Written test of Condensed Matter Physics - January 21st 2020
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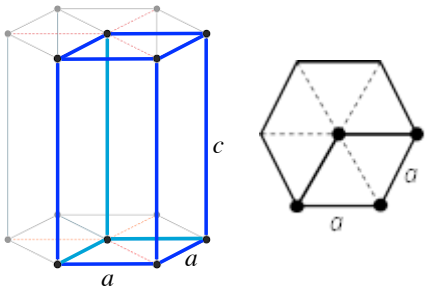
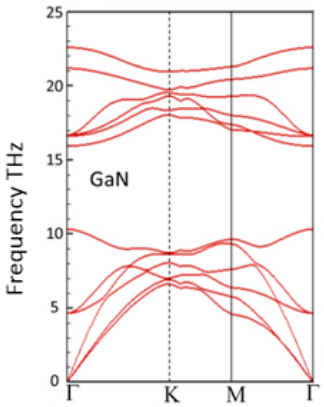
1) Gallium nitride (GaN) is a wide-gap semiconductor with wurtzite crystal structure with basis, the conventional unit cell being a hexagonal prism, with side of the regular hexagonal basis a=0.319 nm and height of the prism c=0.518 nm. The primitive cell is evidenced with the thicker lines in the left panel of the figure below along with the basal plane of the primitive cell. Note that the basis structure is not displayed in those figures.

a) By analyzing the phonon spectrum of GaN shown in the right panel of the figure below, determine the number of atoms in a primitive cell, providing an argument to support your answer.





b) Determine the Debye wavevector k_D of GaN, as it is defined in the Debye model for the acoustic branches.

c) Knowing that the average sound velocity of GaN is c_s=6.51×10^3 m/s, determine the specific heat of GaN at a temperature T=1 K [assume that only the sound modes contribute to the specific heat; the Planck constant is $\hbar = 1.05 \times 10^{-34}$J·s; the Boltzmann constant is k_B=1.38×10^{-23} J/K].

2) Consider a simple cubic semiconductor with lattice constant a=0.5 nm. The conduction and valence bands (E_C and E_V, respectively) feature the following dispersion curves along the k_x direction:

$$E_C = A\left[1 - \frac{1}{2}\sin^2\left(\frac{k_x a}{2}\right)\right]$$

$$E_V = B[\cos(k_x\, a) - 1]$$

where A=1.0 eV and B=0.5 eV.

a) Plot the dispersion curves in the first Brillouin zone along the k_x direction and say whether the semiconductor is direct- or indirect-band gap crystal.

b) In the ideal condition of absence of scattering, evaluate the maximum velocity along the x direction of an electron in the valence band and specify the corresponding point of the first Brillouin zone.

c) Evaluate the effective mass tensor m_{xx} of the electrons at the conduction band minimum and of the holes at the valence band maximum.

d) Evaluate the concentration of electrons and holes in the conduction and valence bands, respectively at T=300 K (the semiconductor is intrinsic, *i.e.*, no impurity is present in the lattice).

e) Evaluate the conductivity σ_{xx} at 300 K knowing that the scattering time of electrons and holes are τ_e=0.3 ps and τ_h=0.1 ps, respectively.

Solutions

Exercise 1

a. Since there are 12 phonon branches, the number of atoms per primitive cell is p=12/3=4.
b. The Debye wavevector is defined as $k_D=(6\pi^2/v)^{1/3}$, where $v=\sqrt{3}\,a^2c/2=0.0457$ nm^3 is the volume of the primitive cell. Hence, k_D=10.9 nm^{-1}.
c. The acoustic-phonon low-temperature contribution to the specific heat is

$$c_V = \frac{2\pi^2 k_B}{5}\left(\frac{k_B T}{\hbar c_s}\right)^3 = 0.443\ \text{J/(K·m}^3\text{)}.$$

Exercise 2

a. Indirect.
b. $v = \frac{1}{\hbar}\frac{\partial E_V}{\partial k_x} = -\frac{1}{\hbar}Ba\sin(k_x a)$, whose maximum magnitude is $\frac{1}{\hbar}Ba = 3.81\times10^5\frac{m}{s}$, and is found at $k_x = \pm\frac{\pi}{2a}$.
c. $m_c = \frac{4\hbar^2}{Aa^2} = 1.10\times10^{-30}\text{kg} = 1.21\,m_0$, $m_v = \frac{\hbar^2}{Ba^2} = 5.51\times10^{-31}\ \text{kg} = 0.604\,m_0$
d. $n_c = p_v = n_i = 2.51\cdot(1.21\cdot0.604)^{3/4}\cdot e^{-\frac{0.5}{2\cdot0.0259}}\times10^{25}\text{m}^{-3} = 1.28\times10^{21}\text{m}^{-3}$
e. $\sigma = n_i e^2\left(\frac{\tau_e}{m_c}+\frac{\tau_h}{m_v}\right) = 14.8\,\Omega^{-1}\text{m}^{-1}$