

Answer on Question #73625 - Chemistry - Physical Chemistry

Question:

Explain powder method for determination of crystal structure.

Solution:

A beam of monochromatic rays falls on a polycrystalline sample. The incident rays are reflected from those crystallites which, with respect to the direction of the incident beam, are oriented so that the Wulf-Bragg condition is satisfied. Two methods for recording a diffraction pattern are used: on a photographic film (photomethod) and with a counter (diffractometric method).

The diffraction pattern on the film appears in this case as a series of concentric circles.

The diffractometer registers the picture as an alternation of the background curve and the interference maxima. The latter arise at certain angles of the counter position 2θ . Using the equation for the measured value of the scattering angle θ , it is possible to calculate the interplanar distances d_{HKL} for any diffraction maximum. Further, an assumption is made as to the type of crystal structure of the given material and the values of the indices of the obtained reflections are determined. Then, if this calculation step is completed, you can determine the dimensions of the unit cell. If the chemical composition and density of the material are known, the number of atoms in the unit cell is calculated. Finally, from the integrated intensity of the diffraction lines, it is possible to establish the detailed arrangement of the atoms in the unit cell.