

SEMESTER 1 EXAMINATION 2012/13

CRYSTALLINE SOLIDS

Duration: 120 MINS

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

A Sheet of Physical Constants will be provided with this examination paper.

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

Only university approved calculators may be used.

Section A

A1. State and justify the Born–Oppenheimer approximation. Sketch the binding potential between two nuclei and mark the important features of the potential.

[4]

A2. One of the two dimensional Bravais lattice is the rhombic or centred rectangular; it consists of a rectangular lattice with an additional lattice point at the centre of every rectangle. Sketch one or more conventional (rectangular) units cells, and mark on the *conventional* $c_{1,2}$ and *primitive* $p_{1,2}$ lattice vectors. Write down expressions for the primitive lattice vectors in terms of the conventional lattice vectors and sketch the conventional and primitive cells. What is the ratio of the areas of these two cells?

[4]

A3. State the Bloch theorem for the eigenfunctions of a translationally periodic Hamiltonian. Sketch, in the extended zone scheme and on the same diagram, the dispersion curves for *free electrons* and for typical *nearly free electrons*.

[4]

A4. Consider x-ray diffraction by a set of crystal planes which are separated by a distance d . What simplifying assumption can we make about the energy of the diffracted x-ray photons compared with that of the incident x-ray photons?

[1]

Give an expression for the magnitude of the crystal momentum $\hbar G$.

[1]

Draw a vector diagram showing the relationship between the incoming and outgoing photon momenta and the momentum transferred by the crystal lattice and give an equation which relates these vectors.

[2]

A5. In an intrinsic semiconductor, where does the Fermi energy fall relative to the bandgap? State whether doping an intrinsic semiconductor with elements containing one more proton than the bulk would *increase* or *decrease* the Fermi energy? [2]

Sketch the Fermi distribution $f(E)$ for absolute zero and for room temperature.

Explain how heating an intrinsic semiconductor affects its conductivity. [2]

Section B

- B1.** (a) Sketch the magnetism M in a **diamagnetic** material as a function of the applied magnetic field B . What property of the electron is responsible for **ferromagnetism**? [2]

Explain with reference to the microscopic structure why a macroscopic sample of iron at room temperature is typically **not** a very strong magnet.

[2]

- (b) Consider a material in which the majority charge carriers are holes and there is a conventional current flow along $+\hat{x}$. A magnetic field is applied along the $+\hat{z}$ direction. Write down a vector equation for the force on a charge carrying hole due to the magnetic field. [1]

- (c) Using classical electromagnetism and the result and geometry from (b), derive an expression for the transverse electric field which will arise in a slab of material due to the magnetic field in terms of the current density and the number density of charge carrying holes. Identify the Hall coefficient and explain how this would change if the majority charge carriers were electrons. [6]

- (d) The average motion of electrons in response to an externally applied electric field is described by the following differential equation:

$$\frac{d\mathbf{v}_d}{dt} + \frac{\mathbf{v}_d}{\tau} = -\frac{q}{m}\mathbf{E}.$$

Define conductivity and, by considering the current density $\mathbf{j} = -nq\mathbf{v}_d$ in the steady-state condition, show that it is given by $\sigma = nq^2\tau/m$. [3]

- (e) Using the equation from (d), calculate the drift velocity for a copper wire of cross-section $A = (1 \mu\text{m})^2$ which carries $I = 1 \mu\text{A}$ and has a charge carrier density of $8.5 \times 10^{28} \text{ m}^{-3}$; you may assume that the effective mass is the same as the free-particle mass. If the resistivity is $\rho = 20 \text{ n}\Omega \cdot \text{m}$, calculate the scattering time. [4]

- (f) What is the name for the quantum of charge oscillations? If the restoring force for a displacement of charge within a material is

$$\mathbf{F} = \frac{-nq^2}{\epsilon_0} \mathbf{x},$$

- give an expression for the oscillation frequency. In metals, to what optical wavelength band does this frequency typically correspond? [2]

B2. (a) Which of the fundamental forces is responsible for bonding in solids? Describe where the electron is most likely to be found in the case of bonding between two identical atoms and state the name given to this type of bond. [3]

(b) Consider the non-identical atoms in a crystal of sodium chloride. The ionisation energy for Na is 5.14 eV and the electron affinity for Cl is 3.62 eV. What is the difference in energy between widely separated neutral Na and Cl atoms, and the ions Na^+ and Cl^- at the same separation? [1]

Treating Na^+ and Cl^- as respectively positive and negative point-like charges, calculate the electrostatic binding energy if the equilibrium separation is $r_0 = 0.24$ nm. [3]

What, therefore, is the overall energy of a Na^+Cl^- molecule as compared with neutral Na and Cl atoms at some large separation? With reference to these calculations, explain whether or not the molecule will form. [2]

(c) List the locations of the lattice points in a body-centred cubic (bcc) lattice, and in a face-centred cubic lattice (fcc) with respect to the conventional cell. If we insist that a 2D lattice has *translational* symmetry, what *rotational* symmetries can it have? What kind of crystal might show a rotational symmetry which is impossible for a translationally symmetric crystal? [4]

(d) The electric field for diffracted x-rays can be expressed as

$$E \propto \sum_n \exp[-i\mathbf{Q} \cdot \mathbf{R}_n] \iiint_{\text{Unit Cell}} \rho_e(\mathbf{r}) \exp[-i\mathbf{Q} \cdot \mathbf{r}] dV$$

Write down an expression for \mathbf{R}_n in terms of the primitive lattice vectors.

State the defining properties of the reciprocal lattice vectors in terms of the real-space lattice vectors, and give a solution for \mathbf{Q} which results in significant diffraction in terms of the reciprocal primitive lattice vectors and the plane (hkl) .

[3]

- (e) Calculate the structure factor for a two atom basis with identical atoms at the positions 000 and $\frac{1}{4}\frac{1}{4}\frac{1}{4}$; assume that electrons associated with each atom are tightly localised around their respective nuclei, and express your answer in terms of the Miller indices (hkl) . What can you infer about the diffracted order from the (110) plane?

[4]

- B3.** (a) Describe the defining property of a semiconductor and explain how the band structure of an insulator differs from that of an intrinsic semiconductor. [3]
- (b) Describe how n- and p-type doping of a semiconductor affect the free charge carriers. Identify the type of doping when a crystal of ${}_{14}\text{Si}$ is doped with ${}_{15}\text{P}$. [2]
- (c) Beginning with the expression for the kinetic energy of a particle with an effective mass m^* , derive an expression for the effective mass in terms of the curvature of the dispersion relation. Sketch the dispersion relation for the valence and conduction bands of an intrinsic semiconductor in which holes are lighter than electrons, and indicate which states are occupied and which are empty at $T = 0\text{ K}$. [4]
- (d) State the Einstein relation for diffusion of charged particles and define all terms in the equation. [2]
- (e) Consider a metal-oxide-semiconductor structure consisting of metal, a layer of insulating SiO_2 , and p-type doped Si. Assuming that the SiO_2 layer is thin, sketch the band edges as a function of distance from the SiO_2 into the bulk p-Si if we apply a voltage just above the switching voltage. Mark on the Fermi energy and describe what happens as the bottom of the conduction band falls below the Fermi energy. [3]
- (f) Consider a sample of n-type semiconductor and a sample of p-type semiconductor which we bring together to form a pn-junction. Sketch this situation showing the carrier concentrations and describing the two effects which act on the charge carriers. Mark on the direction in which the internally generated electric field acts and explain the origin of this field. Explain why charge cannot flow across this junction. [6]

- B4.** (a) Consider a free-electron Fermi gas in three dimensions. Describe the electronic ground state of this system, including in your description an explanation of the allowed k states. Explain what is meant by the terms dispersion relation, Fermi wavevector, and Fermi surface. What shape is the Fermi surface in this system? [6]
- (b) The density of solid gold is $19.3 \times 10^3 \text{ kg/m}^3$, each atom has a mass of 197 atomic mass units, and it forms an fcc lattice. What length is one side of the conventional unit cell? By treating the atoms as close-packed spheres, calculate the effective radius of a gold atom. [6]
- (c) Consider a cube of metal with sides of length L which forms a simple cubic lattice with lattice constant a . Assume that there is one atom per lattice site and that each atom contributes one electron to the free electron Fermi gas. Use the free electron model to derive the radius of the Fermi surface [5]
- (d) For a metal in which the Fermi surface is contained within the 1st Brillouin zone, describe the regions where the surface is most affected by the presence of the crystal lattice. Give a physical justification for these deviations. [3]