

Physics of materials

Collection of questions and problems

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1 Atoms and bonds

1. Describe the photoeffect and the diffraction of electrons. Discuss their importance for the development of modern physics.
(3 points)
2. (R1) A clean tungsten surface is illuminated with light of the wavelength 187 nm leading to the emission of electrons with a maximum energy of 1.2 eV. Calculate the maximum wavelength of the photoelectrons, which can escape from the surface.
(3 points)
3. The emission of photoelectrons from a caesium surface with light of a wavelength of $\lambda = 546.1$ nm is blocked by a bias of 0.374 V. For $\lambda = 312.6$ nm this value amounts to 2.070 V. Calculate the charge of the electron.
(3 points)
4. Give a formula to determine directly the de Broglie wavelength of an electron from the acceleration voltage.
(5 points)
5. a) What is the magnitude of the wavelength of a body having a mass of 1 kg and a speed of 1 m/s.
b) Calculate your own de Broglie wavelength (at the speed of fast walking).
(4 points)
6. Explain the terms uncertainty relation and Pauli principle.
(3 points)
7. Supposed you determine the velocity of an electron to 500 km/s with an error of 0.01 %. What is the principal uncertainty you can determine the position?
(3 points)
8. The uncertainty relation can also be expressed in the form $\Delta E \Delta t \approx \hbar$. If 10^{-8} s is the average lifetime of an electron in an excited state, how big is the uncertainty of the determination of the energy in the excited level? What is the frequency interval the electron will emit during the transition into the ground state?
(4 points)

9. Describe some of the consequences when the Planck constant h would be large, but other physical laws would be still valid.
(3 points)
10. The first four lines of the Lyman series have the wavelengths (in nm)
121.6 102.6 97.2 95.0.
Calculate graphically the Rydberg constant for hydrogen.
(3 points)
11. Do you have an idea, why the fifth line of the Balmer series was not discovered together with the other four?
(3 points)
12. Give the Bohr postulates. Why the Bohr theory is often called semi-classical?
(3 points)
13. What is the binding energy of the electron in the hydrogen atom for the principal quantum number $n = 10$?
(3 points)
14. A photon with a wavelength of 102.6 nm is emitted during the transition from the excited into the ground state. What is the excited state the electron was in?
(3 points)
15. Calculate the current of one electron in the 1st Bohr shell.
(3 points)
16. **(S1)** Calculate the energy levels and radii of the corresponding orbits for the principal quantum numbers $n = 2$ and $n = 3$ in the hydrogen atom.
(4 points)
17. Calculate the number of electrons required to fill all of the energy levels up to and including the 4p sub-shell.
(3 points)
18. Explain why the electrons in the filled electron sub-shells of an atom do not take part in the bonding process.
(3 points)
19. Is the gravitational force between proton and electron in the hydrogen atom of importance compared to the Coulomb interaction? How the ratio between both forces changes from one orbit to the other?
(5 points)

20. If the force between two ions is given by

$$F = -\frac{e^2}{4\pi\epsilon_0 r^2}$$

(e elementary charge, ϵ_0 dielectricity constant, r distance of the ions)
show that the potential energy is given by

$$E_{\text{pot}} = -\frac{e^2}{4\pi\epsilon_0 r}.$$

(4 points)

21. Calculate the fractional change in the magnitude of the repulsive force between two ions as the separation r is increased from $r = r_0$ to $r = 2r_0$. Compare your result with the fractional change in the magnitude of the Coulomb force for the same increase in r . Hence explain why the repulsive force is a short-range force in comparison with the Coulomb force. Assume that the Coulomb force is given as

$$F_C = -C_1 \frac{r_0^2}{r^2}$$

and the repulsive force as

$$F_{\text{rep}} = C_2 \frac{r_0^{10}}{r^{10}}$$

(C_1 and C_2 constants, r_0 equilibrium distance of the ions).

(5 points)

22. If the force between two ions is given by

$$F = -C_1 \frac{r_0^2}{r^2} + C_2 \frac{r_0^{10}}{r^{10}}$$

(C_1 and C_2 constants, r_0 equilibrium distance of the ions)

show that the potential energy is a minimum when $r = r_0$.

(5 points)

23. **(S1)** If the binding energy of an ion in a sodium chloride crystal is $1.29 \cdot 10^{-18}$ J and the equilibrium separation r_0 is 0.281 nm, determine the value of the constant C_1 in the equation of the force

$$F = -C_1 \frac{r_0^2}{r^2} + C_2 \frac{r_0^{10}}{r^{10}}$$

(C_2 constant).

(5 points)

24. The separation between neighboring Na^+ and Cl^- ions in a crystal of NaCl is 0.281 nm, whilst the separation between neighboring Na^+ ions in metallic sodium is 0.372 nm. Given that the ionic radius of Cl^- is 0.181 nm, determine the radius of the Na^+ ions in each case. Explain, why the values are different. (3 points)
25. If the length of a covalent bond between two carbon atoms is 0.154 nm, estimate the length of a polyethylene molecule which contains 25000 CH_2 monomers. (3 points)
26. Estimate the number of carbon atoms in a diamond of mass 0.2 g. (Carbon has a molar mass of 12 g mol^{-1} .) (3 points)
27. The potential energy between two simple, neutral molecules at the separation r is given by

$$E(r) = -C_1 \frac{r_0^6}{r^6} + C_2 \frac{r_0^{12}}{r^{12}}.$$

By obtaining an expression for the force, determine the relationship between the constants C_1 and C_2 . The potential energy can also be written in an alternative form:

$$E(r) = 4E_b \left[\left(\frac{\hat{r}}{r} \right)^{12} - \left(\frac{\hat{r}}{r} \right)^6 \right].$$

Show that the constant \hat{r} is related to the equilibrium distance r_0 by $\hat{r} = 2^{-1/6} r_0$ and E_b is the binding energy.

- (5 points)
28. What is the electron configuration of an atom? Describe how you would determine the electron configuration of silicon (atomic number 14) and iron (atomic number 26). What is the reason that the configuration of iron does not fully meet your expectations? (4 points)
29. **(S1)** Calculate the angles between the bonds in a methane molecule. (3 points)
30. Explain how Bohr's model of the atom is based on the concept of energy quanta. (3 points)
31. **(E1)** Use internet resources* to provide an introduction to the classification of materials.

*e. g. http://www.ccm.udel.edu/Personnel/homepage/class_web/Lecture%20Notes/lecturenotes.htm

2 Crystal lattices

1. What is the atomic radius in face centered and body centered cubic structures if the lattice constant is 0.1 nm?
(4 points)
2. **(S2)** Calculate the fraction of the volume of the unit cell actually occupied by atoms for the three cubic structures.
(5 points)
3. Show that the Madelung constant for a one-dimensional array of ions of alternating sign with a distance a between the ions is $2 \ln 2$.
(5 points)
4. **(S2)** Draw the planes with the Miller indices (112) , $1\bar{1}0$, and $(\bar{1}21)$. What are the intersection points with the x , y , and z axes?
(4 points)
5. **(S2)** Determine the maximum radius of a sphere which can be placed into a body-centered cubic structure without affecting the positions of the other spheres.
(3 points)
6. A plane in a cubic lattice with primitive vectors \mathbf{a} , \mathbf{b} , and \mathbf{c} has intercepts with the coordinate axes at $2\mathbf{a}$, $-\mathbf{b}$, and \mathbf{c} . Use Miller indices to label the lattice plane and the direction perpendicular to the plane.
(3 points)
7. Calculate the packing density for a hexagonal closed packed structure.
(3 points)
8. What is the maximum ratio of radii r_-/r_+ which can have ionic crystals in the
 - a) CsCl and
 - b) NaClstructures?
(5 points)
9. **(R1)** Find all symmetry elements of the C_2H_6 molecule.
(5 points)

10. An fcc structure with the lattice constant a is given.
- Draw the lattice with the primitive unit cell.
 - Calculate the length of the primitive lattice vectors.
 - How many atoms contains the primitive, how many the conventional fcc unit cell?
- (3 points)
11. Determine the ratio of the lattice constants c and a for a hexagonal closed packed crystal structure. Compare the result with the c/a value of the following elements: He: 1.633, Mg: 1.623, Ti: 1.586, Zn: 1.861. What might be the reason for the deviations from the ideal value?
- (5 points)
12. Draw five different primitive unit cell into a two-dimensional rectangular lattice.
- (2 points)
13. What is the meaning of Miller indices? What indicates $\{110\}$?
- (2 points)
14. Determine the Madelung constant for a linear arrangement of positive and negative ions.
- (4 points)
15. Given is a cubic unit cell. Label all six faces with Miller indices (hkl). How do you label the corresponding family of planes?
- (3 points)
16. The origin of a simple cubic lattice with the lattice parameter a is put in a lattice point. The basic translation vectors are along the cartesian axes. Determine the Miller indices for a plane intersecting the x axis at $4a$, the y axis at $3a$, and the z axis at $2a$.
- (2 points)
17. Define the terms short-range and long-range order and explain the differences between crystalline, amorphous, and liquid states.
- (3 points)
18. **(E2)** Discuss the relationship between the structure, the properties and the processing of materials*.

*Use e. g. [1] or corresponding internet resources.

3 Determination of crystal structures

1. Determine the maximum wavelength for which Bragg reflection can be observed from a crystal with an atomic separation of 0.2 nm.
(2 points)
2. The X-ray wavelength used to obtain the data in Fig. 3.1 are 0.15393 (denoted $K\alpha$) and 0.13902 nm ($K\beta$). Decide which of the peaks correspond to the $K\alpha$ radiation. Given that the order of the reflection $n = 1$ and the $K\alpha$ peak is at the angle $\Theta_B = 15.80^\circ$, determine a value of the plane separation d for the sodium chloride crystal used in this experiment. Assuming that there is no error in the measurement of Θ_B and that the width of the peak at half maximum intensity is 0.1° , estimate the uncertainty in the value of d .
(5 points)
3. A simple cubic crystal is illuminated with X-rays of wavelength 0.09 nm at a glancing angle. The crystal is rotated and the angles at which Bragg reflection occurs are measured. Which set of crystal planes will give the smallest angle for first-order reflection? If this angle is 8.9° determine the spacing between these crystal planes. At what angle will first-order reflection be obtained from the (110) crystal planes?
(4 points)
4. Determine the wavelength of an electron with a kinetic energy of 100 keV.
(3 points)
5. * Discuss the advantages and disadvantages of using electron microscopes in comparison with X-ray diffraction for determining the structure of a crystal.
(3 points)
6. (S3) X-rays are reflected at a set of lattice planes under the glancing angles of 3° and 9° in first-order diffraction. What is the separation of the net planes if the X-ray wavelength amounts to 0.1 nm.
(2 points)
7. Under which angle leaves an X-ray beam the crystal when it is diffracted in first order at the (110) planes. Take an fcc lattice with the lattice constant of 0.5 nm

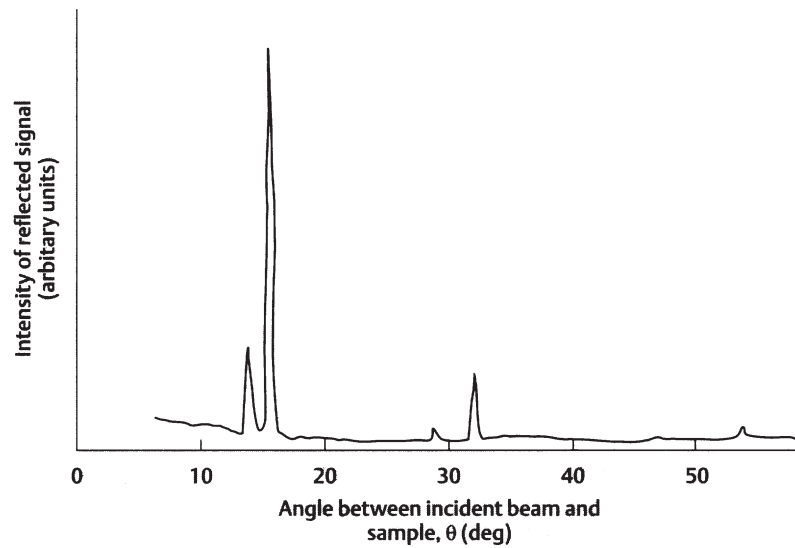


Figure 3.1: Result of X-ray diffraction from the (001) planes of NaCl. The graph shows the intensity of the diffracted signal as a function of the incident angle Θ . Note that the X-ray tube in this instance generates two wavelengths of X-rays, which explains the appearance of the double peak. Three sets of peaks can be seen, corresponding to the order of the diffraction $n = 1, 2, 3$. [6]

and an X-ray wavelength of 0.4 nm.

(2 points)

8. Evaluate the data of a powder diffraction experiment. The distance of a pair of lines amounts to 10 cm, while the camera radius is 24 cm. The wavelength of the X-rays used is 0.16 nm. What is the separation of the diffracting lattice planes in the crystal?
(3 points)
9. (S3) X-rays of the wavelength 0.15497 nm hit a silicon crystal. The first-order Bragg reflection occurs under the angle of 34.5° . What is the separation of the diffracting lattice planes, and are there reflections of higher order?
(3 points)
10. Show that the volume of the first Brillouin zone equals $(2\pi)^3 V_c$, where V_c is the volume of the primitive cell of the lattice. (The volume of a Brillouin zone corresponds to the volume spanned by the primitive translation vectors in the reciprocal space. Use the identity $(\mathbf{c} \times \mathbf{a}) \times (\mathbf{a} \times \mathbf{b}) = \mathbf{c} \cdot \mathbf{a} \times \mathbf{b} \cdot \mathbf{a}$. The primitive translation vectors in the Bravais lattice are \mathbf{a} , \mathbf{b} , and \mathbf{c} .)
(3 points)
11. (S3) The crystal structure of diamond has a basis of eight atoms in the conventional unit cell. Find the structure amplitude \tilde{F} related to this basis. Calculate

when $\tilde{F} = 0$ and discuss the conditions for h , k , and l of allowed reflections.
(5 points)

12. Define the term Brillouin zone!
(2 points)
13. **(R1)** A crystal with a simple-cubic structure ($a = 0.31$ nm) is irradiated with X-rays of the wavelength $\lambda = 0.31$ nm. Determine all lattice planes which fulfill the Bragg condition. Calculate for every reflection the Bragg angle.
(4 points)
14. What is the difference between the reflection of X-rays and the reflection of visible light?
(4 points)
15. Calculate the energy and the momentum of a photon, an electron, and a neutron of the wavelength $\lambda = 0.1$ nm.
(2 points)
16. **(E3)** Explain X-ray diffraction in crystals using the Bragg equation. What is the difference between the "reflection" of X-rays at lattice planes and the reflection of visible light at the surface?
(5 points)
17. What describes the structure amplitude or the structure factor in X-ray diffraction?
(3 points)

4 Crystal defects

1. **(S4)** Supposed the energy to transfer an sodium atom from the interior of a sodium chloride crystal to its surface is 1 eV. Calculate the concentration of Schottky defects at 300 K.
(2 points)
2. Fig. 4.1 shows a microscopical image of a hexagonal growth spiral on the surface of a SiC crystal? Can you explain the formation of such a structure from dislocation theory?
(4 points)
3. Show that the lines of closed packing in fcc structures are $\langle 110 \rangle$ directions.
(4 points)
4. **(S4)** Draw an edge dislocation and indicate the dislocation line, the Burgers vector, and the slip plane.
(3 points)
5. **(R1)** Give the number of octahedral and tetrahedral interstitialcies per unit cell in the fcc and bcc structure. Calculate the size of these positions in relation to the size of atoms on lattice sites.
(5 points)
6. **(S4)** Give the function of the concentration of vacancies on the temperature. Show a suitable graphical representation for different formation energies.
(2 points)
7. **(R2)** Explain the term dislocation and its role in plastic deformation of crystals.
(5 points)
8. What is a dislocation and what quantities are used to characterize such a defect?
(4 points)
9. **(E4)** Discuss the different dislocation types and the significance of dislocations in matter. What are the most important physical quantities to characterize such defects?*

(6 points)

*Use e. g. [1] Sections 4.1–4.3 or other solid-state textbooks.

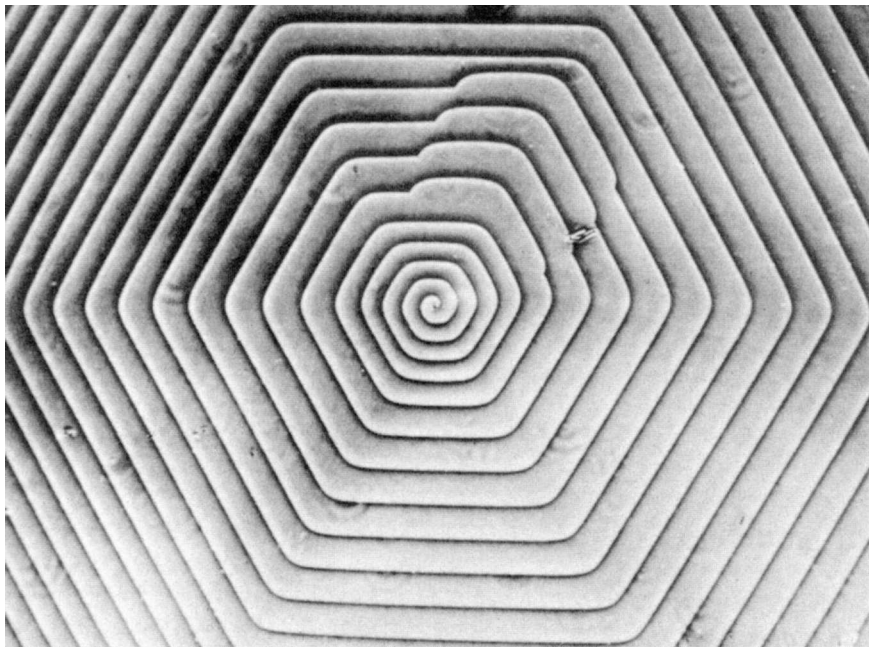


Figure 4.1: Growth spiral on a SiC crystal [3]

5 Phase transitions

1. **(S5)** Determine the degrees of freedom in a Cu–Ni (40 %) alloy at 1300 °C, 1250 °C, and 1200 °C. Use the phase diagram of Fig. 5.1. Use Gibbs phase rule for the condition of constant pressure.
(3 points)
2. **(S5)** Give an interpretation of the cleaning effect of crystals by float-zone melting in terms of a phase diagram of two completely miscible components.
(5 points)
3. **(R3)** Which of the following two-component systems may have a non-limited solubility according to the Hume–Rothery rules?
 - a) Au–Ag,
 - b) Al–Au,
 - c) Al–Cu,
 - d) Mo–Ta,
 - e) Nb–W,
 - f) Mg–Zn,
 - g) Mg–Cd.
(4 points)
4. **(S5)** Determine the liquidus temperature, the solidus temperature, and the temperature of solidification of NiO–MgO ceramics of the compositions given below. Use Fig. 5.2.
 - a) NiO–MgO(30 mol%),
 - b) NiO–MgO(45 mol%),
 - c) NiO–MgO(60 mol%),
 - d) NiO–MgO(85 mol%).
(4 points)
5. Determine the number of phases and their composition in a NiO–MgO ceramics of the compositions at 2400 °C given below. Use Fig. 5.2.

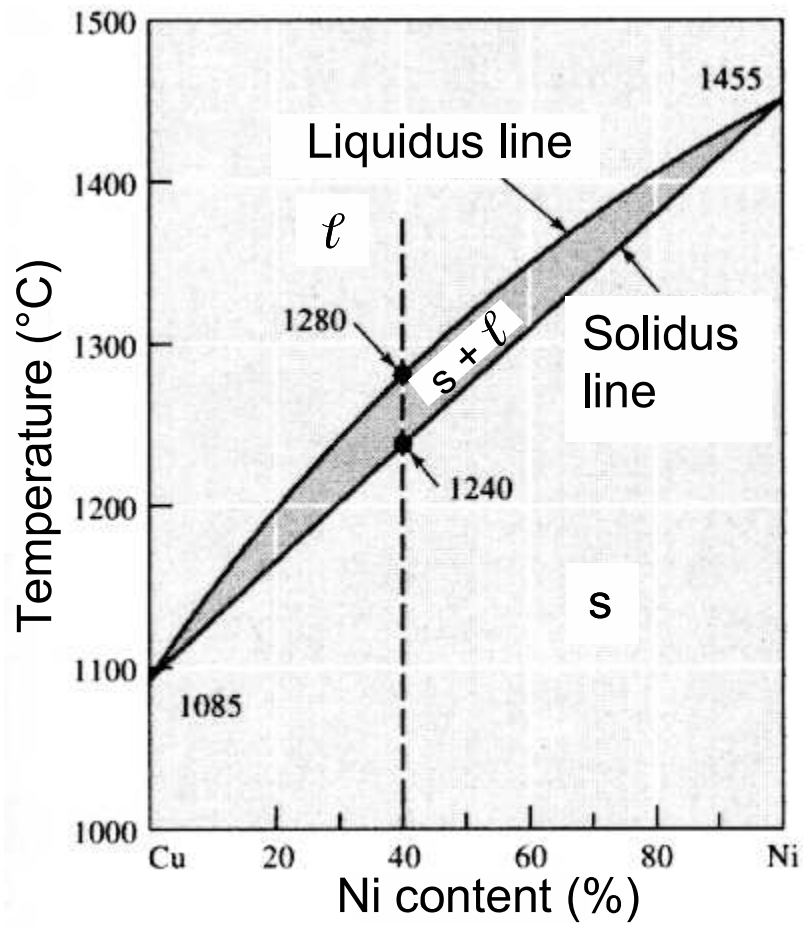


Figure 5.1: Cu-Ni phase diagram [1]

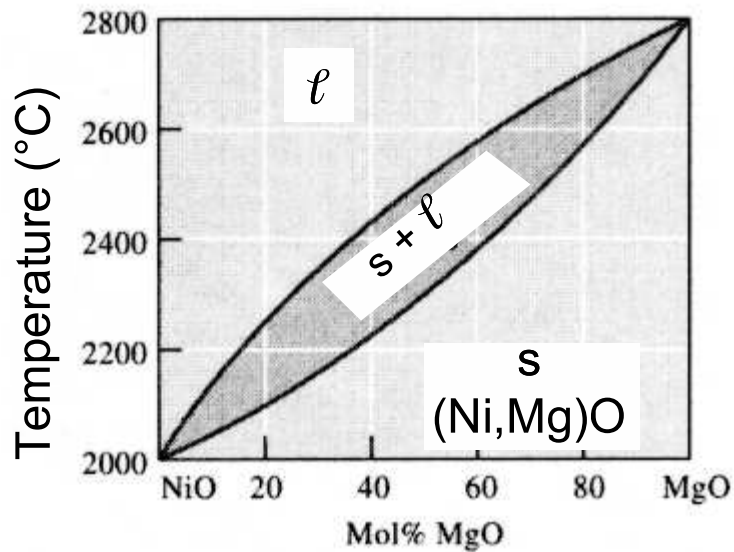


Figure 5.2: NiO–MgO phase diagram [1]

- a) NiO–MgO(30 mol%),
- b) NiO–MgO(45 mol%),
- c) NiO–MgO(60 mol%),
- d) NiO–MgO(85 mol%).

(4 points)

6. How many grams of nickel must be added to 500 g of copper in order to get an alloy with a liquidus temperature of 1350 °C? What is the ratio of the amount of Ni and Cu atoms?

(4 points)

7. Use Gibbs phase rule to explain the triple point of water.

(2 points)

8. Explain the phase diagram of two totally miscible metals? What determined their miscibility?

(4 points)

9. **(E5)** Examine synthesis, processing, and application of ceramic materials.*

(6 points)

*e. g. http://www.ccm.udel.edu/Personnel/homepage/class_web/Lecture%20Notes/lecturenotes.htm

6 Mechanical properties of solids

1. **(S6)** Using the data of Tab. 6.1, determine the strain produced when a mass of 1000 kg is suspended from a steel cable of diameter 1 cm.
(2 points)
2. Use the values of Tab. 6.1 for Young's modulus \tilde{E} and Poisson's ratio $\tilde{\nu}$ to calculate values of the shear modulus \tilde{G} and the bulk modulus \tilde{K} for aluminum and iron. Compare your results with the values in the Table and give a possible explanation for the discrepancies between the figures.
(3 points)
3. **(S6)** A lift cable of diameter 2 cm has a yield stress of $2 \cdot 10^8 \text{ Nm}^{-2}$. Assuming that the empty lift has a mass of 150 kg and that the average mass of a person is 70 kg, determine the maximum number of people that can be carried in the lift given that the safe operation limit is 20 % of the yield stress.
(3 points)
4. Calculate the stress required to break a bar of aluminum by brittle fracture assuming that the most serious surface cracks are of depth $1 \mu\text{m}$ and have a tip radius of curvature of 1 nm. Hence, using the data in Tab. 6.1, explain why aluminum undergoes plastic deformation at room temperature.
(3 points)
5. Given that the yield stress of glass is considerably higher than that of steel (see Tab. 6.1), explain why glass cables are not used in load-bearing applications.
(3 points)
6. **(S6)** Describe the types of deformation that occur for each of the materials listed in Tab. 6.1 and sketch stress-strain diagrams in each case.
(3 points)
7. **(R3)** A polymer rod with a cross section of $2.5 \cdot 5.0 \text{ cm}^2$ and a length of 40 cm elongates under load to a length of 40.5 cm. The elasticity modulus \tilde{E} amounts to $4 \cdot 10^3 \text{ Nmm}^2$. What is the force required for the elongation?
(2 points)
8. A load of $1.8 \cdot 10^5 \text{ N}$ should be raised with a steel cable of a diameter of 3 cm and a length of 15 m. Young's modulus of steel is given in Tab. 6.1. To what length the cable elongates under the given load?
(2 points)

Table 6.1: Typical values of Young's modulus \tilde{E} , the shear modulus G , the bulk modulus \tilde{K} , Poisson's ratio $\tilde{\nu}$, the yield point σ_S , the yield strain ϵ_S , the breaking stress σ_F , and the breaking strain ϵ_F . Note that measured values may differ considerably from the figures in the table depending on parameters such as the impurity content in the sample [Turton:2000].

	\tilde{E} (GPa)	G (GPa)	\tilde{K} (GPa)	$\tilde{\nu}$	σ_S (MPa)	ϵ_S (%)	σ_F (MPa)	ϵ_F (%)
Aluminum	70	24	72	0.33	26	0.04	30	25
Steel	210	84	170	0.29	200	0.1	450	30
Glass	75	23	41	0.22	600	0.8	600	0.8

9. A cylindrical Ti rod with a diameter of 10 mm and a length of 30 cm is loaded under the tension of $2.2 \cdot 10^3$ N. The yield stress of the material amounts to 345 Nmm^{-2} . Young's modulus is $1.1 \cdot 10^5 \text{ Nmm}^{-2}$ and Poisson's constant 0.30. Determine the length and the diameter of the rod under load.
(4 points)
10. According to the bonding strength, metals should be rather soft. Explain, why usually metals show a considerable strength. What are the underlying physical mechanisms?
(4 points)
11. **(E6)** Explain the plastic deformation of single crystals and polycrystals.
(6 points)

7 Lattice vibrations

1. When we find a frequency gap in the vibrational spectra (phonon spectra)?
(2 points)
2. Why we need for the description of the vibrational properties of a crystal only wave vectors \mathbf{K} from the first Brillouin zone?
(2 points)
3. * Define the group velocity of phonons. What is obtained for the long-wave border case?
(3 points)
4. (S7) For small temperatures T the specific heat capacity of metals is given as a sum of vibrational and electronic contributions, $c_V = C_1 T + C_2 T^3$. The values in Tab. 7.1 have been measured for zinc. Determine the constants C_1 and C_2 , and calculate the Debye temperature of zinc. At what temperature the vibrational part of the heat capacity is stronger than the electronic part?
(5 points)
5. (S7) Calculate within the Debye model the molar heat capacity of copper (Debye temperature of 343 K) at the boiling temperature of helium (4.2 K).
(2 points)
6. What is a phonon?
(2 points)
7. (S7) For a system executing simple harmonic motion with an equation of motion of $m \frac{d^2 u}{dt^2} = -\gamma_s u$ (u displacement, γ_s spring constant, m mass, t time), show that the angular frequency of the oscillation is $\Omega = \sqrt{\gamma_s/m}$.
(3 points)

Table 7.1: Measured molar specific heat capacity $c_V = f(T)$ of zinc

T/K	0.6	0.8	1.0	1.4	2.0
$c_V/\text{mJ mol}^{-1} \text{K}^{-1}$	0.402	0.548	0.706	1.063	1.745

8. Show that the expression for the internal energy

$$U_c = 3N_A \frac{\hbar\Omega}{\exp \frac{\hbar\Omega}{k_B T} - 1}$$

(N_A Avogadro constant, \hbar Planck's constant, Ω angular frequency, k_B Boltzmann constant, T temperature)

reduces to the classical value of $U_c = 3RT$ when $k_B T \gg \hbar\Omega$. Explain why we have the classical result even though we have treated the system using quantum theory.

(4 points)

9. Determine the nodes of the equation $\psi = \sin n\pi/L$ in the range of the length $x = 0$ to $x = L$ for the cases $n = 1, 2, 3$.

(2 points)

10. **(R3)** Use the Debye temperature of $\theta_D = 345$ K to estimate the minimum vibrational wavelength in copper. The speed of sound in copper is about 4000 m/s. Compare your result with the atomic spacing, which is about 0.256 nm.

(3 points)

11. What characterizes the Debye temperature?

(2 points)

12. **(E7)** Discuss the experiments of B. AUDOLY and S. NEUKIRCH (IgNobel prize winner 2006) about the formation of deformation waves in spaghetti and their breaking behavior.*

(6 points)

*<http://www.lmm.jussieu.fr/spaghetti/index.html>

8 Electrons in crystals

1. Determine the average thermal velocity of a conduction electron in a metal at a temperature of 295 K. Assuming that the mean free path of the electrons is about 1 nm, calculate the average time between collisions.
(3 points)
2. Use the relaxation time of $\tau_r = 8.2 \cdot 10^{-15}$ s to determine the mobility and drift velocity of an electron in a metal in an electric field of 10 V/m at 295 K. Explain why the drift velocity is much smaller than the thermal velocity.
(4 points)
3. **(R3)** Show that the microscopic form of Ohm's law $J_e = \sigma_e \mathcal{E}$ is equivalent to the more familiar form $U = \mathcal{R}I$ (J_e magnitude of the current density, σ_e conductivity, \mathcal{E} magnitude of the electric field vector, U voltage, \mathcal{R} resistance, I current).
(3 points)
4. **(S8)** A potential difference of 0.3 V exists between the ends of a copper wire of length 5 m. If the cross-sectional area of the wire is 2.5 mm^2 , calculate within the Drude model the mobility and the drift velocity of the electrons in the wire. The conductivity of copper is $6.45 \cdot 10^7 \Omega^{-1} \text{ m}^{-1}$, the number of valence electrons $8.5 \cdot 10^{28} \text{ m}^{-3}$. Also determine the net number of electrons that pass through a given cross section of the wire in 1 s.
(5 points)
5. Show that the Fermi–Dirac equation predicts the same distribution as shown in Fig. 8.1.
(3 points)
6. **(S8)** Using the Fermi–Dirac distribution \tilde{p} , determine the values of energy $E - E_F$ (E_F is the Fermi energy) corresponding to $\tilde{p} = 0.95$ and $\tilde{p} = 0.05$ at a temperature of 300 K.
(3 points)
7. Determine the velocity of a conduction electron at the Fermi energy in copper and aluminum. The Fermi energy of Cu is equal to 7.00 eV and of Al 11.58 eV.
(3 points)
8. **(S8)** * Using the quantum model of conductivity describe what happens to the resistivity of a metal as the temperature is lowered towards absolute zero, In

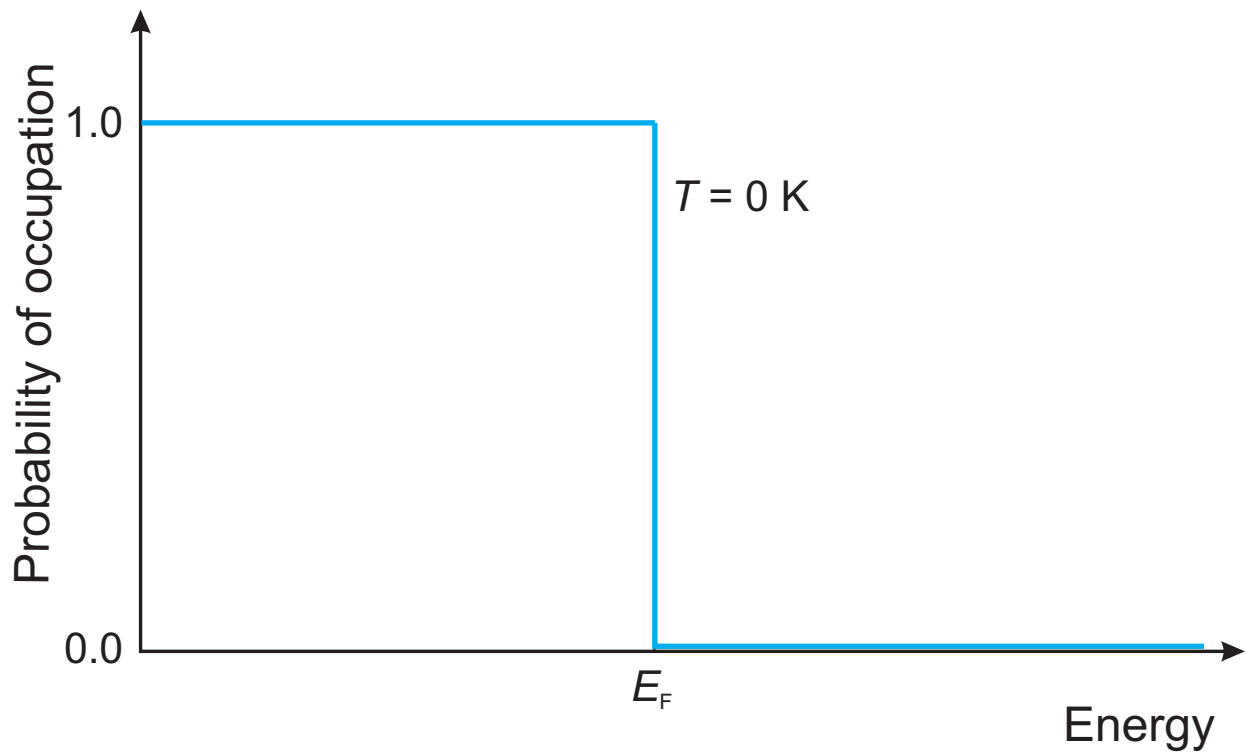


Figure 8.1: The probability distribution for a system of electrons at 0 K. The states are occupied up to the Fermi energy E_F .

particular, does this theory predict that the resistivity goes to zero or remains finite at $T = 0\text{K}$? Give reasons for your answer.

(5 points)

9. Determine the value of the Wiedemann–Franz constant C for copper (thermal conductivity $\Lambda = 400\text{W m}^{-1}\text{K}^{-1}$, electrical conductivity $\sigma_e = 6.45 \cdot 10^7\text{ }\Omega\text{m}^{-1}$ at 273 K), aluminum ($\Lambda = 230\text{W m}^{-1}\text{K}^{-1}$, electrical conductivity $\sigma_e = 4.00 \cdot 10^7\text{ }\Omega\text{m}^{-1}$ at 273 K), and gold ($\Lambda = 310\text{W m}^{-1}\text{K}^{-1}$, electrical conductivity $\sigma_e = 4.88 \cdot 10^7\text{ }\Omega\text{m}^{-1}$ at 273 K).
(3 points)
10. The specific resistivity of InAs is equal to $3 \cdot 10^{-4}\text{ }\Omega\text{m}$. Assuming an electron mobility of $\mu = 3.3\text{ m}^2\text{V}^{-1}\text{ s}^{-1}$ calculate the density of conduction electrons n_e at room temperature.
(3 points)
11. **(E8)** Explain in the reciprocal space (\mathbf{k} -space or Fourier space) the formation of the energy gap in the band structure. Describe the differences of metals and semiconductors.
(6 points)
12. ** In semiconductor physics, we speak about heavy and light holes. Do you have an idea from band theory what could be meant?
(4 points)
13. Characterize the electrical conductivity of silicon and copper over the whole temperature range of the solid state. What are the dominating mechanisms?
(3 points)

9 Dielectric properties

1. **(S9)** The capacitance of a parallel plate capacitor increases from $0.085 \mu\text{F}$ to $0.195 \mu\text{F}$ when a sheet of polyethene is placed between the plates. Use this information to determine the dielectric constant of polyethene.
(2 points)
2. **(R3)** Determine the dipole moment and the displacement of the centroids of positive and negative charge for a neon atom in an electric field of $5 \cdot 10^4 \text{ V/m}$. The atomic polarizability of neon is $4.3 \cdot 10^{-41} \text{ F m}^2$.
(4 points)
3. **(S9)**
 - a) Estimate the dipole moment of a hydrogen chloride molecule assuming that there is a complete transfer of the electron from the hydrogen atom to the chlorine atom. The separation of the hydrogen and the chlorine nuclei is 0.128 nm .
 - b) Given that the measured dipole moment of a hydrogen chloride molecule is $3.3 \cdot 10^{-30} \text{ C m}$, determine the actual amount of charge transferred from the hydrogen to the chlorine atom.
(4 points)
4. Calculate the displacement d between the lattices of positive and negative ions in barium titanate (Fig. 9.1) when the polarization is saturated. The molar volume of BaTiO_3 is $3.8 \cdot 10^{-5} \text{ m}^3$ and the saturation polarization \mathcal{P}_s is 0.26 C m^{-2} .
(4 points)
5. **(S9)** If the type of plastic used for insulating electric wires has a breakdown field of $5 \cdot 10^7 \text{ V/m}$, determine the minimum thickness required to insulate a domestic household supply assuming a voltage of 240 V . Compare this figure with the actual thickness of insulation used in practice, which is typical about 0.5 mm .
(4 points)
6. Explain possible polarization mechanisms in crystals.
(4 points)

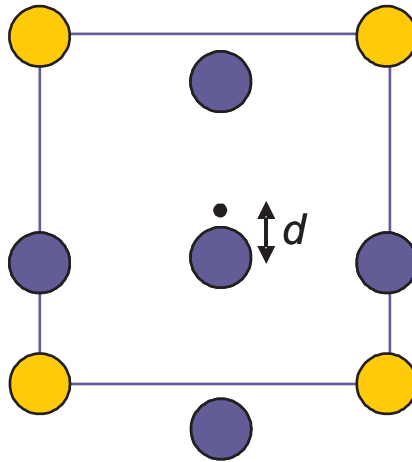


Figure 9.1: Structure of barium titanate indicating the displacement of the negative and the positive ions (Black: Ti, red: Ba, blue: O ions).

7. What is the piezoelectric effect and how it can be explained by the structure of the material?
(4 points)
8. *What materials in Fig. 9.2 are suitable for gate dielectrics in microprocessors? Discuss possible problems.
(4 points)
9. What materials in Fig. 9.2 provide a good stability against electrical breakdown and why?
(3 points)
10. (E9) Explore the role of high- k and low- k materials (*i. e.* materials with a high and a low dielectric constant).
(6 points)

*<http://www.materialstoday.com>

G. BERSUKER, P. ZEITZOFF, G. BROWN, H. R. HUFF: Dielectrics for future transistors. *Mater. today* **7** (2004) 26–33. D. SHAMIRYAN, T. ABELL, F. IACOPI, K. MAEX: Low- k dielectric materials. *Mater. today* **7** (2004) 34–39. B. D. HATTON, K. LANDSKRON, W. J. HUNKS, M. R. BENNETT, D. SHUKARIS, D. D. PEROVIC, G. A. OZIN: Materials chemistry for low- k materials. *Mater. today* **9** (2006) 22–31. B. H. LEE, J. OH, H. H. TSENG, R. JAMMY, H. HUFF: Gate stack technology for nanoscale devices. *Mater. today* **9** (2006) 32–40.

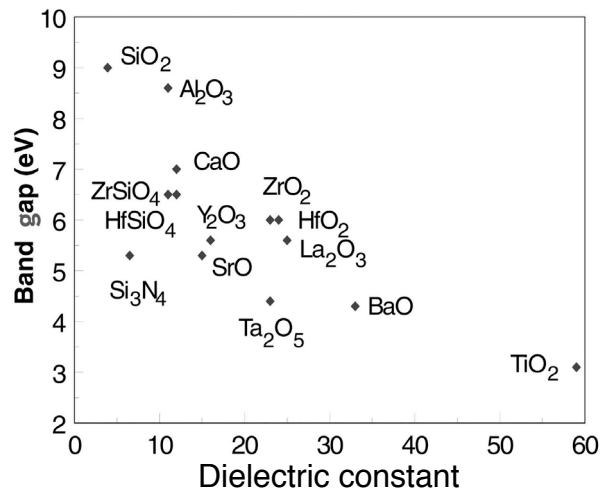


Figure 9.2: Variation of the dielectric constant with the band gap in binary oxides [2]

10 Optical properties

1. The intensity of a phosphorescent material is reduced to 90 % of its original intensity after $1.95 \cdot 10^{-7}$ s. Determine the time required for the intensity to decrease to 1 % of its original intensity.
(3 points)
2. **(S10)** Determine whether an incident beam of photons with a wavelength of 750 nm will cause luminescence in the materials given in Tab. 10.1.
(3 points)
3. Which, if any, of the semiconducting compounds listed in Tab. 10.1 are capable of producing an infrared laser beam?
(3 points)
4. **(S10)** A beam of photons strikes a material at an angle of 25° to the normal of the surface. Which, if any, of the materials listed in Tab. 10.2 could cause the beam of photons to continue at an angle of 18 to 20° from the normal of the material's surface?
(3 points)
5. **(S10)** A laser beam passing through air strikes a 50 mm-thick polystyrene block at a 20° angle to the normal of the block. By what distance is the beam displaced from its original path when the beam reaches the opposite side of the block?
(4 points)
6. **(R3)** A material has a linear absorption coefficient of $5.91 \cdot 10^4 \text{ m}^{-1}$ for photons of a particular wavelength. Determine the thickness of the material required to absorb 99.9 % of the photons.
(3 points)
7. A glass fiber is with the refraction index $\hat{n} = 1.5$ is coated with PTFE (polytetrafluoroethylene – teflon). Calculate the maximum angle that a beam of light can deviate from the axis of the fiber without escaping from the inner portion of

Table 10.1: Energy gap E_g at room temperature for semiconducting compounds

Material	ZnO	GaP	GaAs	GaSb	PbS
E_g/eV	3.20	2.26	1.43	0.67	0.41

Table 10.2: Index of refraction \hat{n} of selected materials for photons of wavelength 589 nm [1]

Material	Air	Water	Quartz	Polytetrafluoroethylene	Polystyrene
\hat{n}	1.00	1.33	1.535	1.35	1.60

the fiber.

(4 points)

8. What voltage must be applied to a tungsten filament to produce a continuous spectrum of X-rays having a minimum wavelength of 0.09 nm.
(3 points)
9. What type of electromagnetic radiation (ultraviolet, infrared, visible) is produced from pure germanium?
(2 points)
10. Determine the wavelength of photons produced when electrons excited into the conduction band of indium-doped silicon
 - a) drop from the conduction band to the acceptor band and
 - b) then drop from the acceptor band to the valence band.

Indium has an acceptor level in Si (energy gap 1.11 eV) of 0.16 eV above the valence band.
(5 points)
11. What is the physical meaning of luminescence?
(3 points)
12. Explain the formation of characteristic X-rays.
(3 points)
13. * Why is the absorption coefficient of a semiconductor with an indirect bandgap very small?
(4 points)
14. What can be said about the bandgap of gold? What are the consequences?
(3 points)
15. Explain the occurrence of a short wavelength limit for the continuous X-ray bremsstrahlung spectrum.
(2 points)
16. **(E10)** Discuss the problems and chances to manufacture light emitting devices (LEDs, lasers) based on silicon. What strategies in topical research are pursued to develop such devices?
(6 points)

17. ** Supposed you are asked to construct an X-ray microscope. What are the basic problems?
(6 points)

11 Magnetic properties

1. (S11) Check that the equations

$$\chi_m \mathbf{B}_0 = \mu_0 \mathbf{M},$$

$$\mathbf{B} = \mathbf{B}_0 + \mu_0 \mathbf{M}$$

(χ_m magnetic susceptibility, \mathbf{B}_0 external magnetic field, μ_0 permeability of the vacuum, \mathbf{M} magnetization) are dimensionally correct.

(2 points)

2. (S11) Show that for a filled electron subshell in an atom the total spin and orbital angular momentum, \hat{S} and \hat{L} , are zero.

(4 points)

3. (R3) Show that if an electron subshell is half filled then the orbital angular momentum $\hat{L} = 0$.

(3 points)

4. Determine the values of the total spin, orbital angular momentum, and the total angular momentum, \hat{S} , \hat{L} , and \hat{J} , for

a) Ni^{2+} , which has eight electrons in the 3d subshell, and

b) Gd^{3+} , which has seven electrons in the 4f subshell. Note that the f subshell corresponds to $l = 3$.

(4 points)

5. Prove that the term $B\mathbf{B}_0/\mu_0$ has units of energy per volume.

(2 points)

6. What is diamagnetism and how a diamagnet behaves in the magnetic field?

(3 points)

7. (E11) Explain the GMR effect and its application in electronic devices.

(6 points)

12 Superconductivity

1. **(S12)** Determine the maximum current density in a lead wire of diameter 4 mm at a temperature of 4.2 K if the wire is to remain superconducting. The relevant values for lead are: critical temperature $T_c = 7.19$ K, and critical magnetic field $B_{\text{crit}} = 8.03 \cdot 10^{-2}$ T. Note that the magnetic field due to a current I in a wire is given by

$$B = \frac{\mu_0 I}{2\pi r},$$

where r is the distance from the center of the wire and μ_0 the permeability of the vacuum.

(4 points)

2. **(S12)** A superconductor with a critical temperature of 20 K obeys the equation

$$\mathbf{B}_{\text{crit}}(T) = \mathbf{B}_{\text{c0}} \left[1 - \left(\frac{T}{T_c} \right)^2 \right]$$

At the temperature $T = 4.2$ K the critical field \mathbf{B}_{crit} is found to be 30 T. Determine the maximum operating temperature if the material is used to make a 10 T superconducting magnet ($\mathbf{B}_{\text{c0}} = \mathbf{B}_{\text{crit}}(0 \text{ K})$, T_c critical temperature).

(2 points)

3. A current is left to flow in a superconducting loop for a period of 2.5 years. At the end of this time the magnitude of the current is found to be unchanged within the experimental uncertainty of 1 %. Use this information to determine a lower limit for the relaxation time. Given that the relaxation time for a normal metal at room temperature is about 10^{-14} s, determine a lower limit for the ratio of the conductivity of a superconductor to that of a normal metal. You may assume that the number density of electrons is the same in each case.

(3 points)

4. A small magnet is placed on the surface of a disc of normal material. Explain what happens when the disc is cooled down so that it becomes superconducting. Can this be explained from a classical viewpoint if we simply treat the superconductor as a material which has zero resistivity?

(2 points)

5. **(R3)** A small magnet of mass 10 g and magnetic moment $m_m = 0.3$ J/T levitates above the surface of a thin disc of type I superconductor. Determine the height

of the magnet above the surface given that the magnetic potential energy for a magnet at distance x from a perfect diamagnet is

$$E = \frac{\mu_0 m_m^2}{32\pi x^3},$$

where μ_0 is the permeability of the vacuum. How will your answer change if the disc is replaced by a type II superconductor in the mixed state?

(5 points)

6. Nb₃Sn is a type II superconductor with an upper critical field of 21 T at 4.2 K. Determine the critical current density for a 1 mm diameter wire of Nb₃Sn at 4.2 K assuming that the only limitation is the magnetic field produced by the current. The measured critical current density turns out to be $1 \cdot 10^9 \text{ A m}^{-2}$. Explain why there is a discrepancy between these results. Note that the magnetic field due to a current I in a wire is given by

$$B = \frac{\mu_0 I}{2\pi r},$$

where r is the distance from the center of the wire and μ_0 the permeability of the vacuum.

(5 points)

7. What is the difference between type I and type II superconductors?
(4 points)
8. **(E12)** Discuss the physical background and possible applications of high-temperature superconductors.*
(6 points).

*e.g. <http://www.atz-gmbh.com>

13 Semiconductors

1. The intrinsic carrier concentrations n_i of various semiconductors at $T = 300$ K are given together with the band gaps E_g in Tab. 13.1. Calculate the value of the constant C in the equation

$$n_i = C \exp\left(-\frac{E_g}{2k_B T}\right)$$

(k_B Boltzmann constant).

(3 points)

2. Use the equation

$$n_i = C \exp\left(-\frac{E_g}{2k_B T}\right)$$

to calculate the intrinsic carrier concentration n_i for diamond at $T = 300$ K. The band gap E_g of diamond amounts to 5.5 eV. The constant C has a value of 10^{25} cm^{-3} . k_B is the Boltzmann constant.

(3 points)

3. Determine the conductivity of silicon at temperatures of 30, 300, and 1000 K, given that the value of C in the equation for the intrinsic carrier concentration

$$n_i = C \exp\left(-\frac{E_g}{2k_B T}\right)$$

(k_B Boltzmann constant, $E_g = 1.11$ eV energy gap)

is $2 \cdot 10^{25} \text{ m}^{-3}$, and the mobility is $0.135 \text{ m}^2 \text{ V}^{-1} \text{ s}^{-1}$. Assume that C and the mobility are constant with temperature T and consider only the conductivity due to conduction electrons. Comment your findings.

(5 points)

Table 13.1: Intrinsic carrier concentrations n_i and band gaps E_g at room temperature

Material	n_i (m^{-3})	E_g (eV)
Ge	$3 \cdot 10^{19}$	0.67
Si	$1 \cdot 10^{16}$	1.11
GaAs	$2 \cdot 10^{13}$	1.43

4. The electrical conductivity of a material is given by the equation

$$\sigma_e = en_e\mu_e,$$

where n is the concentration of electrons and μ_e the mobility. By considering how n_e and μ_e vary as a function of temperature, compare the temperature dependence of conductivity of a semiconductor with that of a metal.

(4 points)

5. Determine the conductivity of intrinsic silicon at 300 K given that the electron and hole mobilities are $0.135\text{ m}^2\text{V}^{-1}\text{s}^{-1}$ and $0.048\text{ m}^2\text{V}^{-1}\text{s}^{-1}$, respectively, and that the concentration of conduction electrons is $1 \cdot 10^{16}\text{ m}^{-3}$.
- (3 points)
6. Assuming that the electron and hole mobilities are constant with temperature, determine the temperature at which the conductivity of intrinsic germanium is double the value at 300 K.
- (4 points)
7. Gallium arsenide has a band gap of 1.43 eV at room temperature. If all of the gallium atoms are replaced with indium, the resulting crystal of indium arsenide has a band gap of 0.36 eV. Assuming that the band gap varies linearly between these two extremes, calculate the percentage of indium that must be used on an alloy of indium gallium arsenide in order to emit light with a wavelength of $1\ \mu\text{m}$.
- (5 points)
8. Explain why silicon is opaque, whereas diamond is transparent. (Hint: consider the minimum frequency of light that is absorbed in each case.)
- (3 points)
9. For an indirect gap semiconductor the difference in wave vector between an electron at the bottom of the conduction band and a hole at the top of the valence band is typically of the order of π/a , where a is the lattice constant. Determine this quantity for silicon for which the lattice constant is 0.357 nm and compare with the wave vector of a photon corresponding to the indirect band gap energy, $E_g = 1.11\text{ eV}$.
- (4 points)
10. a) Use Bohr's model to determine the radius of the donor electron orbit for a phosphorus atom in a silicon crystal.
- b) Estimate the number of silicon atoms in a sphere of this radius. The nearest neighbor separation in silicon is 0.357 nm.

(6 points)

11. Use Bohr's model to determine the energy of the donor state for a phosphorus impurity in germanium. The dielectric constant for Ge is 15.8.
(3 points)
12. Determine the concentration of conduction electrons in a sample of silicon if one in every million silicon atoms is replaced by a phosphorus atom. Assume that every phosphorus atom is singly ionized. Si has a molar mass of $0.028 \text{ kg mol}^{-1}$ and a density of 2300 kg m^{-3} .
(4 points)
13. Determine the conductivity at 300 K of a sample on n-type silicon with a donor concentration of $5 \cdot 10^{22} \text{ m}^{-3}$. Ignore the conductivity of the holes and assume that all of the donors are ionized. The mobility is $0.135 \text{ m}^2 \text{ V}^{-1} \text{ s}^{-1}$.
(3 points)

14. By considering the probability of an electron occupying a state at the valence band edge, show that the concentration of holes in a doped semiconductor is given by

$$p_h = C \exp\left(-\frac{E_F}{k_B T}\right),$$

where C is a constant, E_F the Fermi level, k_B the Boltzmann constant, and T the temperature.

(5 points)

15. A semiconductor has a donor concentration of $6 \cdot 10^{22} \text{ m}^{-3}$ and an acceptor concentration of $6 \cdot 10^{22} \text{ m}^{-3}$. Assuming that all of the impurities are ionized and that the intrinsic carrier concentration is $5 \cdot 10^{15} \text{ m}^{-3}$, calculate the concentration of conduction electrons and holes and identify which are the majority carriers and which are the minority carriers.
(5 points)
16. A sample of n-type silicon 1 cm wide (in the y direction) and 2 mm thick (in the z direction) is subject to a magnetic field along the z direction $B = 0.2 \text{ T}$. If the current in the sample is 1 mA and the Hall voltage (*i. e.* the voltage difference across the sample in the y direction) is $3 \cdot 10^{-4} \text{ V}$, determine the concentration of conduction electrons.
(4 points)
17. How the conductivity of a semiconducting material is controlled? Explain the basic formula for the conductivity σ_e and describe possible ways to influence σ_e .
(3 points)

14 Solid state devices

1. By considering the diffusion of holes across a p–n junction, show that the result is the same as that obtained by considering the diffusion of electrons.
(3 points)
2. Sketch the energy band profile and calculate the contact potential for a silicon p–n junction if the Fermi energy on the n-type side is 150 meV below the conduction band edge and the Fermi energy on the p-type side is 80 meV above the valence band edge. The band edge of silicon is 1.11 eV.
(3 points)
3. Estimate the current gain of an npn bipolar transistor if only 0.3 % of the conduction electrons that enter the base from the emitter recombine in the base region.
(3 points)
4. In 1995 MOSFET circuits containing 64 million devices with a minimum gate length of $0.35\ \mu\text{m}$ came into production. Assuming that the minimum feature size decreases by 11 % per year, determine when circuits with a gate length of $0.1\ \mu\text{m}$ will become available. Estimate the corresponding number of devices per circuit at this date assuming that the area of the circuit increases by 9 % per year.
(3 points)
5. If a MOSFET is scaled so that the linear dimensions are changed by $1/S$, the doping concentrations are changed by S , but the voltages remain constant, determine how this affects the switching time of the devices and power produced per unit area. Note that the electric field does not remain constant in this case.
(5 points)
6. If the dimensions of a MOSFET are scaled down by $1/S$, the doping concentration should be increased by S^3 in order to provide the same number of carriers in the source, gate, and drain regions. Consider the disadvantages of applying this type of scaling. Assume that the voltages are scaled by $1/S$.
(5 points)
7. If the band gap of GaAs is 1.42 eV, the band gap of AlGaAs containing 30 % is 1.80 eV, and the valence band offset is 0.14 eV, determine the magnitude of the conduction band offset. Sketch the alignment of the bands.
(2 points)

8. The band gap of the alloy $\text{GaAs}_{1-x}\text{P}_x$, where x is the proportion of P ions, is given approximately by

$$E_g = (1.42 + 1.3x) \text{ eV.}$$

- Calculate the proportion of P required to produce a material which emits red light with a wavelength of 680 nm.
- Determine the minimum wavelength of light that can be produced with this alloy given that $\text{GaAs}_{1-x}\text{P}_x$ is an indirect semiconductor for $x > 0.44$.

(4 points)

9. A superconductor quantum interference device (SQID) is constructed from a superconducting loop with a radius of 5 mm. If the current in the SQID can be measured to an accuracy of 1 %, determine the minimum change in magnetic field that can be detected with this instrument. Assume that the change in the supercurrent is directly proportional to the change in the magnetic field.

(4 points)

10. **(E14)** Discuss the further development of semiconductor microelectronics. Use the predictions of Moore's law and the International Technology Roadmap for Semiconductors.*

(6 points)

*<http://www.materialstoday.com>

W. ARDEN: Roadmap key challenges. *Mater. today* (2003) 40. A. DODABALAPUR: Organic and polymer transistors for electronics. *Mater. today* **9** (2006) 24. G. MARSH: Moore's law at the extremes. *Mater. Today* (2003) 28. S. E. THOMPSON, S. PARTHASARATHY: Moore's law: the future of Si microelectronics. *Mater. today* **9** (2006) 20.

15 Advanced materials

1. Coiled springs ought to be very strong and stiff. Si_3N_4 is a strong, stiff material. Would you select this material for a spring? Explain.
(2 points)
2. You would like to design an aircraft that can be flown by human power nonstop for a distance of 30 km. What types of material properties would you recommend? What materials might be appropriate?
(2 points)
3. You would like to select a material for the electrical contacts in an electrical switching device which opens and closes frequently and forcefully. What properties should the contact material possess? What type of material might you recommend? Would Al_2O_3 be a good choice?
(2 points)
4. You would like to be able to identify different materials without resorting to chemical analysis or lengthy testing procedures. Describe some possible testing and sorting techniques you might be able to use based on the physical properties of materials.
(2 points)
5. Determine the percentage change in the density that occurs when a monoatomic close-packed crystal, in which the atoms occupy 74 % of the volume, becomes an irregular close-packed liquid, in which the atoms occupy 64 % of the volume.
(3 points)
6. What are the advantages and problems of nanotechnology?
(4 points)

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