Física del Estado Sólido
Tarea 03: Estructura Cristalina, Estructura de Bandas

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Problema 1 *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 2 *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 3 *Reciprocal lattice vectors 2D*

In 3D lattices, the reciprocal lattice vectors are given by,

$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2\times\mathbf{a}_3}{\mathbf{a}_1\cdot\mathbf{a}_2\times\mathbf{a}_3};\quad \mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3\times\mathbf{a}_1}{\mathbf{a}_1\cdot\mathbf{a}_2\times\mathbf{a}_3};\quad \mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1\times\mathbf{a}_2}{\mathbf{a}_1\cdot\mathbf{a}_2\times\mathbf{a}_3}.$$

where $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are the primitive lattice vectors of the lattice, and they fulfill the following condition: $\mathbf{b}_i\cdot\mathbf{a}_j = 2\pi\delta_{ij}$.
Find a similar expresion of the $\mathbf{b}$'s for a 2D lattice.

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Problema 4 *Width of diffraction maximum*

We suppose that in a linear crystal there are identical point scattering centers at every lattice point $\boldsymbol{\rho}_m = m\mathbf{a}$, where m is an integer. The total scattered radiation amplitude will be proportional to $F = \sum \exp[-im\mathbf{a}\cdot\Delta\mathbf{k}]$. The sum over M lattice points is

$$F = \frac{1-\exp[-iM(\mathbf{a}\cdot\Delta\mathbf{k})]}{1-\exp[-i(\mathbf{a}\cdot\Delta\mathbf{k})]},$$

by the use of the series

$$\sum_{m=0}^{M-1} x^m = \frac{1-x^M}{1-x}.$$

(a) The scattered intensity is proportional to $|F|^2$. Show that

$$|F|^2 = F*F = \frac{\mathrm{Sin}^2[M/2(\mathbf{a}\cdot\Delta\mathbf{k})]}{\mathrm{Sin}^2[1/2(\mathbf{a}\cdot\Delta\mathbf{k})]}.$$

(b) We know that a diffraction maximum appears when $\mathbf{a}\cdot\Delta\mathbf{k} = 2\pi h$, where h is an integer. We change $\Delta\mathbf{k}$ slightly and define ϵ in $\mathbf{a}\cdot\Delta\mathbf{k} = 2\pi h + \epsilon$ such that ϵ gives the position of the first zero in $\mathrm{Sin}[M/2(\mathbf{a}\cdot\Delta\mathbf{k})]$. Show that $\epsilon = 2\pi M$, so that the width of the diffraction maximum is proportional to $1/M$ and can be extremely narrow for macroscopic values of M.

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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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Problema 6 *Tight binding model for the simple cubic*

Solve with the tight-binding model the 3D simple cubic structure with only one atomic species in the basis. Consider interactions up to first-nearest neighbors and apply s and p (p_x, p_y, and p_z) orbitals as expansion basis.

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