Determination of Structural Defects in Phyllosilicates by X-Ray Powder Diffraction—I. Principle of Calculation of the Diffraction Phenomenon

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Abstract: This paper describes the calculation of the diffracted intensity for models of powdered minerals with lamellar structure, in order to compare experimental and theoretical X-ray diagrams. The calculation takes into account at the same time (i) the possibility of coexistence of different kinds of layers in the stackings, (ii) the possibility of stacking faults between the layers (translative or rotative ones) and (iii) the unavoidable orientation of particles in the powder sample (the method of determination of the orientation is described).

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