FSK324 Exam 2008 - Suggestions

Time: [ ]	**Total marks:** [ ]

Section A - The crystalline state

1. i.) Distinguish between amorphous, poly-crystalline and single crystal materials [3]

   ii.) Define the terms *vacancy* and *Schottky defect* [2]

2. i.) Define a Wigner-Seitz (WS) unit cell and describe its construction [3]

   ii.) How is the WS unit cell related to a Brillouin zone? [3]

3. Let $\overline{A} = (\overline{a}_1, \overline{a}_2, \overline{a}_3)$ and $\overline{B} = (\bar{b}_1, \bar{b}_2, \bar{b}_3)$ define basis vectors in real and reciprocal lattice spaces respectively. Prove that $\bar{b}_i \cdot \overline{a}_j = 2\pi\delta_{ij}$ where δ_{ij} is Kronecker's delta. [5]

4. FCC gold has density 19.3 gcm^{-3} and atomic number 197. Calculate

   i.) the distance between the (111) planes [3]

   ii.) the atomic radius of the gold atom, assuming hard spheres. [3]

5. Show that for the HCP structure $a = b \neq c$, where $c/a = \sqrt{8/3}$. [8]

6. Sodium undergoes the martensitic transformation from BCC ($a = 0.423\ nm$) to HCP at 23K. Calculate the parameter a for HCP. [10]

7. Determine the density of zinc, which is HCP with atomic mass 65.37 and lattice parameter a=0.266 nm. [4]

Section B - The reciprocal lattice and diffraction

8. Prove that a crystal lattice is invariant to a rotation of $2\pi/n$ for $n \in \{1, 2, 3, 4, 6\}$.

9. The total amplitude of the scattered wave in the direction $\overline{k'}$ for N cells is $F_{\overline{G}} = NS_{\overline{G}}$, where $S_{\overline{G}}$ is the structure factor defined as the integral [10]

$$S_{\overline{G}} = \int_{\text{cell}} n(\overline{r})e^{-\overline{G}\cdot\overline{r}}dV$$

   and $\Delta\overline{k} = \overline{G}$. The lattice vector $\overline{r} = 0$ at one corner. Show that the structure factor for hkl reflections is given by

$$S_{\overline{G}}(hkl) = \sum_{j}^{N} f_j e^{-2\pi i(hx_j + ky_j + lz_j)}.$$

10. The electron density (concentration) is given by the Fourier expansion

$$n(\overline{r}) = \sum_{\overline{G}} e^{i\overline{G}\cdot\overline{r}}.$$

Define $\overline{G}$ mathematically and then prove that the definition meets the translational requirement of a periodic crystal, i.e. $n(\overline{r}) = n(\overline{r} + \overline{T})$. [10]

11. Derive the conditions necessary for diffraction in a BCC lattice if the structure factor is given by [10]

$$S_G = \sum_j f_j e^{(-i\overline{G}\cdot\overline{r}_j)}$$

12. The Bragg angle for a certain reflection of a powdered sample of copper is 47.75^o at 20^oC, and 46.60^o at 1000^oC. Determine the coefficient of linear expansion of copper. [10]

13. A beam of 150 eV electrons is incident on a sample of powdered nickel. If nickel has the FCC structure with $a = 3.25$Å, determine the two smallest angles at which diffraction can occur. [10]

14. Aluminium, which is FCC, has a Bragg angle of 19.2^o for the (111) planes. Calculate

    i.) the (111) inter-planar distance given that $\lambda = 1.54$ Å;

    ii.) Avogadro's number, N_A, given that $\rho_{Al} = 2.7\text{g/cm}^3$ and $M = 27$g.

Section C - The thermal properties of materials

15. The energy of a system in the Debye model is

$$E = 9RT\left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{x^3}{e^x - 1}dx, \quad \text{where } x = \frac{\hbar\omega}{k_B T}. \qquad (1)$$

Determine the specific heat C_v at

    i.) low temperatures [3]

    ii.) high temperatures [3]

16. With regards to specific heat capacity C_v, discuss the failings of

    i.) the classical Petit-Dulong model [3]

    ii.) the Einstein model [3]

17. The wave equation for elastic waves in a rod is given by

$$\frac{\partial^2 u}{\partial x^2} = \frac{\rho}{Y}\frac{\partial^2 u}{\partial t^2}. \qquad (2)$$

    i.) Define *all* the symbols and their S.I. units in equation (2). [3]

    ii.) assuming a solution of the form $u = u(x,t) = Ae^{i(kx-\omega t)}$, show that the dispersion relation is $\omega = v_s k$ where $v_s = \sqrt{Y/\rho}$. [3]

iii.) Normally the wave-number k in a dispersive medium is considered real-valued, such that

$$\omega^2 = \omega_m \sin^2 \frac{ka}{2}. \qquad (3)$$

Show that if k is complex-valued for $\omega > \omega_m$, then the amplitude of vibration is damped by a factor $e^{-\alpha n a}$ where α is real-valued. [4]

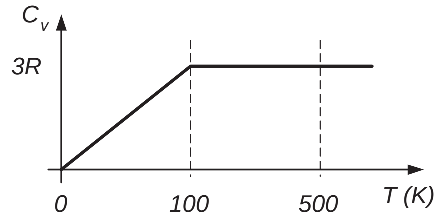

Figure 1: C_v as a function of temperature for some unknown material.

18. Using the data in Fig. 1, calculate the internal energy of 1 mole of the material at 500K. [6]

19. Given that the atomic mass and density of gold are 197 and 19.3 g/cm^3 respectively, determine the Debye temperature of gold if sound travels through it at 2.1 km/s. [6]

Section D - The free–electron model

20. Describe the Hall effect in metals. Use diagrams as necessary. [8]

21. Consider equation (4).

$$\sigma = \frac{ne^2\tau}{m} \qquad (4)$$

i.) Derive equation (4) using Ohm's law as a starting point. [4]

ii.) Derive equation (4) using the classical approach by assuming a free-electron gas under the influence of a viscous force. [4]

22. Copper has a density of 8.95 g/cm^3, atomic mass of 63 and a room-temperature electrical conductivity of $1.55 \times 10^{-8}\ \Omega \cdot m$. Calculate

i.) the concentration of conduction electrons. [2]

ii.) relaxation time, τ. [2]

iii.) the Fermi level, E_F in electron-volts. [2]

iv.) the Fermi velocity, v_F. [2]

(Assume that the effective mass of the electron is the rest mass).

23. Assuming that the Fermi energy level is ε_F,

i.) write down the Fermi-Dirác distribution (FD), [4]

ii.) explain the significance of having an energy equal to ε_F. [2]

iii.) plot a schematic graph of the FD distribution. [2]

24. Discuss the failing(s) of the *free-electron* model. [8]

25. i.) In what essential way does a plasma differ from a gas? [2]

ii.) Describe Matthiessen's law, the "Umklapp" process and the Lorentz number. [6]

Some general information and data

Planck's constant	$h = 6.626 \times 10^{-34}\ J \cdot s$
	$\hbar = h/2\pi$
Avogadro's constant	6.022×10^{23} mol^{-1}
Electronic charge	$e = 1.6022 \times 10^{-19}$ C
Electron mass	$m_e = 9.109 \times 10^{-31}$ kg
Neutron mass	$m_n = 1.675 \times 10^{-27}$ kg
Boltzmann's constant	$k_B = 1.38 \times 10^{-23}\ J/K$
Electron concentration	$N = Z_\nu \rho N_A/M$
Debye frequency	$\omega_D = \nu\sqrt[3]{6\pi^2 n}$
Debye temperature	$\theta_D = \hbar\omega_D/k_B$
Fermi energy	$\varepsilon = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{\frac{2}{3}}$
A useful integral:	$\int_0^\infty \frac{x^3}{e^x-1}dx = \frac{\pi^4}{15}$