Stacking faults type disorder in layered double hydroxides

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Layered double hydroxides (LDH) are a broad group of widely studied materials. The layered character of these materials and their high flexibility for accommodating different metals and anions make them technologically interesting in a range of areas including catalysis, photocatalysis, gas sorption and separation, medicine, pigments, thermal barriers, polymer fillers, and fire retardants. The general formula for an LDH compound is [M1–xIIIMxIII(OH)2][An–]x/n·mH2O, where MII is a divalent metal cation which can be substituted by an MIII trivalent cation, and An– is a charge compensating anion located between positively charged layers. Here we present a comprehensive study on possible structural disorder in LDH. We show how X-ray powder diffraction (XRPD) can be used to reveal important features of the LDH crystal structure such as stacking faults, random interlayer shifts, anion–molecule orientation, crystal water content, distribution of interlayer distances, and also LDH slab thickness. All calculations were performed using the Discus package, which gives a better flexibility in defining stacking fault sequences, simulating and refining XRPD patterns, relative to other commonly used programs such as DIFFaX, DIFFaX+, and FAULTS. Finally, we show how the modelling can be applied to two LDH samples: Ni0.67Cr0.33(OH)2(CO3)0.16·mH2O (3D structure) and Mg0.67Al0.33(OH)2(NO3)0.33 (2D layered structure). The presented examples show how XRPD can be successfully used for both highly crystalline and very disordered materials. In summary, we present a novel way of modelling the structure function, F(Q), to provide a source of structural information for poorly crystalline and 2D flake-type samples of LDH.

Keywords: Layered Double Hydroxides, stacking faults, powder diffraction