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Exercise for Solid State Physics for Nanoscience
SS 2019
Exercise sheet 1

1.1. Structure of GaAs (4 points)

The GaAs structure is composed by two fcc lattices, one for Ga with origin in 0,0,0 and one for As with origin in ¼ ¼ ¼. The lattice parameter is a=b=c =5.653 Å . Calculate the bonding length between Ga and As and the bonding angle Ga – As – Ga. Calculate the mass density ([g/cm³]) of the compound.

1.2. Visualizing of crystal structures (4 points)

Carbon can crystallize in a variety of structures. Both, diamond and graphite, contain only one chemical element (C). The structure of diamond is the same as the structure of GaAs (both Ga and As atoms have to be replaced by C) with the lattice constant a = b = c = 3.57 Å.
At the same time the structure of graphite is described by means of lattice constants a=b=2.46 Å and c=6.70 Å, $\alpha = \beta = 90°$, $\gamma = 120$ °. The fractional atomic positions are C [0 0 0], C [1/3 2/3 0], C [0 0 1/2], C [2/3 1/3 1/2]. Find the position of atoms inside a parallelepiped, containing at least 4 unit cells along in **a** direction, 4 unit cells in **b** direction and 1 unit cell in **c** direction. Plot the resulting structure in projection along **c** axis (use the different sizes and colors to show the atoms with different z-coordinate).

1.3. Debye-Scherrer Experiment (4 points)

Powder-diffraction, also referred to as Debye – Scherrer method, is used to analyze crystal structures and to identify unknown polycrystalline materials. Figure 1 shows a sketch of the experimental setup, in which the opening angle of diffraction cones is measured on an x-ray film or camera.

1. Make a sketch and clarify that this diffraction angle represents 4θ with θ satisfying the Bragg equation $\lambda = 2d_{hkl} \sin \theta$.

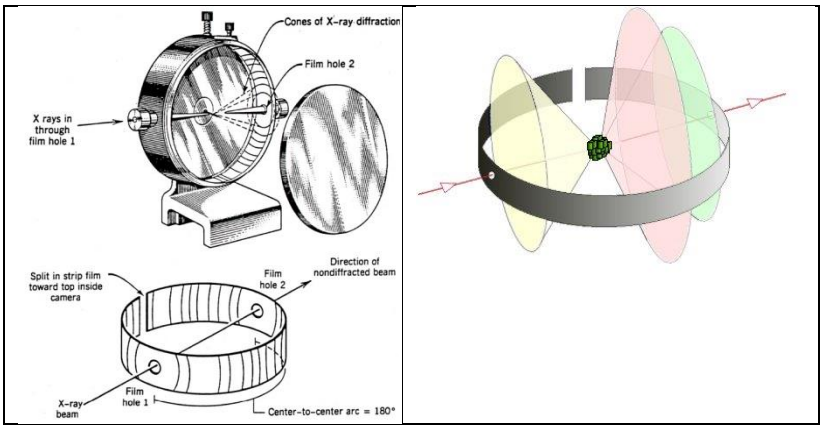

Figure 1: sketch of a Debye – Scherrer camera used for x-ray powder-diffraction. A monochromatic x-ray beam illuminates a powder inside a capillary, placed in the center of a circular x-ray film. The diffraction from the individual crystallites leads to diffraction cones (right), observable on the film.

Using this method, a monoatomic crystal powder was analyzed which is already known to exhibit the diamond crystal structure. The following opening angles of the first five

diffraction cones have been determined: 56.88°; 94.6°; 112.25°; 138.26°; 152.75°, The x-ray analysis was carried out with a wavelength of 1.541Å (Cu-Kα).

2. Determine the lattice constants of the cubic unit cell of the sample. Which substance was measured?