Answer TWO questions.

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.

$$\text{Planck constant } h = 6.63 \times 10^{-34}\text{Js}$$
$$\text{mass of neutron } m_N = 1.67 \times 10^{-27}\text{kg}$$

[Part marks]

1. The potential energy for a pair of inert gas atoms separated by a distance r may be written as the Lennard-Jones potential:

$$U_{pair}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

   (a) Explain the physical origin of these two terms. [2]

   (b) Find the equilibrium atomic separation (r_0) of a pair of atoms and $U_{pair}(r_0)$. [2]

   (c) Sketch $U_{pair}(r)$, clearly labelling σ and ϵ. [2]

   (d) Write down the cohesive energy of an inert gas crystal whose N atoms interact via the Lennard-Jones potential. [2]

   (e) The lattice sums $A_6 = \Sigma_j{}' p_{ij}^{-6}$ and $A_{12} = \Sigma_j{}' p_{ij}^{-12}$, where $p_{ij}r$ is the distance between reference atom i and any other atom j are given in the table below for *bcc* and fcc crystal structures. Calculate which structure is energetically preferred.

	bcc	fcc
A_6	12.2533	14.4539
A_{12}	9.1142	12.1319

[6]

   (f) An ionic solid can be modelled by a line of $2N$ ions of alternating charge $\pm q$, interacting electrostatically. There is also a repulsive potential energy of $\frac{A}{r^n}$ between the nearest neighbours only.
   Show that at the equilibrium separation (r_0), the cohesive energy of this solid is

$$U(r_0) = \frac{-2Nq^2}{4\pi\epsilon_0 r_0} \ln 2 \left(1 - \frac{1}{n}\right)$$ [6]

2. Consider a cubic solid with atoms of mass M separated by a distance a. Planes of atoms are coupled by a force constant C_p between planes at s and $s+p$.

   (a) By considering the equation of motion for atoms in the plane s, show that the dispersion relation $\omega(k)$ for a travelling wave perpendicular to the plane is given by:

$$\omega^2 = \frac{2}{M}\sum_p Cp(1 - \cos pka)$$ [5]

   (b) Sketch the dispersion relation for the case when $C_2 = \frac{1}{2}C_1$, and $C_p = 0$ for $p > 2$. [5]

   (c) For a solid with $C_1 = 15\text{Nm}^{-1}, M = 6.44 \times 10^{-25}\text{kg}, a = 0.485\text{nm}$ and force constants as in (b) above, calculate

      i. the velocity of sound;

      ii. the frequency at the Brillouin zone boundary;

      iii. the energy and crystal momentum of a phonon associated with the maximum frequency; [10]

3. (a) Show that the density of states of a 3-dimensional free electron gas is

$$D(E) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$$

where V is the volume of the gas. [3]

(b) Show that the density of states of a free electron gas of dimensionality d ($d = 1, 2, 3$) may be written as

$$D(E) = A_d E^{\left(\frac{d-2}{2}\right)}$$

Calculate A_d for $d = 1$ and $d = 2$. [4]

(c) Discuss briefly how $D(E_F)$ for a metal can be determined experimentally. [2]

(d) The heat capacity of two materials (A and B) was measured at low temperature with the following results. From appropriate graphs, estimate the coefficient (γ) of the electronic heat capacity in both cases, and comment on your results. [6]

T (Kelvin)	C_A ($\mathrm{mJmol^{-1}K^{-1}}$)	C_B ($\mathrm{mJmol^{-1}K^{-1}}$)
5	0.356	150.1
1.0	0.750	300.5
1.5	1.22	450.6
2.0	1.80	604.0
2.5	2.53	757.8
3.0	3.45	913.5
3.5	4.59	1071.4
4.0	6.00	1232.0
5.0	9.75	1562.5
6.0	15.00	1908.0
7.0	22.05	2271.5
8.0	31.20	2656.0

(e) Drive an expression for the change of the Fermi energy with hydrostatic pressure, in terms of the isothermal compressibility $\kappa_T = -\frac{1}{V}\left(\frac{\delta V}{\delta p}\right)$.
Calculate the hydrostatic pressure required to change the Fermi energy of copper by 1 part in 10^6, given that κ_T for copper is $7.3 \times 10^{-12}\mathrm{Pa}^{-1}$. [5]

END OF PAPER