Diffuse Scattering from Composite Crystals Containing Stacking Faults

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The compound $(Ca_2CoO_3)_{0.62}CoO_2$, a potential candidate for a thermoelectric material, has been revealed to be a misfit-layered compound, which consists of two interpenetrating monoclinic subsystems, CoO_2-part of CdI_2-type sandwiches and Ca_2CoO_3-part of ordered three-atom-thick NaCl-type blocks [1]. Sometimes reflections with specific indices showed rather large line-widths in powder diffraction patterns of the compound. They suggested occurrence of stacking disorder in one subsystem or in two subsystems. In some powder patterns of misfit-layered sulfides such as $(PbS)_{1.12}VS_2$, composed of VS_2 sandwiches and two-atom-thick NaCl-type PbS layers [2], selective broadening of the reflections was observed and occurrence of stacking faults was suggested.

An expression for intensity distribution in powder diffraction from a sample containing stacking faults [3] has been modified in consideration the misfit between two-dimensional lattices of the subsystems, and applied to stacking disorder in composite crystals. The analyses have been made for neutron and X-ray powder patterns of faulted $(Ca_2CoO_3)_{0.62}CoO_2$, and X-ray powder patterns of faulted $(PbS)_{1.12}VS_2$. The experimental results have been interpreted satisfactorily on the basis of stacking disorder model.

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