Problem sheet 2: Symmetry groups, Crystal structures, Lattice planes **18.10.2023**

2.1. Polarity and chirality (3 P)

Determine whether or not the following space groups allow polarity and chirality:

(a) $Pbca$

(b) $P4_122$

(c) $Pma2$

Explain your answer. For polar space groups, indicate the polar direction

2.2. Congestion on the surface (3 P)

Consider the crystal structure of cubic germanium. How many Ge atoms per square cm are there on the:

(a) (100) plane?

(b) (110) plane?

(c) (111) plane?

2.3. Lab investigation (5 P)

A bottle in your lab has partially lost its label. One can distinguish the word "cubic", but chemical composition is impossible to read. X-ray powder diffraction experiment (CuK_α radiation, $\lambda = 1.541$ Å) revealed peaks at $2\theta_1 = 23.40°$, $2\theta_2 = 27.09°$, $2\theta_3 = 38.68°$, as well as some further peaks at higher angles.

(a) Calculate distances between the corresponding lattice planes, assuming that all reflections are of first order ($n = 1$ in Bragg's law)

(b) Determine Miller indices of these planes and the lattice parameter

(c) Use Crystallography Open Database to determine what is in the bottle

Note that you may find several matching entries in the database. Choose those that look realistic.

2.4. The problem of resolution (4 P)

You study an alloy that contains a mixture of two very similar cubic phases with the lattice parameters of $a = 3.433$ Å and $a = 3.435$ Å, respectively.

(a) Several x-ray tubes can be found in the storage room of your lab. They produce MoK_α ($\lambda = 0.709$ Å), CuK_α ($\lambda = 1.541$ Å), and CrK_α ($\lambda = 2.291$ Å) radiation. What are the corresponding x-ray energies?

(b) The resolution of your diffractometer is such that reflections have the full-width-at-half-maximum (FWHM) of $\Delta(2\theta) = 0.05°$. Reflections from the two cubic phases can be resolved if their centers are separated by more than FWHM. At which minimum 2θ angle can you resolve the two cubic phases with each type of x-rays? Which x-ray radiation offers the best resolution?

Hint: VESTA has the option of calculating the x-ray powder pattern

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2.5. Departure from regularity (5 P)

You already know the MgB_2 superconductor. Its sibling compound, also a diboride, had a minor accident and became distorted into the orthorhombic symmetry ($a = 4.684$ Å, $b = 2.872$ Å, $c = 4.076$ Å) with four B atoms per unit cell located at $(\pm x, 0, z)$ and $(\pm x + \frac{1}{2}, \frac{1}{2}, -z)$, with $x = 0.192$ and $z = 0.632$.

(a) Write down the explicit coordinates for all four B atoms lying within one unit cell. Sketch the unit cell (the *ab* projection should suffice), place the atoms, and complete the honeycomb network.

(b) Evaluate the deformation of the honeycomb network. Calculate the nearest-neighbor B–B distances and B–B–B angles. How do they compare to the MgB_2 case?