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New modeling of X-ray diffraction by disordered lamellar structures, such as phyllosilicates

ALAIN PLANÇON*

Institut des Sciences de la Terre d'Orléans, 1a rue de la Férollerie, 45100 Orléans, France

ABSTRACT

The "classical" modeling of powder X-ray diffraction (XRD) patterns of lamellar structures, such as phyllosilicates, assumes that the samples are composed of "crystals" having various thickness and well-defined translations between layers. This model is able to describe the high-angle domain of XRD patterns but sometimes fails in the low-angle region. The new model proposed here considers the samples to be composed of "particles" that have larger sizes than crystals and contain defects such as cracks, inner-porosity, bent layers, edge dislocations, etc. These defects induce variations in the *d*-spacings, introduced in the calculation by distributions of the *d*-spacings. For phyllosilicates, this model is consistent not only with XRD, but also with small-angle X-ray scattering (SAXS) data, transmission electron microscopy (TEM) results, and high-resolution transmission electron microscopy (HRTEM) observations.