Estado Sólido I
Tarea 1: Estructura Cristalina

Dr. Omar De la Peña Seaman

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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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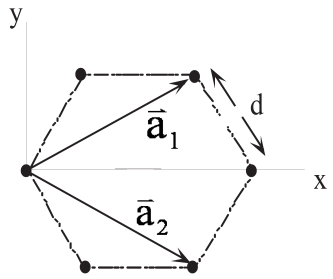
Problema 2 *Graphene structure*

Graphene forms a two-dimensional honeycomb lattice with carbon atoms at the corners of a hexagon separated by a distance d. The primitive lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are shown in the figure.



(a) Find the lattice vector's magnitude $|\mathbf{a}_1|$ and $|\mathbf{a}_2|$ in terms of d, and call this magnitude a.

(b) Rewrite $\mathbf{a}_1$ and $\mathbf{a}_2$ in terms of a, and express them in Cartesian coordinates with unit vectors $\hat{\mathbf{i}}$ and $\hat{\mathbf{j}}$.

(c) How many atoms does graphene have in the conventional and the primitive unit cells? Which are their positions? (in Cartesian coordinates).

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Problema 3 *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 4 *Structure factor of diamond*

Consider the diamond crystal structure as a conventional cubic cell with a basis of eight atoms if the cell, then:

(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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