

# Midterm Exam

1. Consider the structure of NiAs with Ni at the corners of the cell and the centres of the edges and the As atoms (shown as colored) symmetrically placed between two layers of Ni at elevations  $z = 1/3$  and  $z = 2/3$ . All sides of the uni cell are of equal length and all crystallographic angles are  $90^\circ$ .

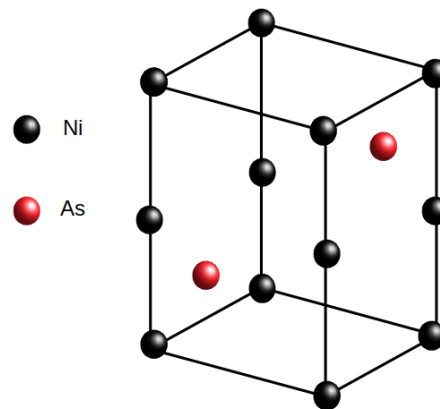


Figure 1

The position of the Ni atoms is shown in the partial stereographic projection.

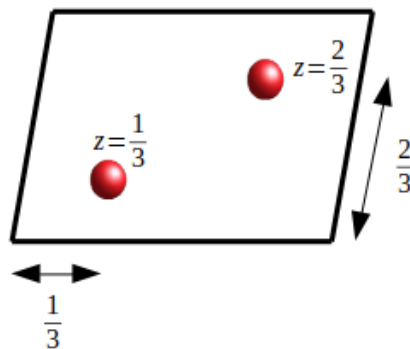


Figure 2

- (a) Complete the stereographic projection showing *all* atoms in the unit cell. [5 marks]
- (b) State the fractional coordinates of *all* atoms in the unit cell. [5 marks]
- (c) What is the Bravais lattice? What is the basis (mention the position vectors) of the atoms in the basis. [5 marks]
- (d) Find the structure factor for the scattering of X-rays. Are there any systematic absences? [20 marks]

2. Show that  $e^{i\vec{G}\cdot\vec{R}} = 1$  where  $\vec{G}$  and  $\vec{R}$  are reciprocal lattice and unit cell translation vectors respectively. [5 marks]

3. The hexagonal unit cell (alongwith 3 neighbours) is shown in the diagram.

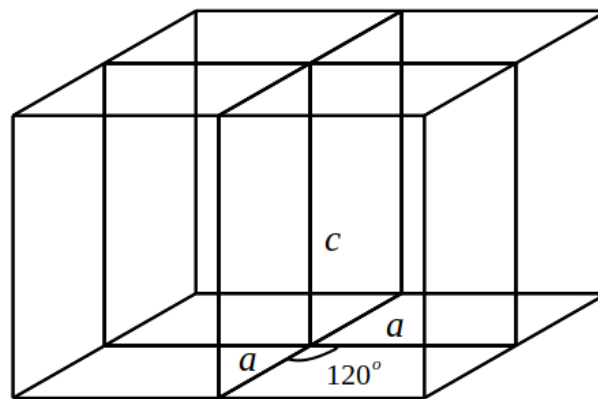


Figure 3

- (a) If  $\hat{i}$ ,  $\hat{j}$  and  $\hat{k}$  are the Cartesian unit vectors, find the unit cell translation vectors  $\vec{a}$ ,  $\vec{b}$  and  $\vec{c}$  in terms of  $\hat{i}$ ,  $\hat{j}$  and  $\hat{k}$ . [5 marks]
- (b) Find the reciprocal lattice vector. What kind of lattice type is it? [10 marks]

4. For electron in a 2D solid, find

(a) the density of states,  $g(E)$ .

(b) the temperature dependence of the chemical potential to first order.

[20 marks]

Note that

$$n = \int_0^\infty dE \Gamma(E) \frac{d\Gamma(E)}{dE} = \Gamma(E)|_\mu + \frac{\pi^2}{6} (k_B T)^2 \frac{d^2\Gamma(E)}{dE^2} \Big|_\mu.$$