

Eðlisfræði þéttefnis I

Dæmablað 3

Skilafrestur 14. September 2017 kl. 15:00

1. Röntgen bylgjubognun – X-ray diffraction (10)

Grindarfasti (lengd tenings) einsatóma bcc kristalls er $a = 4.28 \text{ \AA}$. Reikna skal bylgjubognunarhorn 2θ fyrstu fjögurra toppa (þeirra fjögurra bylgjubognunartoppa sem hafa lægstu 2θ gildi) fyrir duft sýni, þegar beitt er einlitri Röntgen geislun með bylgjulengd $\lambda = 1.5 \text{ \AA}$. (duft sýni þýðir að allar kristallastefnur eru mögulegar í sýninu.)

The lattice constant (length of the conventional cubic cell) of a monatomic bcc crystal is $a = 4.28 \text{ \AA}$. Calculate the diffraction angles 2θ of the first four diffraction peaks (the four diffraction peaks with the lowest 2θ values) from its powder specimen, using monochromatic X-ray with a wavelength $\lambda = 1.5 \text{ \AA}$. (Hint: powder specimen implies that all crystal orientations are possible in the specimen.)

(Próf desember 2016)

2. Röntgen bylgjubeygja – X-ray diffraction (20)

Pólon er eina frumefnið sem kristallast í einfaldan tening. Í bognunartilraun með Röntgengeislum af bylgjulengd 0.1789 nm, beygir fyrstu gráðu toppur, sem tengdur er (110) kristallaplaninu, um hornið 44.51° .

- (a) Hver er grindarfasti pólons ?
- (b) Undir hvaða horni væntir þú þess að finna fyrstu gráðu topp sem svarar til (111) plansins ?
- (c) Undir hvaða horni væntir þú þess að finna annrarar gráðu topp sem svarar til (111) plansins ?
- (d) Í bognunartilraun með rafeindum er 200 keV rafeindageisli notaður til að skoða þunna pólón húð. Reikna hornið sem toppur frá (110) planinu kemur undir.

Polonium is the only element that crystallises in a simple cubic structure. In a diffraction experiment using X-rays of wavelength 0.1789 nm, a first order diffraction peak associated with the (110) crystal plane is deflected through an angle of 44.51° .

- (a) What is the lattice constant of polonium ?
- (b) At what angle would you expect to find the first order peak corresponding to the (111) plane ?
- (c) At what angle would you expect to find the second order peak corresponding to the (111) plane ?
- (d) In an electron diffraction experiment, an electron beam with an energy of 200 keV is used to probe a thin foil of polonium. Calculate the angle through which the (110) diffraction peak is deflected.

(Próf desember 2016)

3. Interplanar separation (10)

Consider a plane hkl in a crystal lattice.

- (a) Prove that the reciprocal lattice vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is perpendicular to this plane.
- (b) Prove that the distance between two adjacent parallel planes of the lattice is $d(hkl) = 2\pi/|\mathbf{G}|$.
- (c) Show for a simple cubic lattice that $d^2 = a^2/(h^2 + k^2 + l^2)$.

4. HCP structure (10)

- (a) Show that the c/a ratio for an ideal hexagonal close-packed structure is $(8/3)^{1/2} = 1.633$. (c is the distance between hexagonally packed planes; a is the distance between nearest neighbors in-plane.) If c/a is significantly larger than this value, the crystal structure may be thought of as composed of planes of closely packed atoms, the planes being loosely stacked.
- (b) Calculate the packing fraction for the ideal close-packed HCP structure.

5. Miller indices (10)

Find the Miller indices for the following planes:

- (a) A plane parallel to both \mathbf{a}_1 and \mathbf{a}_3 .
- (b) The plane containing the points $3\mathbf{a}_1$, $2\mathbf{a}_2$, and $1/2 \times (\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3)$.
- (c) A plane that contains a cube edge and cuts two other cube edges of the same cube at their midpoints, in a simple cubic lattice.