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Problems for *Physik der Materie III*

Due by May 8, 2019

Series 3: Reciprocal Lattice and Diffraction

3.1 Reciprocal lattice

Consider the primitive translation vectors $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ of the body-centered cubic (bcc) lattice.

(1) Show that the corresponding reciprocal lattice is one of the 14 Bravais lattices by determining the primitive translation vectors $\vec{g}_1$, $\vec{g}_2$, and $\vec{g}_3$. Use orthogonal vectors $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$ of unit length.

(2) Sketch the primitive direct and reciprocal translation vectors, respectively, using cubic cells.

3.2 Miller indices and lattice planes

Consider a cubic unit cell with lattice constant a.

1) Sketch the (110), ($\bar{1}$10), and (210) planes.

2) Determine reciprocal lattice vectors $\vec{G}_{hkl}$ which are perpendicular to these planes. Use orthogonal vectors $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$ of unit length.

3) Determine the spacing d_{hkl} of the plane (hkl).

3.3 Structure factor of fcc and NaCl lattices

The *structure factor* for diffraction from periodic crystals is defined as:

$$S_{\vec{G}} = \sum_j f_j \; e^{-i\vec{G}\vec{r}_j},$$

where $\vec{r}_j$ is the position of the atoms in the basis and f_j is the *atomic form factor* which is determined by the internal structure of the atoms.

(1) Construct the structure factor S_{hkl} for the fcc lattice of identical atoms with $f_j = f$ using a simple cubic cell with the basis (0,0,0), ($\frac{1}{2}$,$\frac{1}{2}$,0), ($\frac{1}{2}$,0,$\frac{1}{2}$), (0,$\frac{1}{2}$,$\frac{1}{2}$). Express the result as a function of the atomic form factor f. Determine S_{hkl} for three cases: All indices h, k, and l being even, all indices being odd, and mixed even and odd indices.

(2) Construct the structure factor S_{hkl} of NaCl, which consists of two fcc lattices shifted by ($\frac{1}{2}$,$\frac{1}{2}$,$\frac{1}{2}$). Refer the basis for both atoms to the simple cubic cell as in (1). Express the result as a function of the atomic form factors f_{Na+} and f_{Cl-}. Determine S_{hkl} for two cases: All indices h, k, and l being even and all indices being odd.

(3) KCl has the sodium chloride (NaCl) structure. For X-ray diffraction, the atomic form factors are almost the same: $f_{K+} \approx f_{Cl-}$. Discuss the consequences for the intensities of (hkl) spots of the diffraction pattern.