

1. Number of lattice points

Calculate the number of lattice points within the conventional unit cell in the a) simple cubic, b) bcc and c) fcc lattices. (Notice, for example, that only 1/8 of any point in the corner of the conventional unit cell belongs to that cell.) Show additionally that the conventional unit cell of the zinc blende structure contains an equal number of both types of atoms.

2. Filling factors

Show that the largest volume (percentage of the unit cell) that can be filled with atoms, supposed to be hard spheres, is a) 52 % for simple cubic, b) 68 % for bcc, and c) 74 % for fcc structures. (Hint: determine first the maximum radius of the spheres and then use the results of Problem 2.)

3. Relation between density, atomic mass, lattice structure and lattice constant

The density of aluminium is 2700 kg/m³ and the atomic mass is 26.98 u. What is the particle number density of an aluminium crystal, that is, how many atoms there are in 1 m³? The lattice structure of aluminium is fcc. Use this information to deduce the lattice constant and compare it with the measured value $a = 0.405$ nm.

4. Sphere model for NaCl structure

Assuming that atoms are like hard spheres, calculate the optimal radii ratio of hard spheres in the Na⁺Cl⁻ structure. Start from the assumption that the bigger spheres (Cl⁻) are as large as the size of the unit cell allows, and determine the maximum radius of the small sphere (Na⁺) that fits in between. Answer: $\sqrt{2} + 1 = 2.4$.

5. Fcc as a Bravais lattice

Show that the fcc structure is a Bravais lattice. For this choose appropriate \mathbf{a}_1 , \mathbf{a}_2 and \mathbf{a}_3 so that the expression $\mathbf{r} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, where n_1 , n_2 and n_3 are integers, gives all lattice points of fcc structure within a unit cell, but seems to give no extra points.

1. Measuring the lattice constant

The lattice structure of copper is bcc. By using radiation, which wavelength is 0.1537 nm, the reflection from the (111) planes of copper was observed at the scattering angle $\theta = 21^\circ 40'$ and (200) reflection at $\theta = 25^\circ 13'$. What is the value of lattice constant a ? [The symbol (200) means reflection from the plane (100) corresponding to the order $n = 2$.]

2. Lattice planes

Draw the planes (210) and (111) in the conventional unit cell of a cubic crystal. Show that the distance between the lattice planes in these cases is correctly given by the equation

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}.$$

3. Determination of the lattice structure

In a diffraction measurement the intensity peaks were observed at the following values of the scattering angle θ : 20° , 29° , 36.5° , 43.4° , 50.2° , 57.35° and 65.55° . The wavelength of the radiation was 0.154 nm. Assume that the smallest angle corresponds to a reflection from the (100) planes in a simple cubic structure. Based on this assumption, check whether you can explain all the rest of the intensity peaks?

4. Electron diffraction

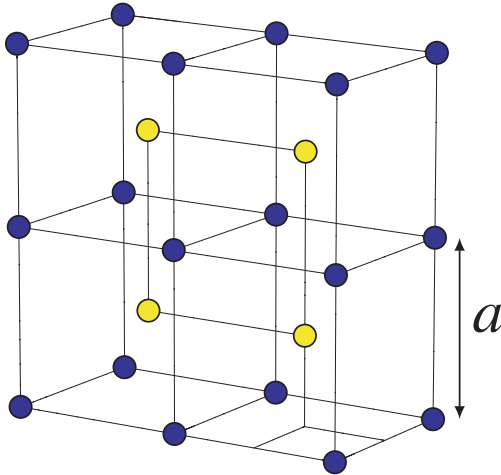
a) A substance is studied by electron diffraction. What is the minimum value of the electron energy so that a diffraction peak is obtained from the crystal, whose lattice constant is 0.2 nm? b) In order to the electrons to penetrate properly to the sample, the energy of 100 keV is used. What is the angle of the lowest order reflection? (Answer: 9.4 eV, 0.56°)

5. Extinction of reflection

Study if planes (100), (110) and (111) have extinguished reflections in body centered cubic structure. Repeat the same in face centered cubic structure.

1. Madelung constant for CsCl structure

CsCl consists of Cs^+ and Cl^- ions placed on every second places in body centered cubic lattice (figure). Verify that the distance between nearest neighbour atoms is $R = \frac{\sqrt{3}}{2}a$. Calculate the first three terms of the Madelung constant for this lattice.



2. Model for ionic bonding

Assume that the potential energy of the interaction between two atoms is

$$U(R) = -\frac{\alpha}{R} + \frac{\beta}{R^8}, \quad (1)$$

where R is the interatomic distance and α and β are positive constants.

- Calculate the force between the atoms. Which of the term describes attraction and which describes repulsion?
- Calculate the equilibrium distance between the two atoms.
- Compare the energies coming from the attraction and repulsion at the equilibrium (a point where the attractive and repulsive forces are equal).

3. Lattice vibrations of long wave length

Show that the equation of motion of a lattice vibration

$$M \frac{d^2 \xi_n}{dt^2} = K(\xi_{n-1} - 2\xi_n + \xi_{n+1}) \quad (2)$$

reduces to the normal wave equation

$$\frac{\partial^2 \xi}{\partial t^2} = c^2 \frac{\partial^2 \xi}{\partial x^2}. \quad (3)$$

in the case of long wavelengths, where ξ_n is a very slowly varying function of n . Hint: Express ξ_{n+1} and ξ_{n-1} in terms of a Taylor expansion of $\xi(x)$ around the point $x = na$.

4. Lattice vibrations for a two-atomic basis

Go through the details of the calculation (presented in the lectures), where the vibrational frequencies of a chain containing two types of atoms (with differing masses) was derived. Calculate the vibrational frequencies for both the acoustic and optic branches in the special cases a) $k = 0$ and b) $k = \pi/a$ assuming $M_1 > M_2$.

5. Estimation of the parameters of lattice vibrations

The speed of sound in copper is 4000 m/s. Estimate the spring constant K between the atoms and the maximum frequency of the lattice vibrations. Estimate the Debye temperature by formula $\Theta_D \approx \hbar\omega_{\max}/k_B$. (copper: fcc, lattice constant 361 pm, mass number 63.55. Assume that the sound propagates in the direction [110], in which case the equilibrium distance between the atoms in our chain model is the lattice constant divided by $\sqrt{2}$.) (Answer: $K = 26$ N/m, $\Theta_D \approx 240$ K.)

6. Specific heat of diamond

Estimate the specific heat (per mole) of diamond at room temperature. Use $\Theta_D = 1860$ K and the figure in the lecture notes (page 13) where the specific heat in the Debye model is plotted as a function of the temperature. [Answer: $C = 5.7$ J/(K mol).]

1. Model for covalent bond

a) An extremely simplified model for an electron in an atom is a deep potential well

$$U(x) = \begin{cases} 0 & , \text{ for } 0 < x < a \\ \infty & \text{ otherwise.} \end{cases} \quad (4)$$

Give the four lowest energy values (corresponding to 8 lowest levels) and plot the energies on a vertical energy axis.

b) Imagine having two potential wells of this kind, completely separated from each other. Justify that the energy values are the same as in a) but now there are double number of levels (= 4) corresponding to each energy value.

c) Now imagine that the potential wells are combined to form a single potential well of width $2a$. Sketch the 8 lowest energy values for this potential well to the energy axis corresponding to the one in a). By comparing the energy levels in b) and c), try to understand which levels correspond to each other and how their energies are changed when potential wells are combined.

d) Assume that there are 2 electrons in each potential well in b). What is the binding energy of the covalent bond in this model? That is, how much energy is released when the separate potential wells are combined?

2. Solution of the Schrödinger equation in a box

Show that the wave function

$$\psi(x, y, z) = A \sin \frac{n_1 \pi x}{L} \sin \frac{n_2 \pi y}{L} \sin \frac{n_3 \pi z}{L} \quad (5)$$

(where n_1 , n_2 and n_3 are positive integers) is a solution of the Schrödinger equation and that it vanishes at the surface of a cube of sides L (the sides are located at x , y , $z = 0$ and L).

3. Accurate counting of energy levels

Let us consider electrons in a deep cubic potential well of volume $V = L^3$. Find all energies that are smaller or equal than $E_r = 6\hbar^2\pi^2/mL^2$. Calculate the number of energy levels (noting that a single wave function corresponds to two levels). Compare the number of levels to the number $n(E)V = (2\sqrt{2m^3V/3\pi^2\hbar^3})E^{3/2}$ estimated in the lectures. [Answer: $n^{\text{true}}(E_r) \approx 0.5n^{\text{estimated}}(E_r)$.]

4. Fermi energies numerically

Calculate the Fermi energy, Fermi temperature, Fermi wave number and Fermi velocity in the free electron model for copper (density 8.96 g/cm^3 , atomic mass 63.55 u , $Z = 1$) and for aluminium (density 2.70 g/cm^3 , atomic mass 26.982 u , $Z = 3$). (Answers: 7.0 and 11.6 eV , $81\,000$ and $130\,000 \text{ K}$, 1.36 and $1.75 \cdot 10^{10} \text{ 1/m}$, 1.57 and $2.02 \cdot 10^6 \text{ m/s}$)

5. **Average energy of free electrons**

Calculate the average energy for free electrons in the ground state (temperature $T = 0$):

$$\langle E \rangle = \frac{1}{n_e} \int_0^{\varepsilon_F} g(E) E dE. \quad (6)$$

(Answer: $\langle E \rangle = \frac{3}{5} \varepsilon_F$.)

1. Bloch wave functions

Derive the formulas presented in the lecture notes

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dx^2} - \frac{i\hbar^2 k}{m} \frac{du}{dx} + U(x)u = \left(E - \frac{\hbar^2 k^2}{2m}\right)u, \quad (7)$$

$$\langle p \rangle = \hbar k + \int u^*(x) \left(-i\hbar \frac{d}{dx}\right) u(x) dx. \quad (8)$$

2. Tight binding method

Fill in the intermediate steps in the calculation of the tight binding model, which gives the dispersion relation $E_k = -\alpha - 2\beta \cos(ka)$. [Hint: calculate the numerator and the denominator of

$$E_k = \left(\int \psi^*(x) \mathbf{H} \psi(x) dx\right) / \int \psi^*(x) \psi(x) dx$$

separately. Write both in the double-sum form $\sum_{n'} \sum_n A_{n'n}$ and calculate all $A_{n'n}$ making use of the periodicity of the lattice potential $U(x)$. Assume that the number of atoms N in the chain is large, which allows you to neglect all possible difficulties caused by the ends of the chain.]

3. Group velocity

Calculate the group velocity v a) for lattice vibrations (assume 1-dimensional lattice with 1-atom basis) and b) for free electrons. c) A wave packet can travel without changing its form if $v(k)$ is constant. When does this happen?

4. Electron motion in ideal crystal

Let's consider the tight binding model, where the dispersion relation is $E(k) = -\alpha - 2\beta \cos(ka)$. Solve $v(k)$, $k(t)$, $v(t)$ and $x(t)$ using the semiclassical equations of motion

$$v = \frac{1}{\hbar} \frac{dE}{dk}, \quad F = \hbar \frac{dk}{dt} \quad (9)$$

assuming a constant force F is acting on the electron, and it starts from rest $k(0) = 0$, $x(0) = 0$. How long does it take for the electron to return to its starting position?

5. Effective mass

In the lectures the effective mass was defined by the equation

$$E \approx E_0 + \frac{\hbar^2 (k - k_0)^2}{2m^*}. \quad (10)$$

Show that the effective mass can also be obtained from the following expression

$$m^* = \frac{\hbar^2}{d^2 E / dk^2}. \quad (11)$$

Calculate m^* in the case of the tight binding model where $E = -\alpha - 2\beta \cos(ka)$. What is the width of the energy band?

1. The mean velocity of charge carriers

We have previously calculated that the density of conducting electrons in copper is $8.5 \times 10^{28} \text{ m}^{-3}$. A current of 100 A flows in a copper wire, whose cross-sectional area is 1 mm^2 . Estimate the mean velocity of conducting electrons and compare the result with the Fermi velocity.

2. Justification of the Drude model

We study the Drude model in the absence of external electric field. In this case the average momentum of the electrons satisfies the equation

$$\frac{d\mathbf{p}}{dt} = -\frac{\mathbf{p}}{\tau}. \quad (12)$$

(a) Show that the solution of the equation (12) with the initial condition $\mathbf{p}(t=0) = \mathbf{p}_0$ is

$$\mathbf{p}(t) = \mathbf{p}_0 e^{-t/\tau}. \quad (13)$$

(b) The previous result can be interpreted as follows: the probability that the electron has not yet been scattered at time t is $F(t) = e^{-t/\tau}$. Calculate the probability density $f(t) = -dF/dt$ that the electron is scattered first time at t .

(c) The average time that the electron spends before scattering is defined by $\langle t \rangle = \int_0^\infty t f(t) dt$. Show that $\langle t \rangle = \tau$.

(c) How long does it take that half of the electrons are scattered?

3. Mean free path in Drude model

The resistivity ρ of copper at room temperature is $1.68 \times 10^{-8} \Omega\text{m}$. What is the relaxation time τ of copper according to the Drude model? Calculate how long distance $l = v_F \tau$ an electron moving at the Fermi velocity travels in this time, and compare the result to the lattice constant 361 pm of copper.

4. A model for a donor impurity in a semiconductor

We study an impurity level in an n-type semiconductor by assuming that the extra nuclear charge e of the impurity atom causes a local Coulomb potential for the electron in the conduction band. In a free hydrogen atom the binding energy in the ground state and the radius of the ground state orbit are

$$E = \frac{m_e e^4}{8\epsilon_0^2 \hbar^2} = 13.6 \text{ eV} \quad , \quad r \approx \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} = 53 \text{ pm}. \quad (14)$$

In a medium we have to take into account that electron effective mass changes $m_e \rightarrow m^*$ and the charge is screened so that the permittivity of the vacuum has to be replaced

$\varepsilon_0 \rightarrow \varepsilon\varepsilon_0$, where ε is the dielectric constant. Estimate the energy gap between the n-type impurity level and the edge of the conduction band, and the radius of the bound impurity state in indium antimonide (InSb), where $m^* = 0.01m_e$ ja $\varepsilon = 17$. Compare the energy with the energy gap $E_g = 0.17$ eV and the radius to the lattice constant 648 pm of InSb.

5. Densities of charge carriers in a semiconductor

For the Fermi function, show that

$$f(E) = \begin{cases} e^{-(E-\mu)/k_B T}, & \text{kun } E - \mu \gg k_B T \\ 1 - e^{-(\mu-E)/k_B T}, & \text{kun } \mu - E \gg k_B T. \end{cases} \quad (15)$$

We study a semiconductor where the electron density in the conduction band is $n_n = \int f(E)g(E)dE$. Here the integration is over the conduction band, whose lower edge is at energy E_n and the upper edge at energy E'_n . We assume the band is wide ($E'_n - E_n \gg k_B T$) and its level density is

$$g(E) = \frac{\sqrt{2}m_n^{3/2}}{\pi^2\hbar^3} \sqrt{E - E_n}, \quad (16)$$

where m_n is the effective mass of the conduction band. Using the approximation above for $f(E)$, show that

$$n_n = Am_n^{3/2}T^{3/2}e^{-(E_n-\mu)/k_B T}. \quad (17)$$

What is the value of the constant A ? The corresponding calculation for holes gives

$$n_p = Am_p^{3/2}T^{3/2}e^{-(\mu-E_p)/k_B T}, \quad (18)$$

where E_p is the energy of the upper edge of the valence band. Using these, derive the formula

$$n_n n_p = A^2(m_n m_p)^{3/2} T^3 e^{-E_g/k_B T}, \quad (19)$$

where E_g is the energy gap between the valence and the conduction bands. Hint: Mathematica calculates $\int_0^\infty \sqrt{x}e^{-x}dx = \sqrt{\pi}/2$.

1. Rectification in a diode

Estimate the relative magnitude of the currents in a forward- and reverse biased n-p junction diode when the applied voltage is 0.5 eV.

2. Materials for a LED and a solar cell

We study a light emitting diode where the semiconductor material is a) Si, b) $\text{Ga}_{0.7}\text{Al}_{0.3}\text{As}$ or c) $\text{In}_{0.3}\text{Ga}_{0.7}\text{N}$. The energy gaps are $E_g = 1.17, 1.82$ ja 2.8 eV, respectively. What is the color of the light emitted by the diode? If the same materials were used for making a solar cell, what advantages and drawbacks the different materials have? Notice that the part of the energy of a photon that exceeds the energy gap is not converted to electricity in a solar cell.

3. Absorption of light

a) Why is diamond transparent? Its energy gap is 5.33 eV.

b) Why is potassium sulphide orange-yellow? Its energy gap is 2.42 eV.

c) Pure KCl is transparent and colorless. In certain circumstances so-called F-centres are formed in the crystal, which absorb photons of energy 2.2 eV. What is the corresponding wavelength? What can you say about the color of the crystal?

4. Electron at a vacancy in a crystal

An F-center in an alkali-halide crystal is a missing negative ion, which is replaced by an electron. Let's model the absorption at energy 2.2 eV in a KCl crystal as an electronic transition between levels that correspond to two lowest energies in an infinitely deep one-dimensional potential well. What is the width of the potential well? Compare it to the lattice constant 0.629 nm. (Answer: 0.72 nm)

5. Paramagnetism of conduction electrons

Calculate the Pauli paramagnetic susceptibility for aluminum in the free-electron approximation. (Use the values calculated in the previous exercises). Compare the result with the measured value 2.1×10^{-5} . Susceptibility is a dimensionless quantity telling how much the field in a sample differs from the magnetizing external field. Interpret your result based on this.

1. Magnetism from magnetic dipole forces

Starting from equations

$$\frac{\mathbf{B}}{\mu_0} = \mathbf{H} + \mathbf{M} \quad \text{and} \quad \mathbf{M} = \frac{\chi}{\mu_0} \mathbf{B}, \quad (20)$$

investigate when the magnetization can spontaneously emerge without the magnetizing field \mathbf{H} . At what temperature this could happen for paramagnetic ions forming a simple cubic lattice with lattice constant 0.3 nm?

2. Magnetic state in a potential well

Let us consider a very deep potential well, whose width is L .

- What are the two lowest energy eigenvalues of the Schrödinger equation?
- The potential well has two electrons whose mutual interaction is neglected. Justify that the ground state is nonmagnetic, i.e. the magnetic moment vanishes in the lowest energy state. How much higher in energy is the lowest magnetized state?

3. Wall between two ferromagnetic domains

The thickness of the interface (domain wall) between two ferromagnetic domains depends on two effects:

- Magnetization favors certain directions in the lattice (in the iron [100]). This cannot be realized in the domain wall, which gives rise to an additional energy $E_1 \approx aLA$, where L is the thickness of the boundary and A is its area.
- Within the domain wall the direction (angle θ) of the magnetization μ changes. This leads to energy density $b(d\theta/dx)^2$. Calculate the energy coming from this effect by supposing that the angle θ changes linearly from zero to π in distance L . Calculate the thickness of the domain wall and the related energy by assuming that they correspond to a minimum of the total energy (from effects 1 and 2) with respect to L . (a and b are positive constants.)

4. A superconducting wire

If a superconductor at temperature T is in an increasing magnetic field, the superconductivity disappears when the magnetic field reaches the critical value

$$B_c = B_0 \left[1 - \left(\frac{T}{T_c} \right)^2 \right], \quad (21)$$

where B_0 is a constant. For lead $B_0 = 0.0803$ T and $T_c = 7.193$ K. How large electric current can maximally flow in a superconducting lead wire of diameter 4 mm at temperature (i) 7.193 K, (ii) 4 K and (iii) 0 K? What is the current density j corresponding to these currents?

Hint: Electric current I flowing in a long, straight wire creates a magnetic field $B = \mu_0 I / 2\pi r$ outside the wire, where r is the radial coordinate measured from the axis of the wire.

Answers (ii) and (iii): 555 and 803 A, and 4.4 and $6.4 \cdot 10^7$ A/m²

5. Flux lines in a type II superconductor

In the lecture notes, there is a figure of flux lines in a type II superconductor. Check that the density of flux lines in the figure corresponds to a magnetic field of 1 T.