Estado Sólido I
Tarea 5: Estructura Cristalina

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Nombre del Estudiante: _____

Problema 1 *Properties of basic crystal structures*

(a) Calculate the first nearest-neighbor distance for the bcc and fcc crystal structures.

(b) Obtain the packing fraction f_e for the bcc and fcc crystal structures.

(c) Show that the c/a ratio for an ideal hexagonal close-packed structure is $(8/3)^{1/2} = 1.633$.

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Problema 2 *Interplanar separation and Bragg condition*

Consider a plane *hkl* in a crystal lattice.

(a) Prove that the recirpocal lattice vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is perpendicular to this plane.

(b) Prove that the distance between two adjacent parallel planes of the lattice is $d(hkl) = 2\pi/|\mathbf{G}|$.

(c) Show for a simple cubic lattice that $d^2 = a^2/(h^2 + k^2 + l^2)$.

(d) Show that the diffraction condition $2\mathbf{k}\cdot\mathbf{G} = G^2$ is an analogous statement of the Bragg condition, $2d\text{Sin}\theta = n\lambda$.

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Problema 3 *Hexagonal space lattice*

The primitive translation vectors of the hexagonal space lattice may be taken as

$$\mathbf{a}_1 = (3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}}; \quad \mathbf{a}_2 = -(3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}}; \quad \mathbf{a}_3 = c\hat{\mathbf{z}}.$$

(a) Show that the volume of the primitive cell is $(3^{1/2}/2)a^2c$.

(b) Show that the primitive translations of the reciprocal lattice are

$$\mathbf{b}_1 = (2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}}; \quad \mathbf{b}_1 = -(2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}}; \quad \mathbf{b}_3 = (2\pi/c)\hat{\mathbf{z}},$$

so that the lattice is its own reciprocal, but with a rotation of axes.

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Problema 4 *Scattering amplitude contributions*

From the scattering amplitude,

$$F = \sum_{\mathbf{G}} \int dV n_{\mathbf{G}} \exp\left[i(\mathbf{G} - \Delta\mathbf{k}) \cdot \mathbf{r}\right],$$

show that F is negligibly small when $\Delta\mathbf{k}$ differs significantly from any reciprocal lattice vector $\mathbf{G}$.

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Problema 5 *Structure factor of diamond*

The basis of the diamond crystal structure consists of eight atoms if the cell is taken as the conventional cube.

(a) Find the structure factor S of this basis.

(b) Find the zeros of S and show that the allowed reflections of the diamond structure satisfy $v_1 + v_2 + v_3 = 4n$, where all indices are even and n is any integer, or else all indices are odd.

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