PROBLEM SHEET 1

Introduction to Condensed Matter Theory

(To be submitted on Wednesday, 29.04.2015 directly to the tutor in the class or alternately you can drop them in the insititute mail box 42, KOMET 337 one day before)

1. Crystal structure of Fe: Iron has a body-centered cubic(bcc) structure (kubisch-raumzentriert).

(a) Draw its crystal structure and mark the basis vectors of the conventional cell (**a'**,**b'**,**c'**) and a primitive unit cell (**a**,**b**,**c**). Remember that a primitive cell is defined as a unit cell with smallest possible volume. Also, determine the number of atoms in the conventional cell. [2]

(b) The lattice constant (Gitterkonstante) of this structure at room temperature is $a = 0.286nm$. If the mass density (Massendichte) $\rho = 7.87x10^3 kg/m^3$ and molar mass (molare Masse) $M = 55.85g/mol$, calculate the Avogadro constant from these quantities. [1]

(c) Express the basis vectors of the primitive cell in terms of the conventional cell. Determine the length of these vectors, the angle between them and the volume of the primitve cell. Specify the number of nearest neighbour and second nearest neighbour for this structure. [2]

2. Crystal structure of Al: Aluminium has a face-centered cubic structure (fcc) (kubisch-flächenzentrierte) with lattice constant (Gitterkonstante) $a = 0.404nm$.

(a) Draw also its lattice structure and mark the basis vectors of the primitve and conventional cell. [2]

(b) Determine the number of atoms in the conventional unit cell. If the molar mass (molaren Masse) $M = 27.98g/mol$, calculate the mass density (Massendichte) of Aluminium. [1]

(c) Just like the previous case, express the basis vectors of the primitive cell in terms of the conventional cell. Determine the length of these vectors, the angle between them and the volume of the primitve cell. How does this volume compare to the volume of the conventional cell? [2]

3. Reciprocal Lattice (Reziproke Gitter): From the lectures, you know that the primitive vectors of the reciprocal lattice is given by

$$\mathbf{b}_i = 2\pi\varepsilon_{ijk}\frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k)}, \quad \mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{i,j} \tag{1}$$

where a_i represents the basis vector of the primitve unit cell of the direct lattice and ε_{ijk} represents the Levi-Civita Symbol.

(a) Show that the vectors of the reciprocal lattice satisfy the following condition.

$$\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3) = \frac{(2\pi)^3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \tag{2}$$

Also, explain what this equation means. [2]

(b)Suppose that the vectors of the primitive cell can be derived from $\mathbf{b}_i$ in the same way as we derived $\mathbf{b}_i$ from $\mathbf{a}_i$. Show that these vectors are given by: [2]

$$2\pi\varepsilon_{ijk}\frac{\mathbf{b}_j \times \mathbf{b}_k}{\mathbf{b}_i \cdot (\mathbf{b}_j \times \mathbf{b}_k)} = \mathbf{a}_i. \tag{3}$$

(c) The Bravais lattice generated by three basis vectors of equal length a and enclosing pairwise equal angles θ is called a rhombohedral lattice (rhomboedrisches) ($a_1 = a_2 = a_3 = a; \alpha = \beta = \gamma = \theta \neq \pi/2$). Show that the reciprocal lattice is also rhombohedral (with lattice constants a^*, θ^*) such that

$$cos\theta^* = -\frac{cos\theta}{1+cos\theta}, \tag{4}$$

$$a^* = \frac{2\pi}{a}(1+2cos\theta cos\theta^*)^{-\frac{1}{2}} \tag{5}$$

Note: It is not necessary to explicitly specify the basis vectors of the direct lattice. Use the formula for the volume of a parallelepiped (Zentralepipedes) with edge lengths a_1, a_2, a_3 and internal angles between them α, β, γ as follows: [2]

$$V = |\mathbf{a}_1||\mathbf{a}_2||\mathbf{a}_3|\sqrt{1+2cos\alpha cos\beta cos\gamma - cos^2\alpha - cos^2\beta - cos^2\gamma} \tag{6}$$

(d)We now consider again the primitive unit cell of a face-centered cubic lattice.
Use your knowledge of the previous tasks to determine the length and angle of the basis vectors of the reciprocal lattice. What type of structure does this reciprocal lattice have? What is the structure of the reciprocal lattice of the body-centered cubic lattice? [2]

(e) Let us look at the hexagonal Bravais lattice (in three dimensions) that was introduced in the lectures. The basis vectors of the primitive unit cell are

$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}}, \quad \mathbf{a}_3 = c\hat{\mathbf{z}}. \tag{7}$$

Calculate the basis vectors of the reciprocal lattice and comment on the structure. [2]