Written exam of Condensed Matter Physics - april 8th 2019
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Exercise 1: X-ray diffraction.

Consider a crystal described as a tetragonal Bravais lattice with lattice parameters a, a, $c = 2a$ [see Fig. 1 (a)], where $a = 0.25\,\text{nm}$. The structure of the crystal is investigated by means of the Debye-Scherrer method, with a radiation of wavelength $\lambda = 0.125\,\text{nm}$.

1. Having adopted the fundamental vectors $\boldsymbol{a}_1 = (a, 0, 0)$, $\boldsymbol{a}_2 = (0, a, 0)$, and $\boldsymbol{a}_3 = (0, 0, c) = (0, 0, 2a)$, determine the reciprocal lattice vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$ of the given lattice.

2. Determine the angles $\phi = 2\theta$ corresponding to the first 5 peaks detected by the Debye-Scherrer method (in order of increasing magnitude of the related reciprocal lattice vectors), and the families of planes (hkl) to which they correspond.

3. Assume now that the crystal hosts a two-atom basis $\boldsymbol{d}_1 = (0, 0, 0)$, $\boldsymbol{d}_2 = (\frac{a}{2}, \frac{a}{2}, \frac{c}{4}) = \frac{a}{2}(1, 1, 1)$, with identical atoms at the two basis points [see Fig. 1 (b)]. Which of the five peaks determined before would now be missing?

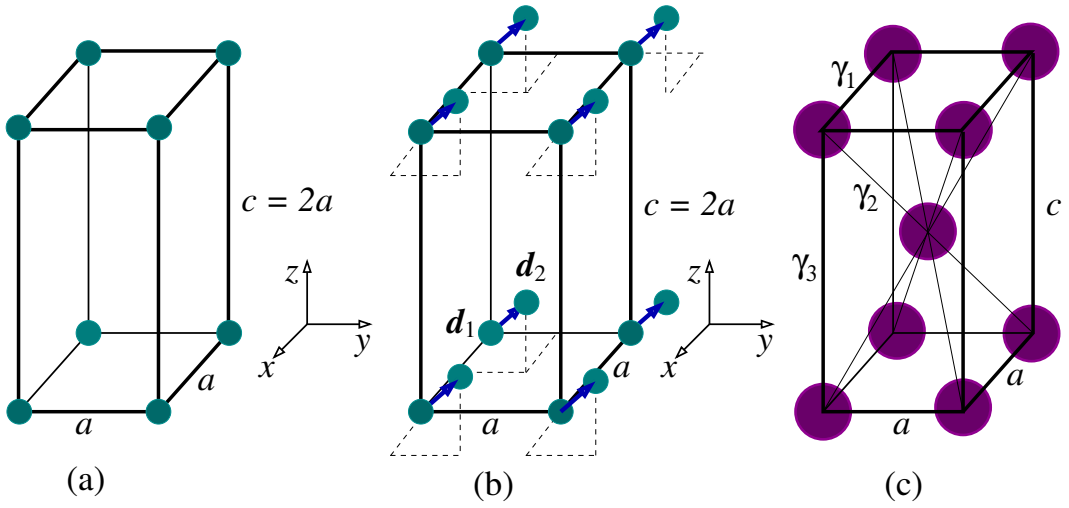

Fig. 1.

Exercise 2: Tight binding.

Consider the body centered tetragonal crystal, whose conventional unit cell is shown in Fig. 1 (c). The lattice sites host s orbitals, the three transfer integrals γ_1, γ_2, and γ_3 are assigned, all the other transfer integrals and all the overlap integrals can be neglected. Here, the standard notation $\gamma_i \equiv \gamma(\boldsymbol{R}_i) = -\int \mathrm{d}\boldsymbol{r}\, \phi_s(\boldsymbol{r}) \Delta U(\boldsymbol{r}) \phi_s(\boldsymbol{r} - \boldsymbol{R}_i)$ is adopted. The energy level of the atomic s orbital is E_s, and $\beta \equiv \gamma(\boldsymbol{R} = 0)$ is the shift of the atomic level.

1. Determine the tight-binding band dispersion for Bloch electrons in the given crystal.

2. Let now $a = 0.3\,\text{nm}$, $c = 0.5\,\text{nm}$, $\gamma_1 = 0.25\,\text{eV}$, $\gamma_2 = 0.2\,\text{eV}$, and $\gamma_3 = 0.15\,\text{eV}$. Determine the effective mass tensor at the Γ point of the first Brillouin zone.

3. Assuming that each atom contributes one electron, calculate the electron density n (number of electrons per unit volume) in the given crystal.

[Note that $1\,\text{eV}$ corresponds to an energy of $1.60 \times 10^{-19}\,\text{J}$; the Planck constant is $\hbar = 1.05 \times 10^{-34}\,\text{J·s}$; the free electron mass is $m_0 = 9.11 \times 10^{-31}\,\text{kg}$].

Solution of the written exam
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Exercise 1.

1. The volume of the unit cell is $\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3) = 2a^3$. The reciprocal lattice vectors are

$$\boldsymbol{b}_1 = 2\pi \frac{(\boldsymbol{a}_2 \times \boldsymbol{a}_3)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(1,0,0), \qquad \boldsymbol{b}_2 = 2\pi \frac{(\boldsymbol{a}_3 \times \boldsymbol{a}_1)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(0,1,0), \qquad \boldsymbol{b}_3 = 2\pi \frac{(\boldsymbol{a}_1 \times \boldsymbol{a}_2)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{\pi}{a}(0,0,1).$$

2. The magnitude of the reciprocal lattice vector $\boldsymbol{K} = h\,\boldsymbol{b}_1 + k\,\boldsymbol{b}_2 + l\,\boldsymbol{b}_3 = \frac{\pi}{a}(2h, 2k, l)$ is $K = |\boldsymbol{K}| = \frac{\pi}{a}\sqrt{4(h^2+k^2)+l^2}$. The magnitude of the wave vector of the radiation is $\kappa = \frac{2\pi}{\lambda}$

The peaks measured by means of the Debye-Scherrer technique are found at scattering angles ϕ that must obey the condition

$$\sin\frac{\phi}{2} = \frac{K}{2\kappa} = \frac{\lambda}{4a}\sqrt{4(h^2+k^2)+l^2} = 0.125\sqrt{4(h^2+k^2)+l^2}.$$

From the expression of K it is evident that the shortest reciprocal lattice vector corresponds to the family of planes (001), for which $4(h^2+k^2)+l^2 = 1$; then come the families (100), (010), and (002) that are indistinguishable with the Debye-Scherrer technique, as they all give $4(h^2+k^2)+l^2 = 4$; the third peak corresponds to the families (101) and (011), for which $4(h^2+k^2)+l^2 = 5$; the fourth peak is produced by the planes (110), (102), and (012) that are indistinguishable with the Debye-Scherrer technique, as they all give $4(h^2+k^2)+l^2 = 8$; the fifth peak corresponds to the families (111) and (003), for which $4(h^2+k^2)+l^2 = 9$. The corresponding angles are $\phi_1 = 14.4°$, $\phi_2 = 29.0°$, $\phi_3 = 32.5°$, $\phi_4 = 41.4°$, and $\phi_5 = 44.0°$.

3. The scalar products between the basis vectors and a generic reciprocal lattice vector are $\boldsymbol{d}_1 \cdot \boldsymbol{K} = 0$ and $\boldsymbol{d}_2 \cdot \boldsymbol{K} = \pi\left(h + k + \frac{1}{2}l\right)$. The structure factor

$$S_{\boldsymbol{K}} = \sum_{j=1,2} \mathrm{e}^{\mathrm{i}\,\boldsymbol{d}_j \cdot \boldsymbol{K}} = 1 + (-1)^{\left(h+k+\frac{1}{2}l\right)}$$

vanishes when $h + k + \frac{1}{2}l$ equals an odd integer. Among the five peaks found before, the second would not be visible, since for all the corresponding families of lattice planes, (100), (010), and (002), one has $h + k + \frac{1}{2}l = 1$.

Exercise 2.

1. Denoting the lattice vectors with $\boldsymbol{R} \equiv (u_1|u_2|u_3) \equiv (u_1\,a, u_2\,a, u_3\,c)$, where the u_i may also be half-integers, having adopted a conventional unit cell, there are four equivalent lattice vectors, $(\pm1|0|0)$ and $(0|\pm1|0)$, associated with the transfer integral γ_1, eight equivalent lattice vectors, $(\pm\frac{1}{2}|\pm\frac{1}{2}|\pm\frac{1}{2})$, associated with the transfer integral γ_2, and 2 equivalent lattice vectors, $(0|0|\pm1)$, associated with the transfer integral γ_3. The tight-binding band dispersion is

$$\begin{aligned}\varepsilon_{\boldsymbol{k}} &= E_s - \beta - \gamma_1 \sum_{\substack{\boldsymbol{R}=(\pm1|0|0),\\ (0|\pm1|0)}} \cos(\boldsymbol{R}\cdot\boldsymbol{k}) - \gamma_2 \sum_{\substack{\boldsymbol{R}=\\ (\pm\frac{1}{2}|\pm\frac{1}{2}|\pm\frac{1}{2})}} \cos(\boldsymbol{R}\cdot\boldsymbol{k}) - \gamma_3 \sum_{\substack{\boldsymbol{R}=\\ (0|0|\pm1)}} \cos(\boldsymbol{R}\cdot\boldsymbol{k}) \\ &= E_s - \beta - 2\gamma_1\left[\cos(k_x a) + \cos(k_y a)\right] - 8\gamma_2 \cos\left(\frac{1}{2}k_x a\right)\cos\left(\frac{1}{2}k_y a\right)\cos\left(\frac{1}{2}k_z c\right) - 2\gamma_3\cos(k_z c).\end{aligned}$$

2. Expanding the band dispersion near the Γ point of the first Brillouin zone one finds

$$\varepsilon_{\boldsymbol{k}} \approx E_s - \beta - 4\gamma_1 - 8\gamma_2 - 2\gamma_3 + a^2(\gamma_1+\gamma_2)(k_x^2+k_y^2) + c^2(\gamma_2+\gamma_3)k_z^2.$$

It is then evident that the inverse mass tensor m_{ij}^{-1} is diagonal, and so is the mass tensor $m_{ij} = \mathrm{diag}\,(m_x, m_y, m_z)$, with

$$m_x = m_y = \frac{\hbar^2}{2a^2(\gamma_1+\gamma_2)}, \qquad m_z = \frac{\hbar^2}{2c^2(\gamma_2+\gamma_3)},$$

consistent with the tetragonal symmetry. Inserting the values given in the text one finds $m_x = m_y = 0.93\, m_0$ and $m_z = 0.43\, m_0$.

3. There are two atoms in the conventional unit cell, and each atom contributes one electron, therefore

$$n = \frac{2}{a^2 c} = 4.44 \times 10^{28}\,\mathrm{m}^{-3}.$$