

SEMESTER 1 EXAMINATION 2013-2014

CRYSTALLINE SOLIDS

Duration: 120 MINS (2 hours)

This paper contains 10 questions.

Answer **all** questions in **Section A** and **only two** questions in **Section B**.

Section A carries 1/3 of the total marks for the exam paper and you should aim to spend about 40 mins on it.

Section B carries 2/3 of the total marks for the exam paper and you should aim to spend about 80 mins on it.

An outline marking scheme is shown in brackets to the right of each question.

A Sheet of Physical Constants is provided with this examination paper.
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Only university approved calculators may be used.

A foreign language translation dictionary (paper version) is permitted provided it contains no notes, additions or annotations.

Section A

- A1.** Describe the nature of van der Waals bonding. How might the number of electrons per atom influence the van der Waals interaction? [3]
- A2.** Explain what is meant by 'ionisation energy'. Explain what is meant by 'electron affinity'. [2]
- A3.** Explain what is meant by 'ionic bonding'. Name the three energies that determine the stability of ionic bonding. Use these to write down the condition that is required for ionic bonding to occur. [3]
- A4.** Explain the Born-Oppenheimer approximation and why it often works very well. [3]
- A5.** Explain what is meant by terms: dispersion relation, Fermi-energy , Fermi-surface, allowed k -state. [4]
- A6.** Explain what is meant by diamagnetism, paramagnetism and ferromagnetism. Draw a graph of the magnetisation M against the applied magnetic field B for each of the three forms of magnetism. [2]
- A7.** Write down and explain Bloch's equation for the electron wavefunction in the periodic potential of a crystal. [3]

Section B

- B1.** (a) Describe the mechanism of the scattering of X-rays in crystals? [2]
- (b) What information can we obtain about a crystal using X-ray diffraction? [4]
- (c) A specific crystal has lattice vectors \mathbf{a}_1 , \mathbf{a}_2 and \mathbf{a}_3 . Using these vectors, define the reciprocal lattice vectors \mathbf{a}_1^* , \mathbf{a}_2^* and \mathbf{a}_3^* . [4]
- (d) The equation that dictates whether X-ray diffraction will occur is given by:

$$\mathbf{Q} = \mathbf{G} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*$$

- where $\mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i$, \mathbf{k}_i is the incident X-ray wavevector and \mathbf{k}_f is the reflected X-ray wavevector. Also h , k and l are Miller indices. Using a single diagram, illustrate the geometry required to measure X-ray diffraction from a single crystal. Indicate the lattice planes and the direction of \mathbf{Q} . [4]
- (e) A simple cubic crystal has unit cell length of 5.4 Angstroms. Write down the equation that determines the angles at which X-ray diffraction will occur. Calculate the Bragg angle for X-ray diffraction from the (110) plane at a wavelength of 1.2 Angstroms. [2]
- (f) The structure factor for a specific crystal is given by:

$$SF = \iiint_{\text{UnitCell}} \rho_e(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} dV$$

- where $\rho_e(\mathbf{r})$ is the electron density. Describe what effect the structure factor will have on the diffraction pattern. Treating the ions as point like, derive the structure factor for caesium chloride with Cs^+ ions at (0,0,0) and Cl^- ions at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ for Miller indices (h, k, l) . Note that the atomic positions are given in fractions of the lattice vectors. [4]

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- B2.** (a) Explain what is meant by ‘electron mobility’. [2]
- (b) Describe the assumptions made in the free electron (jellium) and in the nearly-free electron models. [4]
- A one-dimensional lattice has a unit cell length $a = 0.18$ nm.
- (c) Calculate the momentum of the free electron at the Brillouin zone edge. [4]
- (d) Calculate the kinetic energy of the free electron with this momentum. [4]
- (e) The periodic potential due to the ions has a strength V that is one tenth of the free-electron kinetic energy at the Brillouin zone edge.
- Sketch a graph of the dispersion relation for both free electron and for the nearly free electron models in the reduced zone scheme. Use units of nm^{-1} for k , and eV for E . In each case, label your sketch with the energy of the electrons at the zone edge, and the band gap energy. [6]

- B3.** (a) What is a semiconductor? [2]
- (b) Describe what is meant by an 'intrinsic' and an 'extrinsic' semiconductor. [2]
- (c) Describe what is meant by an 'n-type' and a 'p-type' semiconductor. [2]
- (d) Using simple band theory arguments, explain why extrinsic carriers can appear to be positively charged in a semiconductor doped with acceptor impurities. [6]
- (e) Sketch a band bending diagram of a semiconductor pn-junction in the absence of a potential difference. Ensure that each side of the junction is labelled appropriately and indicate the location of the depletion region. In addition, illustrate what would happen to an electron and a hole soon after they were created by the absorption of a photon in the depletion region. [8]

END OF PAPER