

1 Theoretical questions

(answer them in short and clear sentences including the necessary formulas when needed)

1. Describe the properties of ionic crystals!

Solution:

Ionic crystals

- they are rigid and brittle
- bad heat conductors
- bad electric conductors
- have high melting point
- are diamagnetic

2. What are the properties of covalent crystals?

Solution:

- rigid electronic structure
- hard materials
- bad heat conductors (there are no free electrons available)
- bad electric conductors (same reason)
- high frequency lattice vibrations (with excitation energies in the infrared (IR) range)
- they have a large electronic band gap therefore they are transparent for visible light

3. What are the properties of molecular crystals?

Solution:

- extreme weak bonding
- bad heat conductors
- bad electric conductors
- low melting point
- low boiling point
- easily compressible and deformable

4. What are the properties of an ionic crystals?

Solution:

- they are rigid and brittle
- bad heat conductors
- bad electric conductors
- high melting point
- diamagnetic

5. What do we call an atomic orbital? What is a molecular orbital?

Solution:

An atomic orbital is the wave function of the electron inside the atom. The molecular orbital is the same for a molecule. (In chemistry the same term may be applied to the region of space where the electron is found with suitable high (e.g. 90%) probability.)

6. Define short and long range ordering and the coordination number.

Solution:

- *Short range ordering: First- or second-nearest neighbors of an atom are arranged in the same structure. At distances that are many atoms away, however, the positions of the atoms are uncorrelated.*
- *Long range ordering: Once the positions of an atom and its neighbors are known at one point, the place of each atom is known precisely throughout the material.*
- *Coordination number: the number of nearest neighbors (the number of lattice points which are closest to a selected point) in a lattice.*

7. Define the concepts that are used in the description of crystal structures.

Solution:

The physical structure of the crystal is described by a system of geometrical points, the so called point lattice and the basis containing the atoms or molecules, which are located at every one of these geometrical points.

8. Define the conventional and primitive cells.

Solution:

- *The volume of space that when translated through all of the point lattice vectors just fills the complete space without overlap or without leaving voids is called a primitive cell or primitive unit cell. These are not unique. A primitive cell contains 1 lattice point.*
- *Those non-primitive unit cells that have all of the symmetry of the crystal are called conventional unit cells.*

9. Define the unit cell, primitive cell and conventional cell!

Solution:

A unit cell is a volume of space with which we can fill the entire space without overlap and without leaving voids. A primitive cell is a unit cell that contains only a single point. A conventional cell is a unit cell that has all the symmetries of the crystal

10. Describe at least three point defects in a crystal!

Solution:

Remark: It is enough to write down the names of the defects.

- *Vacancy or Schottky defects are lattice sites which would be occupied in a perfect crystal, but are vacant. In equilibrium all crystals must have them.*
- *Interstitial defects are atoms that occupy a site in the crystal structure at where there is usually no atom. They are generally high energy configurations.*
- *Frenkel pair or Frenkel defect. A nearby pair of a vacancy and an interstitial caused when an ion moves into an interstitial site and creates a vacancy.*
- *Substitutional atoms when a foreign (impurity) atom occupies a lattice position.*
- *Antisite defects. Occur in an ordered alloy or compound when atoms of different type exchange positions.*
- *Topological defects Regions in a crystal where the normal chemical bonding environment is topologically different from the surroundings.*

11. Describe the two main types of a metal-semiconductor junctions!

Solution:

Two kinds of junctions can be present. One is the (non-rectifying) voltage independent ohmic contact, the other one is the (rectifying) Schottky junction.

12. What are holes, and are they present in metals as well as in semiconductors?

Solution:

Holes are positive charge carriers in solids (both metals and semiconductors) which - apart from their opposite sign charge - behave exactly like electrons do. Conduction in a band can be described using either electrons or holes but not with both of them. In semiconductors holes are used in the valence band and electrons in the conduction band, because the other charges do not move.

13. Are there metals with holes as majority charge carriers instead of electrons? If there are then explain how is it possible, if there are not explain why!

Solution:

Yes Mg and Cd for instance have completely filled s-bands overlapped by an empty conduction band. Mobility of electrons in that band is lower than the mobility of the holes remaining in the valence band making hole current the dominant one as it is shown by the Hall effect.

14. What are Bloch-functions, and can they be constructed from localized electronic orbitals?

Solution:

Bloch functions are one electron functions which describe non interacting free electrons in a crystal. They wave functions in one dimension are of the form: $\psi(x) = u(x) e^{ikr}$, where $u(x)$ is a lattice periodic function. They are constructed from localized atomic orbitals in the tight binding model.

15. Does the Sommerfeld nearly free electron model explain the difference between metals and insulators? Explain!

Solution:

No. In the Sommerfeld model the solid is represented by a potential box with free electrons inside it. This model is not valid for insulators, where there are no free charge carriers.

16. Enumerate at least 5 possible symmetries of a crystal lattice. (The one common for all crystals must be included, otherwise the answer is void.)

Solution:

- translational symmetry - the most important one, as every crystal must have it
- 2, 3, 4, 6 -fold rotational symmetry (rotation by 180, 120, 90, 45° respectively)
- mirror symmetry - (reflection across a plane)
- inversion through a point (center of symmetry)
- improper rotation or rotoinversion - (may be defined as "combinations of rotation with a center of symmetry" OR "rotation about an axis and a reflection in a plane perpendicular to the axis" - OR "rotation and inversion in a point".)

(Each rotational symmetry is counted separately, so it is enough to mention them and the translational symmetry, but if they are only

referred to as 'rotational symmetry' that is worth only one. This case 4 symmetries are enough. 1-fold rotation doesn't count.)

17. Enumerate the phenomena that lead to the development of quantum physics.

Solution:

- Black body radiation
- (external) Photoelectric effect
- Compton effect
- Stability of atoms
- Line spectrum of atoms
- Frank-Hertz experiment

18. Give the formula to calculate the average value of an energy physical quantity O in a solid!

Solution:

$$\langle O \rangle = \int_{\text{all } \mathcal{E}} g(\mathcal{E}) f_{FD}(\mathcal{E}) d\mathcal{E} \quad (1.1)$$

19. How can a Bloch electron be moved outside the first Brillouin zone in direct and indirect gap semiconductors?

Solution:

- in an direct gap semiconductor: by colliding with or emitting a photon as the momentum of photon is negligible relative to the momentum of the electron
- in an indirect gap semiconductor: by colliding with or emitting a photon - this provides the energy and absorbing or emitting a phonon - which provides the momentum difference, because the momentum of photon, and the energy of the phonon are negligible relative to those of the electron

20. How can we determine the solution of the time-dependent Schrödinger equation from the solutions of the stationary equation?

Solution:

The eigenfunctions of the time dependent Schrödinger equation are the products of the eigenfunctions of the corresponding stationary Schrödinger equation and the function $e^{-E/\hbar t}$. Therefore the solution of the time dependent equation may be written as a linear combination of such products.

In 1D e.g.:

$$\psi(x, t) = \sum_E \phi_E(x) e^{-E/\hbar t}$$

21. How many Bravais lattices are there and is it possible that a lattice is not a Bravais lattice?

Solution:

There are 14 different Bravais lattices. The lattice of 2D hexagons does not form a Bravais lattice.

22. How many branches are in the dispersion relation of a 1 dimensional diatomic linear chain with a 2-atom basis and what are their characteristics?

Solution:

It has 1 acoustic and 1 optical branch. In the acoustic branch near $k \approx 0$ the atoms vibrate in phase, while in the optical branch their

relative phase is 90° . At the edges of the Brillouin zone the vibration of the two sub-chain of the different atoms is such that one sub-chain is vibrating while the other one is stationary.

23. How many branches does the diatomic linear chain dispersion relation have and what are their characteristics?

Solution:

It has one acoustic and one optical branch. In the acoustic branch near $k \approx 0$ the atoms vibrate in phase, while in the optical branch their relative phase is 90° . At the edges of the Brillouin zone the vibration of the two sub-chain of the different atoms is such that one sub-chain is vibrating while the other one is stationary.

24. How many branches does the dispersion relation of a 3 dimensional diatomic linear chain with a 2-atom basis have and what are their characteristics?

Solution:

It has 3 acoustic and $3N - 3$ optical branches. In the acoustic branches near $k \approx 0$ the atoms vibrate in phase, while in the optical branches their relative phase is 90° . At the edges of the Brillouin zone the vibration of the two sub-chain of the different atoms is such that one sub-chain is vibrating while the other one is stationary.

25. How many branches does the dispersion relation of a 3 dimensional diatomic linear chain with an n -atom basis have and what are their characteristics?

Solution:

It has 3 acoustic (1 longitudinal and 2 transverse) and $3n - 3$ optical ($n - 1$ longitudinal and $2n - 2$ transverse) branch. In the acoustic branches near $k \approx 0$ the atoms vibrate in phase, while in the optical branches their relative phase is 90° . At the edges of the Brillouin zone the vibration of the two sub-chain of the different atoms is such that one sub-chain is vibrating while the other one is stationary.

26. How many branches does the dispersion relation of the diatomic linear chain have and what are their characteristics?

Solution:

It has one acoustic and one optical branch. In the acoustic branch near $k \approx 0$ the atoms vibrate in phase, while in the optical branch their relative phase is 90° . At the edges of the Brillouin zone the vibration of the two sub-chain of the different atoms is such that one sub-chain is vibrating while the other one is stationary.

27. How many branches have the dispersion relation of a 1 dimensional diatomic linear chain with a 2-atom basis have and what are their characteristics?

Solution:

It has 1 acoustic and 1 optical branch. In the acoustic branch near $k \approx 0$ the atoms vibrate in phase, while in the optical branch their relative phase is 90° . At the edges of the Brillouin zone the vibration of the two sub-chain of the different atoms is such that one sub-chain is vibrating while the other one is stationary.

28. "In extrinsic semiconductors the number of the conduction electrons is equal to the number of valence band holes." Is this statement true or false and why?

Solution:

False. Extrinsic semiconductors have dopants (either donor or acceptor atoms present). The overwhelming majority of the charge

carriers come from these. Therefore n_c and p_v will differ.

29. Is it always true that the wave function of a system of electrons must be antisymmetric for the exchange of the coordinates of two electrons? Explain.

Solution:

False. The total wave function (including the spin) of a system of electrons must always be antisymmetric to the exchange of the coordinates of two electrons. This wave function can be written as a product of two functions. One that depend on the spatial coordinates of the electrons the other one depends on their spin. So when the spin dependent part is antisymmetric the spatial coordinate dependent part must be symmetric.

30. Order the following materials according to their approximate band gap separating the valence and conduction bands from smallest to largest: aluminium oxide, copper, diamond, germanium, magnesium, silicon
What type of materials are these?

Solution:

metal: copper (0), magnesium(0), semiconductor: germanium(0.7), silicon (1.1), insulator: diamond(4), aluminium oxide(6,7) All values in braces are in eV, The student is not required to give these and the order in the semiconductor insulator and conductor groups is not important.

31. Prove with a simple argument why the reciprocal lattice of the reciprocal lattice is the direct lattice!

Solution:

In the definition equation $e^{i\mathbf{K}\cdot\mathbf{R}} = 1$, or $\mathbf{K}\cdot\mathbf{R} = 2\pi$ the role of the direct lattice vector \mathbf{R} and the reciprocal lattice vector \mathbf{K} is symmetrical, therefore either of them is the reciprocal vector of the other.

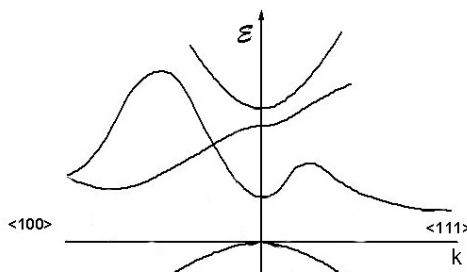
32. The electrical current in a metal ... Delete the invalid statement(s) from below!

- (a) ... can be described as a current of electrons
- (b) ... can be described as a current of holes
- (c) ... is zero for a full band
- (d) ... is proportional to $e^{-\frac{e\phi}{k_B T}}$

Solution:

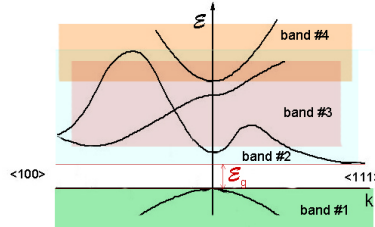
delete only (d)

33. The following picture depicts the valence and conduction bands of a semiconductor. Mark the bands and the forbidden gap on the figure.

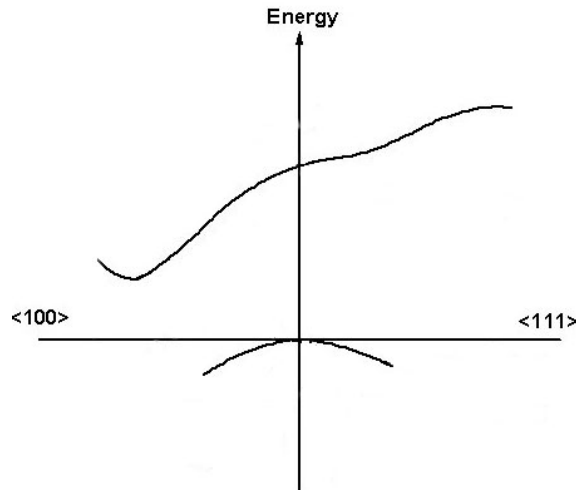


Solution:

The gap is between the x axis (max. value for the valence band edge) and the minimum of the conduction band edge at the right.



34. The following picture depicts the valence and conduction bands of a semiconductor. The electrons or the holes have larger absolute effective mass? Mark the forbidden gap on the figure.



Solution:

a) The curvature of the conduction band edge is larger (approximately a more narrow parabola) than that of the valence band edge ($|1/d^2 E_c/dk^2| < |1/d^2 E_v/dk^2| \Rightarrow$ the effective mass of holes is larger. b) The gap is between the x axis (max. value for the valence band edge) and the minimum of the conduction band edge at the left.

35. The sentence
 “A crystal lattice is described by a and a, the latter is the at any”
 define the crystal lattice. Fill in the spaces!

Solution:

A crystal lattice described by a point lattice and a basis, the latter is the atoms or molecules at any lattice point.”

36. Under which circumstances (and in which types of materials) can the electrical current in a material attributed to both electrons and holes as charge carriers?

Solution:

The current of charge carriers in a single band can be described either as the current of electrons or the current of holes, but not to both of them. Therefore to have a current of both of these the material must have at least two not completely filled bands. These materials are insulators including semiconductors and some metals with overlapping bands, e.g. Mg.

37. Under which condition can we neglect the induced emission?

Solution:

In thermal equilibrium, when $h\nu/k_B T \gg 1$, i.e. for light and higher frequency radiation.

38. What are conventional and primitive cells?

Solution:

- *The volume of space that when translated through all of the point lattice vectors just fills the complete space without overlap or without leaving voids is called a primitive cell or primitive unit cell. These are not unique. A primitive cell contains 1 lattice point.*
- *Those non-primitive unit cells that have all of the symmetry of the crystal are called conventional unit cells.*

39. What are selection rules and what do they mean?

Solution:

Selection rules constrain the possible transitions of a system. They can be formulated for electronic, vibrational or rotational transitions. Examples: for electronic transitions the total angular momentum difference between the initial and final states must be an integer multiple of \hbar . Transitions prohibited by a selection rule may still happen by allowing other kind of interactions taking place. Usually these transitions have a much smaller probability than the one prohibited by the selection rule.

40. What are the assumptions of the Bose-Einstein and of the Fermi-Dirac statistics?

Solution:

Both statistics are valid for indistinguishable particles. Fermi-Dirac statistics is valid for half-spin particles called fermions (like electrons) where no two particles may occupy the same quantum state, while Bose-Einstein statistics is valid for particles of integer spin (bosons), where any number of particles may be in the same quantum state.

41. What are the assumptions of the Drude model of conductivity?

Solution:

- (a) *electrons do not interact with each other (independent electron model)*
- (b) *conduction electrons collide only with the ion cores*
- (c) *these collisions are completely inelastic: electrons lose all of their kinetic energy in a collision*

42. What are the assumptions of the Sommerfeld model of conductivity?

Solution:

In longer form:

- (a) *ion cores are stationary*

- (b) *conduction electrons do not interact with the ion cores, so the metal may be represented by a potential box*
- (c) *electrons do not interact with each other (independent electron model)*
- (d) *even though there are no interactions between electrons still no 2 electrons can be in the same quantum state when we include the spin as a quantum number (Pauli principle)*

In shorter form

- (a) *ion cores are stationary*
 - (b) *the metal is a potential box*
 - (c) *electrons do not interact (independent electron model)*
 - (d) *the Pauli principle is valid*
43. What are the basic elements of a laser?

Solution:

- *pumped amplifier*
- *feedback (frequency relative)*
- *out coupler*

44. What are the characteristics (just keywords please) and application area of the following X-ray diffraction methods? Laue method (1), Rotating crystal method (2), Debye-Sherrer powder method (3)?

Solution:

- (a) *polychrome X-ray ($\lambda_{min} \leq \lambda \leq \lambda_{max}$) – large single crystal, used for determining the orientation of the crystal*
- (b) *monochrome X-ray – single crystal rotated – determine unknown crystal structures*
- (c) *monochrome X-ray – powdered single crystal – determination of lattice constants*

45. What are the characteristics of the acoustic and optical branches of the 3D phonon dispersion relations? How many of them are there in a solid of N atoms basis?

Solution:

- *acoustic branch – $\omega(\mathbf{k} = 0) = 0$, all atoms in the basis vibrate with the same phase, there are 3 of them*
- *optical branch – $\omega(\mathbf{k} = 0) \neq 0$, atoms in the basis are vibrating in different (with a 2 atom basis - opposite) phases. there are $3n - 3$ of them, $n - 1$ longitudinal and $2n - 2$ transverse ones.*

46. What are the crystal momentum and total momentum of the Bloch electrons?

Solution:

The total momentum is

$$p = \hbar k + p_u$$

where $\hbar k$ is the crystal momentum of the Bloch electron.

47. What are the drift velocity and the mobility of the electrons? What is the connection between the conductivity and these?

Solution:

In an \mathbf{E} field the average velocity of the electrons is called the drift velocity. It is small and proportional with \mathbf{E} and the proportionality

factor μ is the mobility:

$$\mathbf{v}_{drift} = \mu \mathbf{E}$$

The conductivity:

$$\sigma = n e \mu$$

where e is the elementary charge and n is the electron density.

48. What is a Bloch–electron and why can't it be excited out of the first Brillouin-zone by a constant electric field?

Solution:

Bloch electrons are independent, non interacting (crystal) electrons. In 1D Bloch electrons wave function in the form:

$$\psi(x) = u(x) e^{ikx}$$

where $u(x + R) = u(x)$. Constant electric fields cannot excite them outside the 1st Brillouin zone because at the zone boundary their momentum is reflected back into the zone.

49. What is a Bravais lattice?

Solution:

Any one of the following is acceptable:

- The infinite set of discrete points with an arrangement and orientation that appears exactly the same, from whichever of the points the array is viewed
- A point lattice that satisfies the condition that if \mathbf{r} is a point in the point lattice then every other points can be reached by using the formulas

$$\mathbf{r}_{\mathbf{R}} = \mathbf{r} + \mathbf{R}, \text{ where}$$

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$$

using all positive and negative numbers for n_1, n_2, n_3

50. What is hybridization?

Solution:

Hybridization means the mixing of atomic orbitals to create orbitals which qualitatively describe the atomic bonding in molecules. Their name is derived from the corresponding atomic orbitals used. Example: an sp^3 orbital is the linear combination of one s and 3 p orbitals (like in CH_4)

51. What is population inversion used for lasers and how can we achieve it?

Solution:

In population inversion the population of the higher level is greater than the one for the lower level. This is achieved by non thermal excitation processes such as: electrical, chemical and optical processes

52. What is the connection between the crystal momentum and the total momentum of a Bloch electron?

Solution:

The total momentum is

$$p = \hbar k + p_u$$

where $\hbar k$ is the crystal momentum of the Bloch electron.

53. What is the coordination number and what is its value for sc, fcc and bcc lattices?

Solution:

The coordination number is the number of the nearest neighbors of a lattice point. sc - 6, fcc - 12, bcc - 8

54. What is the difference between a crystalline and an amorphous solid?

Solution:

Crystalline solids have long range ordering and translational symmetry. Amorphous materials have only short range ordering.

55. What is the difference between intrinsic and extrinsic semiconductors? Which are used in semiconductor devices?

Solution:

Intrinsic semiconductors have no dopants therefore they are more similar to other insulators. In extrinsic semiconductors there are either donor or acceptor atoms present. The overwhelming majority of the charge carriers come from these. In semiconductor devices extrinsic s.c.s are used.

56. What is the reciprocal lattice?

Solution:

each and any of the following answers is acceptable

(a) *The structure of crystals can be studied using EM waves (X-rays) with wavelengths comparable with the lattice constants of a crystal. The reciprocal lattice is a set of those \mathbf{K} vectors that yield plane waves with the periodicity of the lattice.*

(b) *The Fourier transform of the direct lattice*

(c) *A lattice whose base vectors are*

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

where \mathbf{a}_l ($l = 1, 2, 3$) are the base vectors of the primitive cell of the crystal.

57. What is the relationship between the probability per unit time of spontaneous and induced emission between two levels?

Solution:

$$B_{21} = A_{21}\varepsilon(\nu)$$

58. What is the temperature dependance of the specific heat at low temperatures for both electrons and lattice vibrations? Which one of them is dominant at $T \ll \Theta_D$?

Solution:

$$c_v = A(\text{phonons}) \cdot T^3 + B(\text{electrons}) \cdot T$$

at very low T s electron specific heat is the dominant one.

59. Delete the invalid statement(s) from below!

The electrical current in a metal ...

- (a) ... can be described as a current of electrons
- (b) ... can be described as a current of holes
- (c) ... is zero for a full band
- (d) ... is proportional to $e^{-\frac{e\varphi}{k_B T}}$

Solution:

delete only (d)

2 Problems

Useful constants : Planck's constant: $h = 6.63 \cdot 10^{-34} \text{ Js}$,
 elementary charge : $e = 1.6 \cdot 10^{-19} \text{ C}$,
 electron mass : $m_e = 9.1 \cdot 10^{-31} \text{ kg}$,
 Stefan - Boltzman constant : $\sigma = 5.670373(21) \cdot 10^{-8} \text{ Wm}^{-2} \text{ K}^{-4}$,
 Rydberg energy : $1 \text{ Ry} = 13.6 \text{ eV}$
 Avogadro's constant $L = 6.022 \cdot 10^{23} \text{ 1/mol}$

60. Aluminum has three valence electrons per atom, an atomic weight of 0.02698 kg/mol, a density of 2700 kg/m^3 , and a conductivity of $3.54 \cdot 10^7 \text{ S/m}$. Calculate the electron mobility in aluminum. Assume that all three valence electrons of each atoms are free.

Solution:

The number of aluminum atoms per m^3 is

$$\begin{aligned} n_a &= 6.0210^{23} \text{ atoms/mol} \cdot 1/0.02698 \text{ mol/kg} \cdot 2700 \text{ kg/m}^3 \\ &= 6.024 \cdot 10^{28} \text{ atoms/m}^3 \end{aligned}$$

Thus the electron density in aluminum is

$$n = 3 \cdot 6.024 \cdot 10^{28} \text{ atoms/m}^3 = 1.807 \cdot 10^{29} \text{ electron/m}^3$$

$$\mu = \frac{\sigma}{ne} = \frac{3.54 \cdot 10^7}{1.807 \cdot 10^{29} \cdot 1.6022 \cdot 10^{-19}} = 1.22 \cdot 10^{-3} \text{ m/s}$$

61. An electron gun emits electrons with energies between 3.2 keV and 3.3 keV. What is the minimum uncertainty of the position of the electrons?

Solution:

Because

$$U = \frac{p^2}{2 m_e e}$$

$$p = \sqrt{2 m_e e U}$$

and

$$\Delta p \Delta x \geq \frac{\hbar}{2}$$

and

$$\begin{aligned}\Delta p &= p_2 - p_1 = \sqrt{2m_e eU} - \sqrt{2m_e eU} \\ &= 3.1036419 \cdot 10^{-23} - 3.0562553 \cdot 10^{-23} = 4.74 \cdot 10^{-25} \text{ kg m}^2/\text{s}^2 \\ \Delta x &= \frac{\hbar}{2\Delta p} = 1.11 \cdot 10^{-10} \text{ m}\end{aligned}$$

Using $h/2$ instead of $\hbar/2$ would give $6.99 \cdot 10^{-10} \text{ m}$, while with h this would be $1.39 \cdot 10^{-9} \text{ m}$.

62. An electron is confined in a 3D potential box with sides $10\mu\text{m}$, $20\mu\text{m}$ and $30\mu\text{m}$. Give the energy and degeneracy of the 3 lowest states.

Solution:

The possible energy levels in one direction:

$$E_n = \frac{h^2}{8m_e L^2} n^2$$

therefore in 3D

$$\begin{aligned}E_{n_1, n_2, n_3} &= \frac{h^2}{8m_e} \left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2} \right) \\ &= 6.02 \cdot 10^{-28} \left(\frac{n_1^2}{1} + \frac{n_2^2}{4} + \frac{n_3^2}{9} \right) [J] \\ &= 3.76 \cdot 10^{-9} \left(\frac{n_1^2}{1} + \frac{n_2^2}{4} + \frac{n_3^2}{9} \right) [eV]\end{aligned}$$

The 3 lowest lying energy states can be determined by trying out different combinations of the 3 numbers and selecting the 3 smallest values:

n_1	n_2	n_3	factor
1	1	1	1.36
1	1	2	1.47
1	2	1	1.61
2	1	1	2.36
2	2	1	2.61
1	2	2	1.72
1	1	3	1.58

From this table the indices for the 3 lowest levels are: $(1,1,1)$, $(1,1,2)$ and $(1,2,1)$.

The corresponding energies and degeneracies:

Energy level	$E(\times 10^{-28} \text{ J})$	$E(\times 10^{-9} \text{ eV})$	degeneracy
E_{111}	8.20	5.11	1
E_{112}	8.87	5.53	1
E_{121}	12.7	7.94	1
E_{113}	13.6	8.46	1
E_{122}	14.7	9.19	1
E_{211}	26.3	16.39	1
E_{212}	28.3	17.7	1
E_{221}	30.8	19.2	1
E_{222}	32.8	20.47	1

63. Calculate the current density of electrons and holes in the conduction band of a 1D metal “crystal” with the following dispersion relation:

$$\mathcal{E}(k)(\equiv \hbar\omega) = \mathcal{E}_0 + A(1 - \cos\alpha k),$$

where $A = 5.06 \cdot 10^{-19} J$ and $\alpha = 2.78 \cdot 10^8 m$. (In a 1D crystal the numerical factor in the formula for the current is $1/2\pi$ and not $1/8\pi^3$)

Solution:

The current densities in 1D are (the original formulas are in 3D and use the factor $\frac{e}{8\pi^3}$ instead of $\frac{e}{2\pi}$):

$$j_e = -\frac{e}{2\pi} \int_{\text{occupied levels in band}} v(k) dk$$

$$j_h = +\frac{e}{2\pi} \int_{\text{empty levels in band}} v(k) dk$$

In metals the conduction band is half full and $j_e = -j_h$, therefore we only need to calculate j_e .

The velocity :

$$v(k) = \frac{d\omega}{dk}$$

$$= \frac{1}{\hbar} \frac{d\mathcal{E}}{dk} = \frac{1}{\hbar} A \alpha \sin\alpha k$$

$$= \frac{1}{1.055 \cdot 10^{-34}} 5.06 \cdot 10^{-19} \cdot 2.78 \cdot 10^8 \cdot \sin(2.78 \cdot 10^8 k)$$

$$= 1.33 \cdot 10^{-24} \cdot \sin(2.78 \cdot 10^8 k) \text{ m/s}$$

From the dispersion relation $\mathcal{E}_{min} = \mathcal{E}_0 + A(1 - (\text{max of cosine})) = \mathcal{E}_0$, $\mathcal{E}_{max} = \mathcal{E}_0 + A(1 - (\text{min of cosine})) = \mathcal{E}_0 + 2A$ The width of the conduction band is $\Delta\mathcal{E} = \mathcal{E}_{max} - \mathcal{E}_{min} = 2A$. For j_e the limits of the integration are k values corresponding to the minimum and the half of the band. The minimum is \mathcal{E}_0 , where the cosine is 1, i.e. $k_{min} = 0$, while the half of the band is $\mathcal{E}_0 + \frac{1}{2}\Delta\mathcal{E} = \mathcal{E}_0 + A$ which means the cosine is zero, i.e. $k_{max} = \frac{\pi}{2\alpha}$

$$j_e = -\frac{e}{2\pi\hbar} \int_0^{\frac{\pi}{2\alpha}} A \alpha \sin\alpha k dk$$

$$= -\frac{e}{2\pi\hbar} A [-\cos\alpha k]_0^{\frac{\pi}{2\alpha}}$$

$$= +\frac{e}{2\pi\hbar} A (0 - 1) = -\frac{eA}{2\pi\hbar}$$

$$= -\frac{2 \cdot 1.6 \cdot 10^{-19} \cdot 5.06 \cdot 10^{-19}}{\pi \cdot 1.055 \cdot 10^{-34}}$$

$$= -4.894 \cdot 10^{-4} A/m^2$$

($-1.984 \cdot 10^{-4} A/m^2$ for the wrong factor)

and $j_h = -j_e = +4.894 \cdot 10^{-4} A/m^2$

64. Calculate the electron mobility in silver using the Drude model; knowing the following parameters: at $T=293\text{ K}$ conductivity: $\sigma = 6.8 \cdot 10^7\text{ S/m}$, mass density: $\rho_m = 19.5\text{ g/cm}^3$, atomic weight: $A = 107.88\text{ g/mol}$. and as an average every silver atom yields $n_a = 1.3$ conduction electrons.

Solution:

The conduction electron density equals to the number of electrons in a V volume of silver divided by the volume:

$$n = \frac{n(V)}{V} = \frac{1}{V} \frac{V \rho_m}{A} L_A n_a = \frac{19.5\text{ g/cm}^3}{107.88\text{ g/mol}} \cdot 6.022 \cdot 10^{23}\text{ 1/mol} \cdot 1.3$$

$$= 1.415 \cdot 10^{23}\text{ 1/cm}^3 = \underline{1.415 \cdot 10^{29}\text{ 1/m}^3}$$

The mobility:

$$\mu = \frac{\sigma}{n e} \left(= \frac{\sigma A}{e \rho_m L_A n_a} \right) = \frac{6.8 \cdot 10^7}{1.6 \cdot 10^{-19} \cdot 1.415 \cdot 10^{29}} = \underline{2.999 \cdot 10^{-3} \cdot \frac{\text{m}^2}{\text{V s}}}$$

65. Copper has the electron configuration $[\text{Ar}] 3d^{10} 4s^1$, an atomic weight of 0.06355 kg/mol , a density of 8960 kg/m^3 , and a conductivity of $5.960 \cdot 10^7\text{ S/m}$. Calculate the electron mobility in copper. Assume that the valence electrons of each atoms are free.

Solution:

The number of copper atoms per m^3 is

$$n_a = 6.0210^{23}\text{ atoms/mol} \cdot 1/0.06355\text{ mol/kg} \cdot 8960\text{ kg/m}^3$$

$$= 8.491 \cdot 10^{28}\text{ atoms/m}^3$$

and this equals to the electron density. The mobility:

$$\mu = \frac{\sigma}{n e} = \frac{5.960 \cdot 10^7}{8.491 \cdot 10^{28} \cdot 1.6022 \cdot 10^{-19}} = \underline{\underline{4.381 \cdot 10^{-3} \frac{\text{m}^2}{\text{V s}}}}$$

66. Calculate the distance of the (123) lattice planes in a simple cubic lattice if the lattice constant is 5 nm !

Solution:

The distance of the lattice planes (hkl) can be calculated using the length of the reciprocal vector g_{hkl} :

$$d_{hkl} = \frac{2\pi}{|\mathbf{g}_{hkl}|} = \frac{1}{\sqrt{\frac{h^2}{a_1^2} + \frac{k^2}{a_2^2} + \frac{l^2}{a_3^2}}}$$

Now $a_1 = a_2 = a_3 = 5\text{ nm}$, so $d_{hkl} = \frac{5}{\sqrt{1^2+2^2+3^2}} = 1.34\text{ nm}$

67. Determine the distance between neighboring (110) lattice planes in an fcc lattice if the lattice constant is 0.483 nm .

Solution:

a) using the Bravais cell

the (110) planes are perpendicular to the bottom plane of the cell determined by \mathbf{a}_1 and \mathbf{a}_2 and one of them goes through the face diagonal. The nearest parallel lattice planes go through the center points of the faces perpendicular to bottom face. Therefore they divide the face diagonal in 4 equal part, so the distance of these is one

quarter of the face diagonal: $a\sqrt{2}/4 = 0.1708 \text{ nm}$

b) using the primitive cell

in this case the the three primitive vectors may point to the center points nearest to the corner of the fcc cube selected as the origin. They are perpendicular to each other (which can easily be proved by writing the base vectors as linear combinations of unit vectors in a Cartesian system) and have a length of $1/2$ of the body diagonal. The (100) plane then again perpendicular to the plane of \mathbf{a}_1 and \mathbf{a}_2 and the distance of two neighboring plane is the face diagonal of the cube created by \mathbf{a}_1 , \mathbf{a}_2 and \mathbf{a}_3 : $|\mathbf{a}_1|\sqrt{(2)} = a/4 \cdot \sqrt{(2)} = 0.1708 \text{ nm}$

68. Determine the possible diffraction angles for a 25 keV X-ray from the (100) planes of a bcc lattice, if the lattice constant is $a = 4.7 \text{ \AA}$.

Solution:

The wavelength of the X-ray:

$$E = h\nu = \frac{hc}{\lambda} \Rightarrow \lambda = \frac{hc}{E} = \underline{4.96 \cdot 10^{-11} \text{ m}}$$

Bragg's law:

$$2d \sin\theta = n\lambda$$

The distance between planes (100) is $d = \frac{a}{2} = 0.235 \text{ nm}$.

The possible diffraction angles are determined by:

$$\sin\theta = n \frac{\lambda}{2d} = n \cdot \frac{4.96 \cdot 10^{-11}}{2 \cdot 0.235 \cdot 10^{-9}} = n \cdot 1.055 \cdot 10^{-1} = \underline{0.106 \cdot n}$$

Here $n = 1, 2, 3, 4$, i.e. the angles are

$6.05^\circ, 12.18^\circ, 18.45^\circ, 24.97^\circ, 31.84^\circ, 39.28^\circ, 47.71^\circ, 57.58^\circ$ and 71.74°

69. In a direct gap intrinsic semiconductor the dispersion relation near the band edges can be approximated by the form $\mathcal{E}_{v,c}(k) = A_{v,c}k^2 + B_{v,c}$, where $A_{v,c}$, and $B_{v,c}$ are constants, and the indices c and v denotes the band. Determine these four constants, knowing that the band gap is 0.9 eV and the effective masses in the bands are

$$m_{eff}^{(c)} = -0.832 \cdot m_e, m_{eff}^{(v)} = 1.260 \cdot m_e$$

Solution:

Select the energy zero be at the top of the valence band, then

$B_c \equiv \mathcal{E}_{gap} = 0.9 \text{ eV} = \underline{1.442 \cdot 10^{-19} \text{ J}}$ and $B_v = 0$.

An equivalent solution would be: $B_c - B_v = 0.9 \text{ eV}$ From the definition of the effective mass:

$$\frac{1}{m_{eff}} = \frac{1}{\hbar^2} \frac{d^2\mathcal{E}}{dk^2}$$

With \mathcal{E} in the given form the second derivative is $2A_{c,v}$

$$\frac{1}{m_{eff}^{(c,v)}} = \frac{1}{\hbar^2} 2A_{c,v}$$

$$\underline{A_c} = \frac{\hbar^2}{2 m_{eff}^{(c)}} = \underline{\underline{-7.337 \cdot 10^{-39} J m^2}}$$

$$\underline{A_v} = \frac{\hbar^2}{2 m_{eff}^{(v)}} = \underline{\underline{4.845 \cdot 10^{-39} J m^2}}$$

70. The Zeeman components of a 500 nm spectral line are 0.0116 nm apart when the magnetic field is 1.00 T. Find the e/m_e ratio for the electron from these data.

Solution:

The magnitude of the energy shift from the given $\Delta\lambda$ value is

$$\Delta E_B = h \Delta \nu = h \left(\frac{c}{\lambda_2} - \frac{c}{\lambda_1} \right) = \frac{c h}{\lambda_1 \lambda_2} (\lambda_1 - \lambda_2) = -\frac{c h \Delta \lambda}{\lambda_1 \lambda_2}$$

Where $\lambda_{1,2} = \lambda \pm \Delta\lambda/2$. But $\Delta\lambda \ll \lambda$ therefore in the denominator $\lambda_1 \lambda_2 \approx \lambda^2$.

$$|\Delta E_B| = \frac{h c \Delta \lambda}{\lambda^2} = \frac{6.63 \cdot 10^{-34} \cdot 3 \cdot 10^8 \cdot 0.0116 \cdot 10^{-9}}{(500 \cdot 10^{-9})^2} = 9.22 \cdot 10^{-24} J$$

For the Zeeman effect

$$\Delta E_B = \frac{e}{2m_e} \mathbf{L} \cdot \mathbf{B}$$

$$\frac{e}{m_e} = \frac{2 |\Delta E_B|}{L \cdot B}$$

Substituting ΔE_B and taking L and B parallel, $B = 1 T$ and $L = 1 \hbar$

$$\frac{e}{m_e} = \frac{2 \cdot 9.22 \cdot 10^{-24}}{1.05 \cdot 10^{-34}} = 1.748 \cdot 10^{11}$$

The exact value is $1.76 \cdot 10^{11}$

71. The conductivity of silver is $6.8 \cdot 10^7$ S/m at $T=293$ K. The density of silver is 10.5 g/cm^3 . Every silver atom gives an average of 1.3 conduction electrons. The atomic weight of silver is 107.88 g/mol . Calculate the electron mobility in silver using the Drude model.

Solution:

$$\mu = \frac{\sigma}{n e}$$

Notations: Let m_1, M and M_1 denote the mass of 1 mol (i.e. L_A atoms), mass of 1 kmol (i.e. $L : L_A \cdot 1000 = 6.022 \cdot 10^{26}$ atoms) and M_1 mass of 1 m^3 of Ag respectively, while let $s := 1.3$ to be the number of electrons from one atom, and N_{km} the number of moles in 1 m^3 of Ag! $\rho = 10.5 \text{ g/cm}^3 = 10.5 \text{ kg/m}^3$, $m = 107.88 \text{ g}$, $M = 107.88 \text{ kg}$, $M_1 = \rho \cdot 1 \text{ m}^3 = 10,500 \text{ kg}$, $N_{km} = 10\,500/107.88 = 97.3 \text{ kmol}$. We only need to calculate the n electron density:

$$n = \frac{\text{number of electrons in a given volume}}{\text{volume}}$$

$$= N_1 \cdot L \cdot s$$

$$= 97.3 \cdot 6.022 \cdot 10^{26} \cdot 1.3 = 7.62 \cdot 10^{28} \text{ 1/m}^3$$

The mobility:

$$\mu = \frac{\sigma}{n e} = \frac{6.8 \cdot 10^7}{7.62 \cdot 10^{28} \cdot 1.6 \cdot 10^{-19}} = 5.57 \cdot 10^{-3} \frac{m^2}{V s}$$

72. The conductivity of silver is $6.8 \cdot 10^7$ S/m at $T=293$ K. The density of silver is 19.5 g/cm³. Every silver atom gives an average of 1.3 conduction electrons. The atomic weight of silver is 107.88 g/mol. Calculate the electron mobility in silver using the Drude model.

Solution:

A cubic meter of silver has a mass of 19,500 kg.

A kg-mole of silver weighs 107.88 kg.

So a cubic meter contains $19\,500/107.88 = 180.76$ kg-moles of silver.

A kg-mole of anything contains $6.023 \cdot 10^{26}$ atoms (or molecules).

So a cubic meter of silver contains $180.76 \cdot 6.023 \cdot 10^{26} = 1.0885 \cdot 10^{29}$ atoms

So it contains $1.3 \cdot 1.0885 \cdot 10^{29} = 1.4151 \cdot 10^{29}$ electrons

The mobility:

$$\mu = \frac{\sigma}{n e} = \frac{6.8 \cdot 10^7}{1.4151 \cdot 10^{29} \cdot 1.6 \cdot 10^{-19}} = 2.999 \cdot 10^{-3} \frac{m^2}{V s}$$

(The number 19.5 g/cm³ was a typing error as the correct density of silver is 10.5 g/cm³. With the correct density the result would be $5.57 \cdot 10^{-3} m^2/V s$)

73. The dispersion relations of electrons in the valence and conduction bands near the band edges are approximated by the following functions:

$$\mathcal{E}_v(k) = -3.024 \cdot 10^{-20} (k - 2.4510^8)^2 + 13 \quad [eV]$$

$$\mathcal{E}_c(k) = 4.65 \cdot 10^{-20} k^2 + 11.9 \quad [eV]$$

Express the effective masses of electrons in units of the free electron mass $m_e = 9.1 \cdot 10^{-31} kg$.

Solution:

In 1D

$$\frac{1}{m_{eff}} = \frac{1}{\hbar^2} \frac{d^2 \mathcal{E}(k)}{dk^2}$$

The energies (in eV) converted to Joule are:

$$\mathcal{E}_v(k) = 4.845 \cdot 10^{-39} (k - 2.4510^8)^2 + 2.08 \cdot 10^{-18} \quad [J]$$

$$\mathcal{E}_c(k) = -7.450 \cdot 10^{-39} k^2 + 1.91 \cdot 10^{-18} \quad [J]$$

The second derivative of both functions gives twice the coefficient of the 2nd order terms, and so the electron effective masses in the conduction and valence bands are:

$$m_{eff}^{(c)} = \frac{\hbar^2}{1.490 \cdot 10^{-38}} = 7.46 \cdot 10^{-31} [kg] = 0.819 m_e$$

$$m_{eff}^{(v)} = -\frac{\hbar^2}{9.690 \cdot 10^{-39}} = -1.14 \cdot 10^{-30} [kg] = -1.260 m_e$$

74. The donor concentration in an n-type silicon cube of sides $l = 0.7\text{cm}$ is $2.5 \cdot 10^{15}$ atom/cm³, (the density of Si atoms is $5 \cdot 10^{26}$ atom/m³) A voltage of 1.5 V is applied between two opposite faces of the cube. Determine the hole concentration, the resistivity and the current through this cube. The intrinsic electron concentration in silicon is $n_i = 1.5 \cdot 10^{16} \text{m}^{-3}$. The electron mobility is $\mu_e = 0.13 \text{m}^2 \text{V}^{-1} \text{s}^{-1}$.

Solution:

$$n\text{-type: } N_a \approx 0, n_c = N_d = 2.5 \cdot 10^{21} \text{atom/m}^3$$

$$p_v = n_i^2 / N_d = 9 \cdot 10^{10} \text{1/m}^3, \text{ because}$$

$$p_v \ll n_c \Rightarrow \sigma = e n_c \mu_e = 5.207 \cdot 10^3 \text{ S/m} \Rightarrow \rho = 1/\sigma = 0.000192 \Omega \text{ m}$$

$$I = U/R = U \sigma A/l = U \sigma l^2/l = U \sigma l = 1.5 \cdot 5.207 \cdot 10^3 \cdot 0.007 = 7.8 \cdot 10^{-1} \text{ A}$$

75. The donor concentration in an n-type silicon cube of sides $l = 0.7\text{cm}$ is $2.5 \cdot 10^{15}$ atom/cm³, (the density of Si atoms is $5 \cdot 10^{26}$ atom/m³) A voltage of 1.5 V is applied between two opposite faces of the cube. Determine the hole concentration, the resistivity and the current through this cube. The intrinsic electron concentration in silicon is $n_i = 1.5 \cdot 10^{16} \text{m}^{-3}$. The electron mobility is $\mu_e = 0.13 \cdot \text{m}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$.

Solution:

$$\text{In an n-type semiconductor } N_a \approx 0 \text{ and } n_c = N_d = 2.5 \cdot 10^{21} \text{atom/m}^3.$$

From the law of mass action

$$n_c \cdot p_v = \text{const} = n_i^2 \text{ i.e.}$$

$$p_v = n_i^2 / N_d = \underline{9 \cdot 10^{10} \text{1/m}^3}$$

As $p_v \ll n_c$, so approximately

$$\sigma = e n_c \mu_e = 52.07 \text{ S/m} \Rightarrow \underline{\underline{\rho = \frac{1}{\sigma} = 1.92 \cdot 10^{-2} \Omega \text{ m}}}}$$

$$I = U/R = U \sigma A/l = U \sigma l^2/l = U \sigma l \\ = 1.5 \cdot 52.07 \cdot 0.007 = \underline{0.55 \text{ A}}$$

76. The lattice constant of a bcc lattice is $a = 0.352 \text{nm}$. Calculate the atom density on lattice planes (100) and (110)!

Solution:

There are 4 atoms on the (100) plane, 1/4th of each belongs to this cell:

$$\rho = \frac{4 \text{atom}}{a^2} = 8.071 \frac{1}{\text{nm}^2} = \underline{\underline{8.071 \cdot 10^{18} \frac{1}{\text{m}^2}}}$$

There are 5 atoms on the (110) plane. 1/4th of the corner atoms plus the center atom belong to the cell:

$$\rho = \frac{2}{\sqrt{2} a^2} = 11.41 \frac{1}{\text{nm}^2} = \underline{\underline{1.141 \cdot 10^{19} \frac{1}{\text{m}^2}}}$$

77. The lattice constant of an fcc lattice is 0.228 nm. Calculate the surface density of atoms for lattice planes (001) and (110).

Solution:

- Plane (001) is the plane that goes through one face of the cube
There are 5 atoms in this plane but only 1/4th of the 4 corner

atoms, and the middle atom belong to this cell therefore the total number of atoms on this plane that belong to the face of the cube is 2.

The area is $a^2 = 5.20 \cdot 10^{-20} \text{m}^2$, the atom density :

$$n_a = 2/a^2 = \underline{3.846 \cdot 10^{19} \text{m}^{-2}} = 38.46 \text{nm}^{-2}$$

- The (110) plane goes through the face diagonal. It contains $4 \cdot 1/4 = 1$ atoms at the corners and $2 \cdot 1/2 = 1$ atom at the center. The area of $a \cdot a\sqrt{2} = 7.352 \cdot 10^{-20} \text{m}^2$, the atom density is: $n_a = 2/7.352 \cdot 10^{-20} = \underline{2.72 \cdot 10^{19} \text{m}^{-2}} = 27.2 \text{nm}^{-2}$.

78. The lattice constant of an fcc lattice is 0.228 nm. Calculate the surface density of atoms for lattice planes (100) and (110).

Solution:

- Plane (100) is the plane that goes through one face of the cube There are 5 atoms in this plane but only 1/4th of the 4 corner atoms, and the middle atom belong to this cell therefore the total number of atoms on this plane that belong to the face of the cube is 2.

The area is $a^2 = 5.20 \cdot 10^{-20} \text{m}^2$, the atom density :

$$n_a = 2/a^2 = \underline{3.846 \cdot 10^{19} \text{m}^{-2}} = 38.46 \text{nm}^{-2}$$

- The (110) plane goes through the face diagonal. It contains $4 \cdot 1/4 = 1$ atoms at the corners and $2 \cdot 1/2 = 1$ atom at the center. The area of $a \cdot a\sqrt{2} = 7.352 \cdot 10^{-20} \text{m}^2$, the atom density is: $n_a = 2/7.352 \cdot 10^{-20} = \underline{2.72 \cdot 10^{19} \text{m}^{-2}} = 27.2 \text{nm}^{-2}$.

79. The lattice constant of an fcc lattice is 0.34 nm. Calculate the surface density of atoms for lattice planes (010) and (101).

Solution:

- Plane (010) is the plane that goes through one face of the cube There are 5 atoms in this plane but only 1/4th of the 4 corner atoms, and the middle atom belong to this cell therefore the total number of atoms on this plane that belong to the face of the cube is 2.

The area is $a^2 = 1.16 \cdot 10^{-20} \text{m}^2$, the atom density :

$$n_a = 2/a^2 = \underline{.10^{19} \text{m}^{-2}} = 173 \text{nm}^{-2}$$

- The (101) plane goes through a face diagonal. It contains $4 \cdot 1/4 = 1$ atoms at the corners and $2 \cdot 1/2 = 1$ atom at the center. The area of $a \cdot a\sqrt{2} = 1.635 \cdot 10^{-19} \text{m}^2$, the atom density is: $n_a = 2/1.635 \cdot 10^{-19} = \underline{1.223 \cdot 10^{19} \text{m}^{-2}} = 12.23 \text{nm}^{-2}$.

80. The lattice constant of an fcc lattice is 0.457 nm. Calculate the surface density of atoms for lattice planes (100) and (110).

Solution:

a) The Lattice plane (100) is the plane that contains one face of the cube There are 5 atoms in this plane but only 1/4th of 4 of them belongs to this cell therefore the total number of atoms on this plane that belongs to the cube is 2, the area is $a^2 = 2.088 \cdot 10^{-19} \text{m}^2$, the atom density is $2/a^2 = 9.58 \cdot 10^{18} 1/\text{m}^2$

b) The (110) plane goes through the face diagonal. It contains $4 \cdot 1/4 = 1$ atoms at the corners and $2 \cdot 1/2 = 1$ atom at the diagonal an area of $a \cdot a\sqrt{2} = 2.95 \cdot 10^{-19} \text{m}^2$, the atom density is: $2/2.95 \cdot 10^{-19} = 6.77 \cdot 10^{18} 1/\text{m}^2$.

81. The part of the EM radiation we call visible light is in the wavelength range of $400 \dots 600 \text{nm}$. Are the following crystals

material	Band gap (eV)
Aluminum nitride	6.0
Diamond	5.5
Silicon dioxide	9.0
Copper oxide	1.1

transparent in this frequency range?

Solution:

The energy range for visible light is

$$\begin{aligned} \mathcal{E}_{min} &= h\nu_{min} = \frac{hc}{\lambda_{max}} = \\ &= \frac{6.626 \cdot 10^{-34} \cdot 2.998 \cdot 10^8}{6 \cdot 10^{-7}} \\ &= 3.311 \cdot 10^{-19} \text{ J} = 2.066 \text{ eV} \end{aligned}$$

$$\begin{aligned} \mathcal{E}_{max} &= h\nu_{max} = \frac{hc}{\lambda_{min}} = \\ &= \frac{6.626 \cdot 10^{-34} \cdot 2.998 \cdot 10^8}{4 \cdot 10^{-7}} \\ &= 4.966 \cdot 10^{-19} \text{ J} = 3.100 \text{ eV} \end{aligned}$$

All of these materials are insulators, they have a full valence band, therefore to absorb EM radiation the EM wave must be able to excite electrons from the top of the valence band through the gap. It follows that only materials with a band gap wider than 3.10 eV are transparent in the whole visible range, therefore

material	transparent
Aluminum nitride	yes
Diamond	yes
Silicon dioxide	yes
Copper oxide	no

(Remark: real crystals mus always contain vacancies, which creates levels in the gap, therefore thick slabs of these materials are not necessarily transparent.)

82. The un-normalized wave function of an electron is $\psi(x) = 12x^2 - 8x$ Calculate the kinetic energy of this electron.

Solution:

The kinetic energy is determined from the formula:

$$\langle E_{kin} \rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x) \frac{\hat{p}^2}{2m_e} \psi(x) dx}{\int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx}$$

where the denominator contains the normalization factor. For our wave function both integrals are infinite, so this function is not a

physical wave function in the whole space. After integration the numerator contains 3rd and 2nd powers of x , while the one in the denominator (the normalization factor) contains 5th and 4th power of x too. If we now set the limits of the integration to $\pm a$ and calculate the limit of this fraction as a tends to ∞ we may see that the denominator goes faster to infinity than the numerator does, i.e. the value of kinetic energy tends to 0.

83. The width of the band gap in silicon is about 1.1 eV. Calculate the ratio of probabilities of electron excitation from the valence to the conduction band in Si at room temperature and at 430 °C!

Solution:

The temperatures are: $T_{room} = 293\text{ K}$ (or 300 K), $T_{430\text{ C}} = 503\text{ K}$, the width of the gap is $\Delta \mathcal{E}_g = 1.1\text{ eV} = 1.76 \cdot 10^{-19}\text{ J}$ The probability

is proportional to the Boltzmann-factor: $\mathcal{P}(T) \propto e^{-\frac{\Delta \mathcal{E}_g}{k_B T}}$

$$\mathcal{P}(293) \propto e^{-\frac{1.76 \cdot 10^{-19}}{1.38 \cdot 10^{-23} \cdot 293}} = 1.20 \cdot 10^{-19} \quad (\text{or } 3.32 \cdot 10^{-19})$$

$$\mathcal{P}(503) \propto e^{-\frac{1.76 \cdot 10^{-19}}{1.38 \cdot 10^{-23} \cdot 503}} = 9.74 \cdot 10^{-12}$$

$$\frac{\mathcal{P}(503)}{\mathcal{P}(293)} = 7.80 \cdot 10^7 \quad (\text{or } 2.83 \cdot 10^7)$$

84. We model the vibrations of an infinite 3D crystal with a 3D set of just 27 atoms using periodic boundary conditions. How many optical branches are in the dispersion relation?

Solution:

For N atoms there are $3N$ branches of the dispersion relation 3 of them is in the acoustic branches, therefore there are $3(N - 1)$ in the optical branches. In our case $N = 27$ so there are 78 optical branches.

85. What are the Miller indices of the following plane? Determine the distance between two such neighboring planes, if all three the lattice constants are 0.372 nm.

Solution:

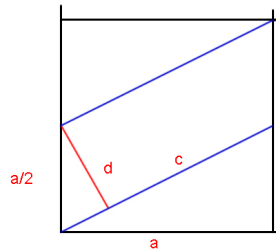
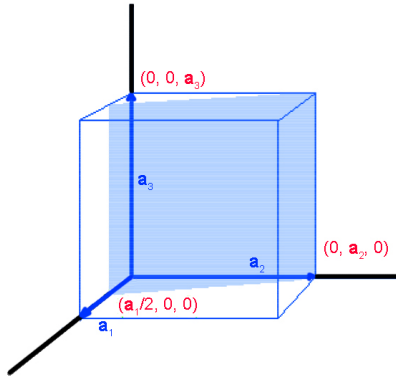
The intersection points of the plane with the axes are $(\frac{a_1}{2}, a_2, \infty)$ ¹ so the Miller indices are (210) The next two parallel planes nearest to this plane go through the point pairs $(0, 0, 0)$ and $(-\mathbf{a}_1/2, -\mathbf{a}_2, 0)$ or $(\mathbf{a}_1, 0, 0)$ and $(\mathbf{a}_1/2, \mathbf{a}_2, 0)$. Because all lattice constants are the same the distance between these two planes is

$$d = \frac{a}{\sqrt{k^2 + l^2 + m^2}} = \frac{a}{\sqrt{2^2 + 1^2 + 0}} = \frac{a}{\sqrt{5}}$$

or equivalently (see figure):

$$\frac{d}{a/2} = \frac{a}{\sqrt{a^2 + (a/2)^2}} \Rightarrow d = \frac{a}{\sqrt{5}} = 0.166\text{ nm}$$

1. $(\frac{a_1}{2}, a_2, \text{none})$



86. What are the Miller indices of the plane given by the following 3 vectors: $4 \mathbf{a}_1$, $3 \mathbf{a}_2$ and $2 \mathbf{a}_3$?

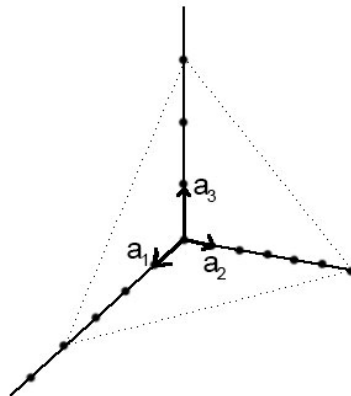
Solution:

The vectors marks the intersections with the three axes at $4 a_1$, $3 a_2$ and $2 a_3$. Then the inverse intercepts in lattice vector units are:

$$\frac{1}{4}, \frac{1}{3}, \frac{1}{2}$$

To get integer numbers we have to calculate the lowest common denominator of this fraction, which is 12. Multiplying each fraction with 12 gives the three Miller indices: (346)

87. What are the Miller indices of the plane on the next figure:



Solution:

The axes cross the plane at $4\mathbf{a}_1$, $6\mathbf{a}_2$ and $3\mathbf{a}_3$. The reciprocals:

$$\frac{1}{4}, \frac{1}{6}, \frac{1}{3}$$

multiply with the least common denominator which is 12 \Rightarrow The Miller indices are (324).

88. What is the acceleration voltage in an electron gun, if the average wavelength of the emitted electrons is 3.1 nm?

Solution:

$$p = \frac{h}{\lambda}, \quad E = \frac{p^2}{2m_e} = e\Delta U \quad \Rightarrow \quad \Delta U = \frac{p^2}{2m_e e} = \frac{h^2}{2m_e e \lambda^2}$$

$$\Delta U = \frac{(6.63 \cdot 10^{-34})^2}{2 \cdot 9.1 \cdot 10^{-31} \cdot 1.6 \cdot 10^{-19} \cdot (3.1 \cdot 10^{-9})^2} = 0.16V$$

89. What is the distance between lattice planes (234) if the base vectors are 0.41 nm, 0.52 nm and 0.43 nm long

Solution:

Distance of the lattice planes is

$$d_{hkl} = \frac{2\pi}{|g_{hkl}|} = \frac{1}{\sqrt{\frac{h^2}{a_1^2} + \frac{k^2}{a_2^2} + \frac{l^2}{a_3^2}}}$$

In our case

$$d_{234} = \frac{1}{\sqrt{\frac{4}{0.41^2} + \frac{9}{0.52^2} + \frac{16}{0.43^2}}} = \underline{\underline{0.08345 \text{ nm}}}$$

90. What is the donor concentration in n-type silicon if when a voltage of 1.5 V is applied between two opposite faces of a cube of this material with sides $l = 0.7 \text{ cm}$ a current of 109.35 mA flows through it? The intrinsic electron concentration in silicon is $n_i = 1.5 \cdot 10^{16} \text{ m}^{-3}$, while the electron mobility is $\mu_e = 0.13 \text{ m}^2 \text{ V}^{-1} \text{ s}^{-1}$.

(for comparison: the density of Si atoms is $5 \cdot 10^{26} \text{ atom/m}^3$)

Solution:

Let N_d be the unknown donor concentration!

$$R = \frac{U}{I} = \frac{1.5}{0.10935} = 13.718 \Omega \quad \text{and}$$

$$R = \rho \cdot \frac{\ell}{A} = \frac{1}{\sigma} \cdot \frac{\ell}{\ell^2} = \frac{1}{\sigma \cdot \ell}$$

$$\sigma = \frac{1}{R \cdot \ell}$$

But in an n-type semiconductor $N_a \approx 0$, $n_c = N_d$, thus $\sigma = e n_c \mu_e$, where n_c is the concentration of the conduction electrons. Therefore

$$e n_c \mu_e = e N_d \mu_e = \frac{1}{R \cdot \ell}$$

$$N_d = \frac{1}{e \cdot \mu \cdot R \cdot \ell} = 5.000 \cdot 10^{20} \text{ m}^{-3}$$

91. What is the lattice constant of a simple cubic lattice if the distance between two neighboring (111) planes is 0.2 nm?

Solution:

In an sc crystal all 3 lattice constants are the same. The distance of two lattice planes with the Miller indices (hkl) is $d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$, where a is the lattice constant. From this formula: $a = d_{hkl}\sqrt{h^2+k^2+l^2} = 0.2 \cdot \sqrt{3} = 0,34nm$

92. What is the quasi-free electron density in copper? Calculate the Fermi velocity and momentum too! The Fermi energy of copper is $\mathcal{E}_F = 4.1eV$.

Solution:

$$N_e = 2 \frac{k_F^3}{6\pi^2} V \quad \Rightarrow \quad n(\equiv \frac{N_e}{V}) = \frac{k_F^3}{3\pi^2}$$

$$\mathcal{E}_F (= \mathcal{E}_{max,occupied}) = \frac{\hbar^2 \pi^2}{2m_e a^2} \frac{s}{2}$$

$$n = \frac{(2m_e \mathcal{E}_F)^{3/2}}{2\pi^2 \hbar^3} = 5.655 \cdot 10^{28} \frac{electron}{m^3}$$

$$v_F = 1.2 \cdot 10^6 m/s = 0.004 c \quad k_F = 1.0 \cdot 10^{11} 1/m$$