Solid State Physics

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Assignment I: Crystal Structure, X-Ray Diffraction

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Q.1) **(a)** Primitive translation vector of hcp lattice is

$$\mathbf{a} = \frac{\sqrt{3}}{2}a\hat{i} + \frac{a}{2}\hat{j}, \quad \mathbf{b} = -\frac{\sqrt{3}}{2}a\hat{i} + \frac{a}{2}\hat{j}, \quad \mathbf{c} = c\hat{k}.$$

Compute the volume of the primitive cell. **(b)** In a fcc dimeric crystal made of A and B atoms, A atoms reside at the corner of the unit cell while B atoms reside at the face centers. One of the A atoms is missing from one corner of the unit cell *[topological defect generated due to broken translational symmetry]*). Show that the simplest formula for the crystal is A_7B_{24}.

Q.2) **(a)** What is the **similarity** and **difference** between Diamond and Sodium Chloride crystal structure? **(b)** Show that for a fcc crystal structure, lattice constant is

$$a = \left(\frac{4M}{\rho N}\right)^{1/3},$$

where M is the gram molecular weight of molecules at lattice points, ρ is the density and N is Avogadro's number.

Q.3) Show that the maximum radius of the sphere R that can just fit into the void at the body centre of the fcc structure coordinated by the facial atoms is $R = 0.414r$, where r is the radius of the atom.

Q.4) Find the Miller indices of a plane that makes an intercept of $3\mathring{A}, 4\mathring{A}$, and $5\mathring{A}$ on the coordinate axes of an orthorhombic crystal with $a : b : c = 1 : 2 : 5$.

Q.5) **(a)** Calculate the angle between normals to the planes (111) and (101) in a simple cubic unit cell. **(b)** Sketch these planes and hence determine the Miller indices of the directions common to both the planes. **(c)** Show that m^{th} order reflection from $\{hkl\}$ planes overlap with the 1^{st} order reflection from $(nh\, nk\, nl)$ planes.

Q.6) Define

$$\mathbf{a}^{**} = 2\pi\frac{\mathbf{b}^* \times \mathbf{c}^*}{\mathbf{a}^* \cdot \mathbf{b}^* \times \mathbf{c}^*}, \mathbf{b}^{**} = 2\pi\frac{\mathbf{c}^* \times \mathbf{a}^*}{\mathbf{a}^* \cdot \mathbf{b}^* \times \mathbf{c}^*}, \mathbf{c}^{**} = 2\pi\frac{\mathbf{a}^* \times \mathbf{b}^*}{\mathbf{a}^* \cdot \mathbf{b}^* \times \mathbf{c}^*},$$

as three vectors generated by primitive vectors $\mathbf{a}^{**}, \mathbf{b}^{**}, \mathbf{c}^{**}$. Firstly, check that

$$\mathbf{a}^* \cdot \mathbf{b}^* \times \mathbf{c}^* = \frac{(2\pi)^3}{\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}},$$

and then show that $\mathbf{a}^{**} = \mathbf{a}, \mathbf{a}^{**} = \mathbf{a}, \mathbf{b}^{**} = \mathbf{b}, \mathbf{c}^{**} = \mathbf{c}$.

Q.7) Molecular weight of rock salt (NaCl crystal) is 58.5 $\mathsf{Kg/kilomole}$ and density is $2.16 \times 10^3\ \mathsf{kg/m^3}$. Calculate the grating spacing d_{100}. Using that, compute wavelength of X-rays, if in 2^{nd} order, angle of diffraction is 26°.

Q.8) **(a)** If X-rays with wavelength $\lambda = 0.5\text{Å}$ is diffracted at 5° in 1^{st} order, what is the spacing betweenadjacent planes of a crystal? At what angle will the second maximum occur? **(b)** Bragg angle for 1^{st} order reflection from (111) plane of a crystal is 60°, when X-rays with wavelength $\lambda = 1.8\text{Å}$ is diffracted. Calculate the interatomic spacing in the unit cell. **(c)** Electrons are accelerated by 844 volts and are reflected from a crystal. The reflection maximum occurs when the glancing angle is 58°. Determine the interatomic spacing of the crystal.