Written test of Condensed Matter Physics - January 22nd 2019
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Exercise 1. Using the powder (or Debye-Scherrer) method with a radiation of wavelength $\lambda = 0.1\,\text{nm}$, a given cubic crystal shows two diffraction peaks corresponding to the following scattering angles $\phi = 2\vartheta$: $28.53°$ and $40.78°$.

a. Say if the crystal is a face-centered cubic or a body-centered cubic lattice.

b. Determine the size a of the conventional unit cell.

c. Determine the next two scattering angles corresponding to the observation of the diffraction maxima.

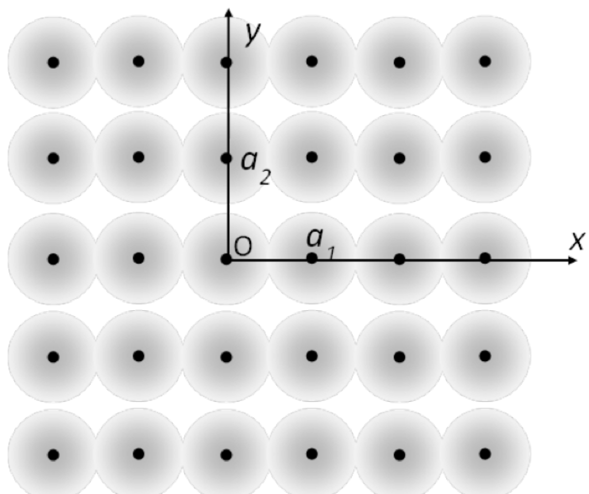

Fig. 1.

Exercise 2. A two-dimensional crystal is formed by a rectangular lattice with atoms having one valence electron of s-type. Fig, 1 shows the lattice constants $a_1 = 0.20\,\text{nm}$ and $a_2 = 0.25\,\text{nm}$.

a. Determine the dispersion of the band $E(k_x, k_y)$, taking into account the contribution of the first three nearest neighbors only. Neglect the overlap integrals, indicate as γ_i $(i = 1, 2, 3)$ the pertinent "transfer integrals" $[\gamma_i \equiv \gamma(\boldsymbol{R}_i) = -\int \mathrm{d}\boldsymbol{r}\, \phi_s(\boldsymbol{r}) \Delta U(\boldsymbol{r}) \phi_s(\boldsymbol{r} - \boldsymbol{R}_i)]$, as E_s the energy level of the atomic s orbital, and let $\beta = \gamma(\boldsymbol{R} = 0)$.

b. Evaluate the electron effective mass and mobility at $(k_x, k_y) = (0, 0) = \Gamma$, along the x and y directions, m_{xx}, m_{yy} and μ_{xx}, μ_{yy}, respectively.

Values of the parameters: $\gamma_1 = 1\,\text{eV}$, $\gamma_2 = 0.3\,\text{eV}$, $\gamma_3 = 0.05\,\text{eV}$; relaxation time $\tau = 2 \times 10^{-15}\,\text{s}$; $1\,\text{eV}$ corresponds to an energy of $1.60 \times 10^{-19}\,\text{J}$, the Planck constant is $\hbar = 1.05 \times 10^{-34}\,\text{J}\cdot\text{s}$, the elementary charge is $e = 1.60 \times 10^{-19}\,\text{C}$. The values of E_s and β are not needed in the numerical calculations.

Solution of the written test
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Exercise 1.

a. Let

$$\beta = \frac{\sin\vartheta_2}{\sin\vartheta_1} = \frac{0.348}{0.246} = 1.416 = \frac{d_1}{d_2} = \left(\frac{h_2^2+k_2^2+l_2^2}{h_1^2+k_1^2+l_1^2}\right)^{1/2}.$$

Given the selection rule table shown in Fig. 2, one expects $\beta = \sqrt{2}$ for bcc and $\beta = 2/\sqrt{3}$ for fcc, hence the crystal is bcc.

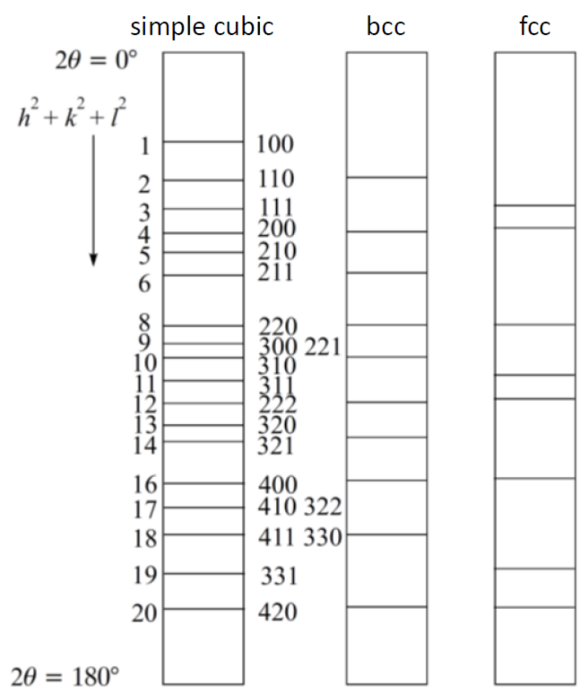

Fig. 2.

b. From Bragg's relation we obtain, e.g.,

$$2d_1\sin\vartheta_1 = \lambda, \qquad \Rightarrow \qquad a = \frac{\lambda}{2\sin\vartheta_1}\sqrt{h_1^2+k_1^2+l_1^2} = \frac{\lambda\sqrt{2}}{2\sin\vartheta_1},$$

hence the size of the conventional unit cell is $a = 2.87\,\text{Å}$.

c. For the given bcc lattice

$$\sin\vartheta_s = \sin\vartheta_1\left(\frac{h_s^2+k_s^2+l_s^2}{h_1^2+k_1^2+l_1^2}\right)^{1/2} = 0.174\sqrt{h_s^2+k_s^2+l_s^2}, \qquad s = 2,3,4,\ldots$$

For $s = 3$, $(hkl) = (211)$, hence $\sin\vartheta_3 = 0.427$ and $\phi_3 = 2\vartheta_3 = 50.53°$. For $s = 4$, $(hkl) = (220)$, hence $\sin\vartheta_4 = 0.493$ and $\phi_4 = 2\vartheta_4 = 59.05°$.

Exercise 2.

a. We have

$$E(k_x, k_y) = E_s - \beta - \sum_{i=1,2,3} \gamma(\boldsymbol{R}_i)\, \mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{R}_i},$$

where $\boldsymbol{R}_1 = (\pm a_1, 0)$, $\boldsymbol{R}_2\,(0, \pm a_2)$, $\boldsymbol{R}_3 = (\pm a_1, \pm a_2)$, and $\boldsymbol{k} = (k_x, k_y)$. Then,

$$E(k_x, k_y) = E_s - \beta - 2\gamma_1 \cos(k_x a_1) - 2\gamma_2 \cos(k_y a_2) - 4\gamma_3 \cos(k_x a_1) \cos(k_y a_2).$$

b. Expanding the band around the Γ point we find

$$E(k_x, k_y) \approx E_s - \beta - 2(\gamma_1 + \gamma_2 + 2\gamma_3) + (2\gamma_1 + 4\gamma_3)\, \frac{a_1^2 k_x^2}{2} + (2\gamma_2 + 4\gamma_3)\, \frac{a_2^2 k_y^2}{2},$$

hence

$$m_{xx} = \frac{\hbar^2}{2a_1^2(\gamma_1 + 2\gamma_3)} = 7.83 \times 10^{-31}\,\mathrm{kg}, \qquad m_{yy} = \frac{\hbar^2}{2a_2^2(\gamma_2 + 2\gamma_3)} = 1.38 \times 10^{-30}\,\mathrm{kg}.$$

Therefore, the required mobilities are

$$\mu_{xx} = \frac{e\tau}{m_{xx}} = 4.09 \times 10^{-4}\,\mathrm{m}^2 \cdot \mathrm{V}^{-1} \cdot \mathrm{s}^{-1}, \qquad \mu_{yy} = \frac{e\tau}{m_{yy}} = 2.32 \times 10^{-4}\,\mathrm{m}^2 \cdot \mathrm{V}^{-1} \cdot \mathrm{s}^{-1}.$$