

Structure of Matter II
20 June May 2022, 16.00-18.00, Exam Hall 1 A1-H12

KEY

Write your name and student number on every sheet
Extra-time students: 10 minutes per hour => 20 min extra

PROBLEM 1. Crystal lattices [12 pts]

Consider a rectangular 3D lattice with the atomic lattice distances in x, y, and z direction equal to a , $2a$ and $3a$, respectively.

- a) Calculate the reciprocal unit vectors corresponding to this lattice. [4 pts]
- b) Calculate the volumes of the Wigner-Seitz unit cell and the (first) Brillouin zone cell. [3 pts]
- c) Consider the planes described by the Miller indices (1,2,3). Determine the distance between these planes. [3 pts]
- d) What is Bloch's theorem? [2 pts]

PROBLEM 2. Electrons and crystals [11 pts]

- a) Explain why we get band gaps in the energy-momentum relationship of crystals. [4 pts]
- b) Do these band gaps become more or less wide when the interaction between the electrons and the atoms increases? explain your answer. [2 pts]

In the course, we have seen that the density-of-states, g , in a 3D electron gas is related to the energy ε by $g(\varepsilon) \propto \sqrt{\varepsilon}$.

- c) Now consider a **1D** crystal and derive the allowed k values. [2 pts]
- d) Calculate the density-of-states g of such a **1D** electron gas. [3 pts]

PROBLEM 3. Doping and pn-junctions [13 pts]

Consider a pn-junction in equilibrium.

- a) What is the electrical charge (positive, negative, or neutral) of a small volume of the semiconductor in the p-region, far away from the interface? explain your answer. [2 pts]
- b) What is the electrical charge (positive, negative, or neutral) of a small volume of the semiconductor in the n-region, within the depletion region (i.e. close to the interface)? explain your answer. [2 pts]
- c) Show that the conductivity of a p-doped semiconductor can be written as

$$\sigma = \frac{pe^2\tau}{m^*},$$

where τ is the average time between scattering events and m^* is the effective mass. [3 pts]

- d) Suppose you need a piece of p-doped silicon with a conductivity of 100 S/cm. Calculate the required distance between the Fermi level and the valence band edge. Assume $\tau = 1$ ns and $m^* = 0.1 m_e$. [4 pts]

e) This image shows a cut-out of the periodic table of the elements:

5 B 10.81	6 C 12.011	7 N 14.007
13 Al 26.982	14 Si 28.085	15 P 30.974
31 Ga 69.723	32 Ge 72.63	33 As 74.922

Which elements can be used to p-dope silicon. Explain your answer. [2 pts]

**Please check whether your name and student number are on every sheet
Please hand in the exam questions (cannot be taken home!)**

Some constants

$$m_e = 9.1096 \times 10^{-31} \text{ kg}$$

$$e = 1.6022 \times 10^{-19} \text{ C}$$

$$\text{for silicon: } N_C = 3.22 \times 10^{19} \text{ cm}^{-3} \text{ and } N_V = 1.83 \times 10^{19} \text{ cm}^{-3}.$$

$$kT = 25 \text{ meV (near room-temperature)}$$

ANSWERS

Q1 a & b are swapped!!

- a) $\vec{a}_1, \vec{a}_2,$ and \vec{a}_3 are perpendicular to each other
so the directions of a_i are the same as b_i
(reciprocal vectors).

Using this information we get:

$$\vec{b}_i = \frac{2\pi}{\|\vec{a}_i\| \|\vec{a}_j\|} \vec{a}_i$$

So

$$b_1 = \frac{2\pi}{a} \hat{x}$$

$$b_2 = \frac{2\pi}{2a} \hat{y}$$

$$b_3 = \frac{2\pi}{3a} \hat{z}$$

- b) ~~the~~ The volume then becomes: (first Brillouin zone cell)

$$V = \frac{2\pi}{a} \cdot \frac{2\pi}{2a} \cdot \frac{2\pi}{3a} = \frac{8\pi^3}{6a^3} = \frac{4\pi^2}{3a^3}$$

The same result can be obtained using the standard
~~the~~ formula for reciprocal vectors.

$$b_i = 2\pi \frac{\vec{a}_j \times \vec{a}_k}{\vec{a}_i \cdot (\vec{a}_j \times \vec{a}_k)}, \text{ etc...}$$

Wigner Seitz cell:

$\vec{a}_1, \vec{a}_2,$ and \vec{a}_3 are perpendicular, so

$$V = \|\vec{a}_1\| \cdot \|\vec{a}_2\| \cdot \|\vec{a}_3\| = a \cdot 2a \cdot 3a = 6a^3$$

- c) use $d = \frac{2\pi}{\|\vec{g}\|}$, where $\|\vec{g}\| = \sqrt{n_1^2 b_1^2 + n_2^2 b_2^2 + n_3^2 b_3^2}$

first calculate $\|\vec{g}\|$:

$$\begin{aligned} \|\vec{g}\| &= \sqrt{1 \cdot \frac{4\pi^2}{a^2} + 4 \cdot \frac{4\pi^2}{4a^2} + 9 \cdot \frac{4\pi^2}{9a^2}} \\ &= \sqrt{\frac{12\pi^2}{a^2}} \\ &= 2\sqrt{3} \frac{\pi}{a} \end{aligned}$$

so

$$d = \frac{2\pi a}{2\sqrt{3}\pi} = \frac{a}{\sqrt{3}}$$

d This states that any wave functions of electrons in a crystal are of the form

$$\Psi = e^{ikr} u_{k(r)},$$

where $u_{k(r)}$ is a function that has the periodicity of the lattice.

OR:

if l is a lattice vector, then

$$\Psi = e^{ikr} u_{k(r)},$$

Q2

a) The zone boundaries (or at the edges of the Brillouin zone), we get scattering of electrons such that the electron density either piles up at the positions of the atoms, or in between two atoms (in a standing wave). Due to the attraction between the electron and the atoms, the former has a lower energy than the latter. Hence the gap.

b). Stronger interaction => energy difference (as outlined in a) becomes larger => band gap is wider.

c) Simply apply the Born-von Karman boundary condition: and we find that

$$k = \frac{2\pi n}{L},$$

where n is an integer and L is the length of the crystal.

d. First, calculate how to put N electrons into this crystal and calculate the corresponding wave number (and energy):

$N = 2(\text{for spin}) 2 k_F (L/2\pi)$. Now we still have that

$$\varepsilon_F = \frac{(\hbar k_F)^2}{2m}$$

so

$$N = \frac{4L}{h} \sqrt{2m\varepsilon}$$

and

$$g = \frac{dN}{d\varepsilon} = \frac{2L}{h} \sqrt{\frac{2m}{\varepsilon}}$$

Note: if student takes g per length ("volume"), then that's fine as well. Also note, there are other possibilities to write this in an acceptable form if the students keeps \hbar .

Q3

a. it's neutral as there are nearly as many holes as there are ionized dopants (=acceptors).

b. it's positive as it corresponds to the charge of the ionized donors.

c. holes (or electrons, doesn't matter) pick up momentum in an applied electric field E .

So: $dp/dt = eE$. In time τ , that means that the momentum changes by $eE\tau$. This yields a current density $J = e p (eE\tau)/m^* = \sigma E$, so indeed

$$\sigma = \frac{pe^2\tau}{m^*},$$

d. $p = \sigma m^*/(e^2 \tau) = 3.55 \times 10^{17} \text{ m}^{-3}$. It's silicon, so $N_v = 1.83 \times 10^{19} \text{ cm}^{-3}$ and $kT = 25 \text{ meV}$. Thus: distance between E_F and $E_V = 0.1 \text{ eV}$.

e. we need elements with 1 fewer VALENCE electrons: B, Al, Ga.