

Written exam of Condensed Matter Physics - June 20th 2023
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Exercise 1: X-ray scattering and phonons.

Germanium (Ge) crystallizes with the diamond structure. When its structure is investigated by means of X-ray scattering, with a radiation of wavelength $\lambda = 0.1542$ nm, the first Bragg peak is observed at an angle $\theta_1 = 13.647^\circ$. When its phonon spectrum is investigated by means of inelastic neutron scattering, the dispersion curves showed in the two left panels of Fig. 1 are found, along the two high-symmetry directions $\langle 111 \rangle$ and $\langle 100 \rangle$ (notice that in the two left panels of Fig. 1 the frequency $\nu = \omega/2\pi$ is plotted vs. $q/2\pi$).

1. [4 points] Determine the numerical value of the side a of the conventional cubic cell of Ge, and of the distance d within the family of lattice planes that produces the observed Bragg peak.
2. [3 points] Determine the numerical value of the Bragg angle θ_5 that corresponds to the fifth peak of the X-ray scattering pattern of Ge (probed with the same wavelength λ), specifying the corresponding Miller indices hkl .
3. [2 points] Specify the degeneracy of each of the phonon branches (TA, LA, LO, TO; T/L=transverse/longitudinal, A/O=acoustic/optical) reported in the two left panels of Fig. 1, motivating your answer.
4. [6 points] Determine the velocity of longitudinal and transverse acoustic phonons, $v_\ell(\Omega)$ and $v_t(\Omega)$, along the two directions reported in the two left panels of Fig. 1 ($\Omega = \langle 111 \rangle, \langle 100 \rangle$); estimate the average velocity of longitudinal and transverse acoustic phonons as the arithmetic average of the values along the two directions; determine the Debye average sound velocity v_D and the Debye temperature Θ_D of the sound modes of Ge.

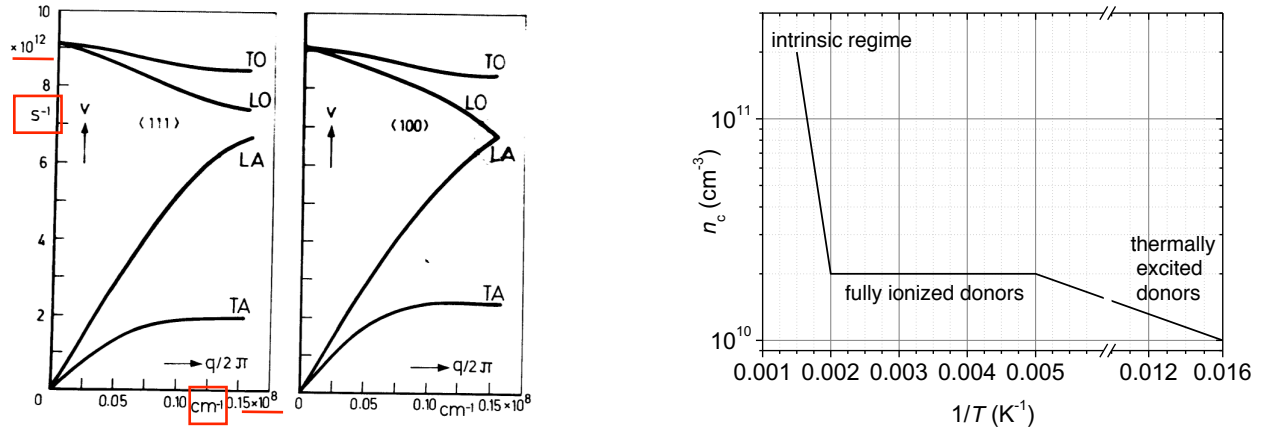


Fig. 1.

Exercise 2: Semiconductors.

In an n -type semiconductor the carrier density in the conduction band n_c is plotted as a function of the inverse of temperature $1/T$ in the right panel of Fig. 1.

1. [4 points] Determine the numerical value of the band gap energy E_g of the semiconductor.
2. [2 points] Determine the numerical value of the donor concentration N_d .
3. [4 points] Determine the numerical value of the donor binding energy ε_d (with respect to the bottom of the conduction band, taken as the reference energy level).
4. [5 points] The static relative dielectric constant of the material is $\varepsilon_r = 12$ and the carrier scattering time at a temperature $T = 250$ K is $\tau = 10^{-13}$ s for all carriers. Determine the numerical value of the electrical conductivity σ at $T = 250$ K and explain why the hole contribution is negligible [hint: use for ε_d the hydrogenoid expression, with effective mass m^*].

[Useful constants and conversion factors: the reduced Planck constant is $\hbar = 1.055 \times 10^{-34}$ J·s, the Boltzmann constant is $\kappa_B = 1.381 \times 10^{-23}$ J·K $^{-1}$, the free electron mass is $m_0 = 9.109 \times 10^{-31}$ kg; 1 eV corresponds to a temperature of 1.160×10^4 K or to an energy of 1.602×10^{-19} J].

Solution
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Exercise 1.

1. According to the selection rules of the diamond lattice, the first Bragg peak corresponds to the Miller indices 111. Then, from the Bragg formula

$$\sin \theta = \frac{\lambda}{2a} \sqrt{h^2 + k^2 + \ell^2} \quad \Rightarrow \quad a = \frac{\lambda}{2 \sin \theta_1} \sqrt{3} = 0.5660 \text{ nm.}$$

The distance within the family of lattice planes that produces the first Bragg peak is $d = a/\sqrt{h^2 + k^2 + \ell^2} = 0.3268 \text{ nm}$.

2. According to the selection rules of the diamond lattice, the fifth Bragg peak corresponds to the Miller indices 331 (and permutations). Then

$$\theta_5 = \arcsin \left(\frac{\lambda}{2a} \sqrt{19} \right) = 36.425^\circ.$$

3. In crystals with the diamond structure, there are three acoustic and three optical branches. Along high-symmetry directions of the first Brillouin zone, the transverse modes can be degenerate, so in the phonon spectra reported in the two left panels of Fig. 1 the TA branch is doubly degenerate, the LA branch is singly degenerate, the LO branch is singly degenerate, the TO branch is doubly degenerate.

4. Calculating the slope of the various acoustic phonon branches near the Γ point we find $v_\ell(\langle 111 \rangle) = 5500 \text{ m/s}$, $v_\ell(\langle 100 \rangle) = 5500 \text{ m/s}$, $v_t(\langle 111 \rangle) = 2500 \text{ m/s}$, $v_t(\langle 100 \rangle) = 3500 \text{ m/s}$. Then, taking the arithmetic averages, $v_\ell = 5500 \text{ m/s}$ and $v_t = 3000 \text{ m/s}$. The Debye sound velocity is

$$v_D = \left[\frac{1}{3} \left(\frac{1}{v_\ell^3} + \frac{2}{v_t^3} \right) \right]^{-1/3} = 3346 \text{ m/s.}$$

Then, the Debye temperature of the sound modes is

$$\Theta_D = \frac{\hbar v_D q_D}{\kappa_B} = (24\pi^2)^{1/3} \frac{\hbar v_D}{a \kappa_B} = 279.4 \text{ K.}$$

Exercise 2.

1. The band gap energy can be determined from the slope of n_c vs. $1/T$ in the high-temperature intrinsic regime, i.e., in the temperature interval between $T_1 = 666.67 \text{ K}$ ($1/T_1 = 0.0015 \text{ K}^{-1}$ and $n_{c1} = 2 \times 10^{11} \text{ cm}^{-3}$) and $T_2 = 500 \text{ K}$ ($1/T_2 = 0.002 \text{ K}^{-1}$ and $n_{c1} = 2 \times 10^{10} \text{ cm}^{-3}$). Indeed, from $n_c = A e^{-E_g/(2\kappa_B T)}$, we find

$$\ln \frac{n_{c1}}{n_{c2}} = -\frac{E_g}{2\kappa_B} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \quad \Rightarrow \quad E_g = \frac{2\kappa_B}{\frac{1}{T_2} - \frac{1}{T_1}} \ln \frac{n_{c1}}{n_{c2}} = 0.794 \text{ eV.}$$

2. The donor concentration can be determined in the regime of fully ionized donors, that corresponds to the plateau region of n_c , hence, $N_d = 2 \times 10^{10} \text{ cm}^{-3}$.

3. The donor binding energy ε_d can be determined from the slope of n_c vs. $1/T$ in the low-temperature regime, where the carrier are thermally excited from the donor levels, i.e., in the temperature interval between $T_3 = 200 \text{ K}$ ($1/T_3 = 0.005 \text{ K}^{-1}$ and $n_{c3} = 2 \times 10^{10} \text{ cm}^{-3}$) and $T_4 = 62.5 \text{ K}$ ($1/T_4 = 0.016 \text{ K}^{-1}$ and $n_{c4} = 10^{10} \text{ cm}^{-3}$). Indeed, from $n_c = B e^{-\varepsilon_d/(2\kappa_B T)}$, we find

$$\ln \frac{n_{c3}}{n_{c4}} = -\frac{\varepsilon_d}{2\kappa_B} \left(\frac{1}{T_3} - \frac{1}{T_4} \right) \quad \Rightarrow \quad \varepsilon_d = \frac{2\kappa_B}{\frac{1}{T_4} - \frac{1}{T_3}} \ln \frac{n_{c3}}{n_{c4}} = 10.9 \text{ meV.}$$

4. From the hydrogenoid formula $\varepsilon_d = m^*/(m_0 \epsilon_r^2) \cdot 13.6 \text{ eV}$ we deduce the electron effective mass $m^* = 0.115 m_0$. From the right panel of Fig. 1, at $T = 250 \text{ K}$ ($1/T = 0.004 \text{ K}^{-1}$) we deduce that $n_i \ll n_c$, hence $p_v = n_i^2/n_c \ll n_c$, therefore the contribution of holes in the valence bands to the conductivity is negligible and

$$\sigma = \frac{n_c e^2 \tau}{m^*} = 4.90 \times 10^{-4} \Omega^{-1} \cdot \text{m}^{-1}.$$