Problem sheet 3: Reciprocal lattice and Structure factor **24.10.2023**

3.1. Reciprocal rules for the lattice centering (5 P)

Derive reciprocal lattice for the bcc and fcc lattices. Use two methods:

(a) Obtain reciprocal lattice vectors from lattice vectors of the conventional unit cell (**a**, **b**, and **c**) and analyze extinction conditions for the structure factor. What is the centering of the reciprocal lattice in each case?

(b) Obtain reciprocal lattice vectors from lattice vectors of the primitive cell ($\mathbf{a}_p$, $\mathbf{b}_p$, and $\mathbf{c}_p$). Confirm that the result is same as in (a).

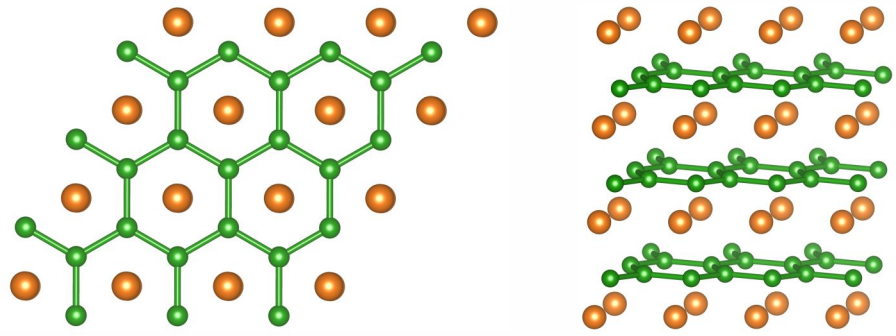
(c) What is the period of the reciprocal lattice (for both fcc and bcc) if you consider it as a lattice with centering?

3.2. Your favorite hexagonal crystal (5 P)

Consider MgB_2 from problem sheet 1.

(a) Draw lattice vectors of the direct lattice and reciprocal lattice. Calculate parameters of the reciprocal lattice: a^*, b^*, c^* and α^*, β^*, γ^*.

(b) Obtain a general expression for $1/d_{hkl}^2$ of a hexagonal crystal and use it to calculate d_{100}, d_{001}, d_{110}, and d_{101} of MgB_2.



You can draw lattice vectors directly on top of these figures, or prepare your own figure in VESTA, or make a sketch of the unit cell by hand

3.3. Ordinary extinctions (4 P)

Obtain reflection conditions for the structure factor of the following crystals,

(a) gypsum ($CaSO_4 \cdot 2H_2O$)

(b) litharge (PbO, tetragonal polymorph)

(c) vanadite ($Pb_5[VO_4]_3Cl$)

In each case, explain how the reflection conditions arise from the lattice centering and symmetry elements of the crystal.

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3.4. Non-ordinary extinction (6 P)

Consider the crystal structures of SnTe and GeTe, both fcc.

(a) Compute d_{111} and d_{200} for each of the two structures

(b) Compute F_{111} and F_{200} for each of the two structures. Atomic form factors can be found here (use values for atoms, not for ions)

(c) Why is F_{111} so low in SnTe?