

Summary of lectures

- I. Review of Bonding in Solids
- II. Crystal Lattices
- III. Elastic Scattering of Waves
- IV. Atomic Vibrations
- V. Electrons in Crystals



Aim of this lecture

- To look at past examination questions.

The examination paper will last for 1 hr 30 mins

There will be a choice of 3 from 5 questions

Each question has 20 marks

There will be one question from each section of the course



Question 1, example I.

Describe the characteristic properties of a material in which ionic bonding occurs. Explain the observation that ionic compounds consisting of ions of approximately equal size crystallize in one of the close-packed structures. [3,3]

Layers of identical atoms, treated as hard spheres, can pack together to form two distinct structures, one of which is the hexagonal close-packed structure. Name the other structure and explain how the two structures come about. [2,4]

Define what is meant by atomic coordination number and atomic packing fraction. [2]

What is the coordination number of the two close-packed structures? [1]

Calculate the packing fraction of the hexagonal close-packed structure. [5]



Question 1, example II.

(i) Describe the nature and properties of **metallic** and **covalent** bonds. In each case, discuss the mechanical properties of solids characterised by such bonds, and give one example of a solid that exhibits the bond. [5,5]

(ii) The crystal structure of diamond consists of a lattice and a basis of two atoms.

(a) Name and sketch the lattice. [3]

(b) Specify the basis. [2]

(c) What is the atomic coordination number? [1]

(d) Calculate the atomic packing fraction. [4]



Question 1 example III.

- (i) Explain the meaning of the terms **packing fraction** and **co-ordination number** in the context of the structure of solids.[4]
- (ii) Describe the nature of metallic and covalent bonds. In each case, discuss the mechanical properties of solids characterised by such bonds, and give one example of a solid that exhibits the bond. [5,5]
- (iii) Calculate the packing fraction of a face-centred cubic structure. [6]



Question 2 example I

A crystal structure can be described using the concepts of a **lattice** and a **basis**. Define the terms in bold. [3]

What is meant by a **symmetry operation**? Give three examples of such operations. [5]

For the two-dimensional triangular lattice:

(a) Draw a portion of the lattice, and indicate a pair of primitive lattice vectors. [2]

(b) Write down the conditions on the relative lengths of the primitive lattice vectors and on the angle between them. [2]

(c) Mark on your drawing a primitive unit cell. [2]

(d) Describe all the point symmetry operations of the lattice. [4]

(e) On a separate drawing, construct a Wigner-Seitz primitive unit cell. [2]⁶



Question 3 example I

Write down expressions for the primitive reciprocal-lattice vectors in terms of primitive real-space-lattice vectors. [3]

Write down a set of primitive real-space-lattice vectors for the face-centred cubic lattice with conventional cube side of length a . [3]

Hence obtain expressions for the primitive reciprocal-lattice vectors. Identify the type of the reciprocal lattice. [3,1]

Solid molybdenum has the body-centred cubic structure. Molybdenum powder is irradiated with X-rays of wavelength 0.154 nm, and the smallest angle with respect to the incoming X-rays at which a diffracted beam is observed is 40.4° . Find the length of the side of the conventional cubic unit cell. [6]

At what other angles, up to 90° , are diffracted beams observed? [4]



Question 3 example II.

(i) The crystal structure of rock salt (NaCl) consists of a lattice which is **cubic-F** (face-centred cubic) with a basis of Na(0,0,0) and Cl $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$.

(a) Make a sketch of a portion (one conventional cube) of the underlying lattice. Mark on the sketch the positions of all the 27 atoms within and on the cube, and identify one set of basis atoms. [2,1,1]

(b) Write down the fractional coordinates of the atoms which would be used as the basis when the rock salt structure is viewed as a cubic-P (simple cubic) lattice with a basis. [4]

(ii) The structure factor $S(hkl)$ for the $(h k l)$ diffracted beam from a crystalline solid can be written as

$$S(hkl) = \sum_p f_p \exp\{-2\pi i(hu_p + kv_p + lw_p)\}$$

Define the terms in this equation. [4]

Obtain expressions for the structure factors relating to the (hkl) reflection for:

(a) the face-centred cubic structure viewed as a simple cubic lattice with a suitable basis;

[2]

(b) the rock salt structure viewed as a cubic-F lattice with the basis defined at the beginning of the question. [2]

Hence show that the allowed reflections of the rock salt structure satisfy the condition that h, k, l are all even or all odd, and comment on the observation that the reflections for which h, k, l are all odd are weak. [4]



Question 4, example I.

(i) Discuss what is meant by the term **first Brillouin zone**. Include in your discussion a definition and description of its physical significance. [5]

(ii) The dispersion relation for longitudinal vibrations of a long diatomic chain of atoms, alternately with masses M_1 and M_2 and with adjacent atoms a mean distance $a/2$ apart, is

$$\omega^2 = \frac{C(M_1 + M_2)}{M_1 M_2} \pm C \left[\left(\frac{M_1 + M_2}{M_1 M_2} \right)^2 - \frac{4}{M_1 M_2} \sin^2 \left(\frac{ka}{2} \right) \right]^{1/2}$$

(a) What do ω and k represent? [2]

(b) What is the significance of C ? [1]

(c) Sketch the dispersion curves for a range of k encompassing the first two Brillouin zones. [4]

(d) By considering the equations of motion of the atoms in the chain, obtain expressions for the ratios of the amplitudes of motion of each type of atom for vibrations at the Brillouin-zone centre. [6]

(e) Discuss how the dispersion curve will change as $M_1 \rightarrow M_2$. [2]



Question 4, example II.

Assuming that only nearest-neighbour interactions are significant, and the resulting forces obey Hooke's law with force constant C , the dispersion curve for longitudinal vibrations of a long linear chain of identical atoms of mass M and mean spacing a is given and drawn below for a specific system

$$\omega = \left(\frac{4C}{M}\right)^{1/2} \left| \sin\left(\frac{ka}{2}\right) \right|$$

|

Mark on a sketch of this dispersion relation the boundaries of the 1st Brillouin zone. [2]

Describe the motion of the atoms for vibrations close to $k=0$ and for vibrations at the edge of the first Brillouin zone. [2,2]

Using the values given on the graph, calculate the mean separation between adjacent atoms, and the value of the factor $(4C/M)^{1/2}$. Obtain an expression for the group velocity of long-wavelength oscillations and calculate its value. [2,2,4]

Every other atom in the chain is then replaced by an atom of slightly different mass m , all other parameters remaining the same. Draw an annotated sketch of the resulting dispersion relation, highlighting its essential features. Comment on the size of the Brillouin zone compared with that for the original monatomic chain. [6]



Question 5 example I.

In the free-electron model electrons are assumed to obey Fermi statistics and have a parabolic dispersion relation. Explain the physical origin of the Fermi distribution and sketch its shape. **[4]**

A metallic crystal of volume V is assumed to behave as a free electron gas such that the number of electrons occupying states up to an energy E is

$$N = \frac{V}{3\pi^2} \left(\frac{2mE}{\hbar^2} \right)^{3/2}$$

If the metal has an electron concentration of $8.5 \times 10^{28} \text{ m}^{-3}$, calculate the Fermi energy **[4]**

Show that the Fermi velocity is $1.6 \times 10^6 \text{ m s}^{-1}$. **[2]**

Describe how the dispersion relation assumed in the free-electron model is modified by the presence of a weak periodic potential, as assumed in the nearly-free-electron model. Discuss how the phenomenon of Bragg scattering influences the electrons' group velocities and energies close to the Brillouin zone edge. **[10]**

