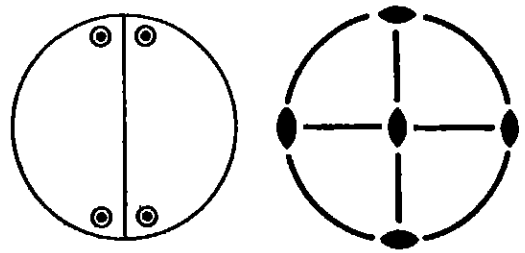


**Exercise 1. (17 pts)**

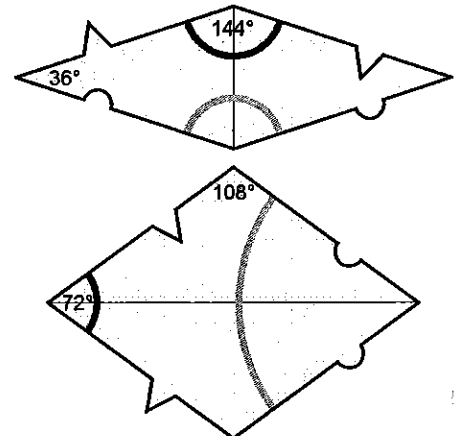
On the right a representation of the  $mmm (D_{2h})$  point group is given.



- To which types of Bravais lattices is this point group connected? (1 pt)
- Suppose we combine this point group with a lattice of C type to obtain the space group  $Cmc2_1$ . When we put one atom on the general  $x,y,z$  coordinate, how many equivalent atomic positions will be occupied by the same type of atom within the unit cell of this space group? Explain your answer in about two sentences (2 pts)
- What do the different symbols  $Cmc2_1$  in the space group exactly mean? (4 pts)
- When we distort a face-centered cubic lattice by changing the length of only one of the diagonals of the square faces by a factor  $(1+\delta)$ , what (new) Bravais lattice will be formed? What are the lattice parameters of the new Bravais lattice in relation to the ones of the initial lattice. (4 pts) (Hint: Draw a schematic representation of the initial lattice projected along a viewing direction perpendicular to the square face in which you elongate one diagonal and then notify what will be the highest symmetry solution after the distortion.)
- Suppose we have a(nother) point group (and thus also space group) that combines a 4-fold rotation axis with two distinct 2-fold rotation axes. To which types of Bravais lattices is this point group connected? Which angles have to be present between these three different rotation axes? Note that this can be calculated using the so-called Euler equation:

$$\cos\left(\hat{AB}\right) = \frac{\cos\frac{\gamma}{2} + \cos\frac{\alpha}{2}\cos\frac{\beta}{2}}{\sin\frac{\alpha}{2}\sin\frac{\beta}{2}}. \quad (3 \text{ pts})$$

- Explain why the Penrose tiling on the right can be associated with quasicrystals. Include the specific angles of the corners of these tiles in your answer. Explain the role of the matching rules for the two tiles. (3 pts)



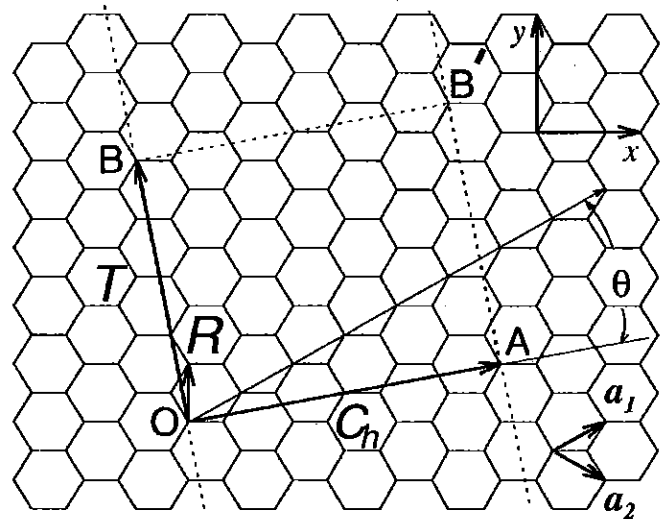
**Exercise 2. (16 pts)**

- Calculate the ratio of the surface energies of  $\{100\}$  and  $\{111\}$  for the fcc (face-centered cubic) structure based on a nearest-neighbor broken bond model, where the maximum number of bonds (coordination) in the bulk is 8. The equilibrium shape of fcc particles based on these energies is the truncated octahedron. (3 pts)
- With the information from a., does it make sense to draw the 2D Wulff plot for fcc particles for viewing along a  $\langle 100 \rangle$  (projection) direction? Explain your answer (2 pts)
- The same as b., but now for viewing along a  $\langle 110 \rangle$  (projection) direction. (2 pts)
- Calculate for the *tetrahedron* (read accurately here!) the ratio of surface area to volume ( $A/V$ ). (4 pts)
- Derive the equation that relates the pressure inside nanoscale tetrahedrons as a function of their size. (3 pts)

- W f. When we increase the size of CdSe nanocrystals from 4 to 8 nm, does a blue or red shift occurs in the luminescence of the nanoparticles? Explain your answer. (2 pts)

### Exercise 3. (16 pts)

- Draw schematically the density of (electron) states (DOS) as a function of energy (around zero energy) for a metallic and for a semiconducting nanowire? (4 pts)
- Why do wires get stronger when their diameter reduce from the micrometer scale to the nanometer scale and finally to the atomic scale. (2 pts)
- Single-wall carbon nanotubes are described on the basis of the vector in the graphene plane that exactly defines the circumference (i.e. perpendicular to the length) of the tube. i.e. the so-called chiral vector  $\vec{C}_h = n\vec{a}_1 + m\vec{a}_2 \equiv (n,m)$ , where the vectors  $\vec{a}_1$  and  $\vec{a}_2$  define the unit cell of graphene (see figure to the right). Write the  $\vec{C}_h$  vector for the general  $(n,m)$  CNT in terms of the  $x$  and  $y$  vectors. (3 pts)
- The SWCNT can also be defined on the basis of the chiral angle  $\theta$ , which is the angle between the chiral vector  $\vec{C}_h$  and the  $\vec{a}_1$  vector (see figure to the right). Derive for the general  $(n,m)$  CNT an equation that relates  $\theta$  to  $n$  and  $m$ . (3 pts)
- We compare the following three SWCNTs:  $(17,0)$ ,  $(13,4)$  and  $(12,5)$ . Which one has the smallest bandgap? Which one has the largest bandgap? Explain both answers. (4 pts)



### Exercise 4. (15 pts)

- Oxide glasses and metallic glasses have rather different atomic structures. Describe these differences. (3 pts)
- Materials used for their (bulk) magnetic properties are subdivided in soft and hard magnetic materials. In what way do the magnetic properties differ for soft and hard magnets? (2 pts)
- Which (micro)structures are used for soft magnetic materials in low and high frequency applications? Explain your answers. (3 pts)
- Explain why phase transformations like solidification and crystallization (of an amorphous phase) show a maximum transformation rate at a certain undercooling below the melting temperature and lower transformation rates at lower and higher (levels of) undercooling. (3 pts)
- Phase transformations proceeding via nucleation and growth can generally be described by the following equation of the JMAK theory describing the fraction transformed  $x$  as a function of time  $t$  at a constant temperature:  $x(t) = 1 - \exp(-kt^n)$ . When the isothermal transformation occurs at various temperatures generally only the factor  $k$  depends on temperature. The factor  $n$  is called the Avrami exponent. Derive the Avrami exponent within the framework of the JMAK theory for a constant nucleation rate and for isotropic crystal

growth in a thin film, when the crystals have a size clearly larger than the film thickness (i.e. when growth is 2-dimensional). (4 pts)

**Exercise 5. (11 pts)**

- a) During thin film growth basically three types of film morphologies can develop, i.e. a distinction is made between Frank - Van der Merwe growth, Volmer - Weber growth and Stranski - Krastanov growth. Describe these three types of morphologies and explain in simple terms when they occur. (3 pts).

When a few unit cells of (001)-oriented  $\text{LaAlO}_3$  are grown on (001)-oriented  $\text{SrTiO}_3$ , the interface between these two good insulators shows metallic characteristics.

- b) One of the mechanisms proposed to explain the observed conduction at the interface is the so-called 'polar catastrophe'. Explain in detail why and how this mechanism works and why it gives rise to conductivity. (5 pts)
- c) The electronic densities measured experimentally at such interface are of the order of  $n = 10^{17} \text{ cm}^{-2}$ . Is this value in agreement with the polar catastrophe theory? Why? Both materials have perovskite cubic lattice with lattice parameters  $a = 0.390 \text{ nm}$ . (3 pts)