SiO_2; this sample is expected to give a diffuse scattering signal up to at least $Q = 40\,\mathrm{Å^{-1}}$. (2)

(d) Determination of the crystal structure of a new polymorph of a pharmaceutical compound, $C_{10}H_{13}N_5O_4$; the only crystal available has dimensions $0.15 \times 0.1 \times 0.1\,\mathrm{mm^3}$. (2)

Problem 4: Symmetry in crystal structures (8 marks)

(a) Show that, if a crystal structure has a mirror plane perpendicular to **a**, its diffraction pattern will have a mirror plane perpendicular to $\mathbf{a}^*$. (4)

(b) Is the converse true? That is, if a diffraction pattern has a mirror plane perpendicular to $\mathbf{a}^*$, is it necessarily true that the crystal structure has a mirror plane perpendicular to **a**? Explain your reasoning. (4)