

Written exam of Condensed Matter Physics - January 24th 2022
Profs. S. Caprara and A. Polimeni

Exercise 1: X-ray scattering and phonons [15 points].

KAlSi_3O_8 (orthoclase) crystallizes in the monoclinic system (see Fig. 1), with sides of the primitive cell $a = 0.86$ nm, $b = 1.3$ nm, $c = 0.72$ nm, and an angle $\beta = 64^\circ$ (the other two angles are right angles in the monoclinic system). The longitudinal and transverse sound velocities of KAlSi_3O_8 (averaged over the directions) are $v_\ell = 4.68 \times 10^3$ m/s and $v_t = 2.39 \times 10^3$ m/s, respectively.

1. Taking $\mathbf{a}_1 = a\hat{x}$, $\mathbf{a}_2 = b\hat{y}$, and $\mathbf{a}_3 = c(\sin\beta\hat{z} + \cos\beta\hat{x})$ as the primitive vectors, \hat{x} , \hat{y} , and \hat{z} being the unit vectors of the corresponding axes, determine the expression of the primitive reciprocal lattice vectors \mathbf{b}_1 , \mathbf{b}_2 , \mathbf{b}_3 of KAlSi_3O_8 . Indicating with $\mathbf{K} = h\mathbf{b}_1 + k\mathbf{b}_2 + \ell\mathbf{b}_3$ the generic reciprocal lattice vector (with $h, k, \ell \in \mathbb{N}$), determine the angle φ that corresponds to the first reflection from the family of lattice planes 100, observed when the structure of the crystal is investigated by means of the Debye-Scherrer technique with a radiation of wavelength $\lambda = 0.125$ nm [7 points].

2. Determine the average sound velocity \bar{v} within the Debye model, the Debye wave-vector q_D of the sound modes, and the Debye temperature Θ_D of the sound modes of KAlSi_3O_8 [5 points].

3. Determine the specific heat c_V of KAlSi_3O_8 at $T = 1$ K, assuming that the contribution of the optical modes can be neglected altogether [3 points].

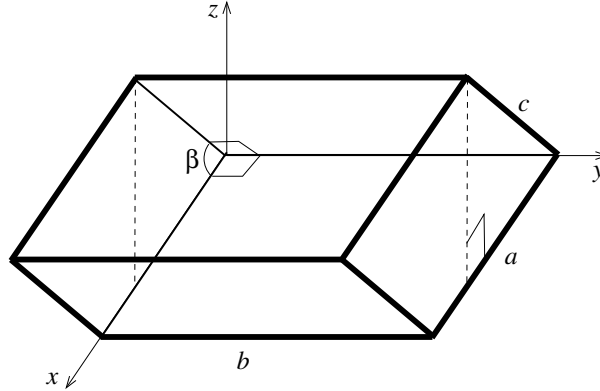


Fig. 1.

Exercise 2: Semiconductors [15 points].

An intrinsic semiconductor is formed by a linear chain of atoms with even valence, such that the topmost energy states are described by a valence band, whose maximum has energy E_v , and by a conduction band, whose minimum has energy E_c . The semiconductor band gap is $E_g = E_c - E_v$. The electron states of the semiconductor can be described within the nearly free electron model, so that the (energy vs. quasi-momentum) dispersion laws of the valence and conduction bands are well approximated by parabolic relations over the entire first Brillouin zone. Let m_c and m_v be the electron and hole effective mass, respectively.

1. Provide the analytical expression of the energy density of states per unit length, $g_c(E)$ and $g_v(E)$, in the conduction and valence band, respectively [5 points].

2. Assuming that $E_c - \mu \gg \kappa_B T$ and $\mu - E_v \gg \kappa_B T$ (μ is the chemical potential), provide the analytical expression of the electron and hole concentration, n and h , at a given temperature T . Recall that $\int_0^\infty x^{-\frac{1}{2}} e^{-x} dx = \sqrt{\pi}$ [5 points].

3. At $T = 300$ K, the chemical potential μ is at 0.450 eV above the top of the valence band E_v . Determine the value of the band gap energy E_g , knowing that $m_c/m_v = 0.100$ [5 points].

[Note that 1 eV corresponds to an energy of 1.602×10^{-19} J; the Planck constant is $\hbar = 1.055 \times 10^{-34}$ J·s; the Boltzmann constant is $\kappa_B = 1.381 \times 10^{-23}$ J·K⁻¹].

Solution of the written exam
Prof. S. Caprara and A. Polimeni

Exercise 1.

1. Taking the primitive vectors $\mathbf{a}_1 = a \hat{\mathbf{x}}$, $\mathbf{a}_2 = b \hat{\mathbf{y}}$, $\mathbf{a}_3 = c(\sin \beta \hat{\mathbf{z}} + \cos \beta \hat{\mathbf{x}})$, one has $\mathcal{V} = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = abc \sin \beta = 7.23 \times 10^{-28} \text{ m}^3$ (volume of the primitive cell), and

$$\mathbf{b}_1 = \frac{2\pi}{\mathcal{V}} (\mathbf{a}_2 \times \mathbf{a}_3) = \frac{2\pi}{a \sin \beta} (\sin \beta \hat{\mathbf{x}} - \cos \beta \hat{\mathbf{z}}), \quad \mathbf{b}_2 = \frac{2\pi}{\mathcal{V}} (\mathbf{a}_3 \times \mathbf{a}_1) = \frac{2\pi}{b} \hat{\mathbf{y}}, \quad \mathbf{b}_3 = \frac{2\pi}{\mathcal{V}} (\mathbf{a}_1 \times \mathbf{a}_2) = \frac{2\pi}{c \sin \beta} \hat{\mathbf{z}}.$$

The reciprocal lattice vector $\mathbf{K} = h \mathbf{b}_1 + k \mathbf{b}_2 + \ell \mathbf{b}_3$, for $h = 1$, $k = 0$, $\ell = 0$, has magnitude

$$K = |\mathbf{K}| = |\mathbf{b}_1| = \frac{2\pi}{a \sin \beta}.$$

All the other reciprocal lattice vectors associated with the same family of lattice planes have magnitude $K_n = nK$, $n = 2, 3, 4, \dots$, and produce higher-order reflections. According to the Debye-Scherrer formula,

$$\sin \frac{\varphi}{2} = \frac{\lambda K}{4\pi} = \frac{\lambda}{2a \sin \beta} = 0.0809,$$

hence $\varphi = 9.28^\circ$.

2. The average sound velocity is

$$\bar{v} = \left[\frac{1}{3} \left(\frac{1}{v_l^3} + \frac{2}{v_t^3} \right) \right]^{-1/3} = 2.68 \times 10^3 \frac{\text{m}}{\text{s}}.$$

The Debye wave-vector of sound modes is

$$q_D = \left(\frac{6\pi^2}{\mathcal{V}} \right)^{1/3} = \left(\frac{6\pi^2}{abc \sin \beta} \right)^{1/3} = 4.34 \times 10^9 \text{ m}^{-1}.$$

The Debye temperature of the sound modes is

$$\Theta_D = \frac{\hbar \bar{v} q_D}{\kappa_B} = 88.9 \text{ K}.$$

3. Since $\Theta_D \gg T = 1 \text{ K}$, and the text says that the contribution of the optical modes can be neglected, we can calculate the specific heat using the low-temperature asymptotic Debye formula for sound modes

$$c_v = \frac{12\pi^4 \kappa_B}{5\mathcal{V}} \left(\frac{T}{\Theta_D} \right)^3 = 6.35 \frac{\text{J}}{\text{K} \cdot \text{m}^3}.$$

Exercise 2.

1. The number of states dN^{1D} within the k -space line element $2dk$ (the factor 2 comes from the “angular” integral in one dimension) is given by $dN^{1D} = 2 \times 2dk/(2\pi/L) = (2L/\pi)dk$, where the spin degeneracy is taken into account, $2\pi/L$ is the k -space length per allowed k value and L is the length of the one-dimensional crystal. Given that $E = \hbar^2 k^2/2m$ and $dk = \frac{1}{2\hbar}\sqrt{2m/E}dE$, one gets the energy density of states for the conduction and valence bands

$$g_c(E) = \frac{1}{L} \frac{dN_c^{1D}}{dE} = \frac{1}{\pi\hbar} \sqrt{\frac{2m_c}{E - E_c}}, \quad \text{for } E > E_c; \quad g_v(E) = \frac{1}{L} \frac{dN_v^{1D}}{dE} = \frac{1}{\pi\hbar} \sqrt{\frac{2m_v}{E_v - E}}, \quad \text{for } E < E_v.$$

2. The electron concentration is given by

$$n(T) = \int_{E_c}^{+\infty} \frac{g_c(E)}{e^{\beta(E-\mu)} + 1} dE \approx \frac{\sqrt{2m_c\kappa_B T}}{\pi\hbar} e^{-\beta(E_c-\mu)} \int_0^{+\infty} x^{-\frac{1}{2}} e^{-x} dx = \frac{\sqrt{2m_c\kappa_B T}}{\sqrt{\pi}\hbar} e^{-\beta(E_c-\mu)},$$

where $\beta = 1/\kappa_B T$ and the change of variable $x = \beta(E - E_c)$ was adopted in the integral over dE . Similarly, one finds for the hole concentration

$$h(T) = \int_{-\infty}^{E_v} \frac{g_v(E)}{e^{\beta(\mu-E)} + 1} dE \approx \frac{\sqrt{2m_v\kappa_B T}}{\pi\hbar} e^{-\beta(\mu-E_v)} \int_0^{+\infty} x^{-\frac{1}{2}} e^{-x} dx = \frac{\sqrt{2m_v\kappa_B T}}{\sqrt{\pi}\hbar} e^{-\beta(\mu-E_v)},$$

where now the change of variable $x = \beta(E_v - E)$ was adopted.

3. At equilibrium $n(T) = h(T)$ and we obtain the chemical potential from the equation

$$\frac{\sqrt{2m_c\kappa_B T}}{\sqrt{\pi}\hbar} e^{\beta(\mu-E_c)} = \frac{\sqrt{2m_v\kappa_B T}}{\sqrt{\pi}\hbar} e^{\beta(E_v-\mu)},$$

whence

$$\mu = \frac{E_v + E_c}{2} + \frac{\kappa_B T}{4} \log \frac{m_v}{m_c} = E_v + \frac{E_g}{2} + \frac{\kappa_B T}{4} \log \frac{m_v}{m_c}.$$

For $T = 300$ K and $\mu - E_v = 0.45$ eV, one finds $E_g = 0.885$ eV.