Texture analysis of a turbostratically disordered Ca-montmorillonite

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ABSTRACT

Turbostratic disorder, consisting in a disorder in which different layers have different rotations with respect to an axis, is commonly found in montmorillonite. The effect of this kind of disorder on diffraction profiles is significant and must be taken into account, especially in quantitative phase analysis. The effect of the turbostratic disorder in textured materials has never been investigated. In the present work, we have developed a strategy to perform quantitative texture analysis on turbostratically disordered Ca-montmorillonite aggregates that were uniaxially compressed. Synchrotron diffraction images were analyzed with a Rietveld method and disordered and ordered models are compared. The method proved to be reliable and ready for further applications.

Keywords: Texture analysis, turbostratic disorder, Rietveld method, montmorillonite, synchrotron X-rays

INTRODUCTION

In layered crystalline materials, different kinds of disorder can be present. A fairly common kind is turbostratic disorder, a stacking disorder in which different layers have no regular rotational or translational relationship. This kind of disorder has a systematic effect on diffraction patterns that cannot be modeled using a conventional definition of crystal structure and space group only. Here we describe a new strategy to perform a Rietveld texture analysis of turbostratically disordered montmorillonite.

Among clay minerals, smectites are important for understanding diagenesis, where the smectite-to-ilite transformation is a key process in sedimentary basins (e.g., Cuadros 2006). Also, smectites are studied in material science because of their ion exchange ability and in novel nanostructured materials such as organoclays (e.g., Letaief and Ruiz-Hitzky 2003). Thus, a better understanding of the role of disorder in smectites is important.

Among the smectite group, the most common member is the dioctahedral clay mineral montmorillonite, with an ideal formula R2Si₄O₁₀(OH)₂. Real montmorillonite shows a variable charge in the layers, balanced by cations in the interlayer, where water molecules are present (Moore and Reynolds 1989). The interlayer plays a key role in the physical and chemical properties of montmorillonite because water molecules can be easily added, extracted, or substituted. In addition, cations in the interlayer are very mobile, and this well-known property makes montmorillonite a good ion exchange material (e.g., Abollino et al. 2008).

The crystal structure of montmorillonite is strongly layered: the basic building unit consists of an octahedral sheet with tetrahedral sheets on both sides (this unit is commonly called “T-O-T” layer). These layers are divided by an interlayer containing water and cations to balance the framework charge. The different layers are bonded with weak Van der Waals forces and, therefore, are subject to stacking disorder. Different kinds of disorder have been described in sheet silicates, such as regular rotational and/or translational shifts between layers (see e.g., Bailey 1988 or Artioli et al. 1995 for kaolinite-type structures and Gualtieri 1999 or Kogure et al. 2006 for talc-type structures).

In turbostratic stacking disorder, single layers in the crystal structures are statistically rotated with respect to the stacking axis. Turbostratic disorder is common in montmorillonite, but has also been observed in other layered materials such as graphite (Warren and Bodenstein 1965), boron nitride (Andreev and Lundström 1994; Hubáček et al. 1996), molybdenite (Borsella et al. 1998), and cobalt hydroxide (Ramesh et al. 2003).

The typical effect of turbostratic disorder on X-ray diffraction powder patterns is the strongly asymmetric shape of some peaks, whereas peaks for diffraction planes perpendicular to the stacking axis are symmetrical. In the specific case of montmorillonite, where the stacking axis is parallel to c*, (00l) peaks are not affected and show a symmetrical shape, whereas (hkl) peaks are the most asymmetric. In addition (hkl) reflections with l ≠ 0 and h or k ≠ 0 are extinct (Drits et al. 1984). The particular shape of peaks in a material containing this kind of disorder is shown in the diffraction pattern of Ca-montmorillonite (Fig. 1): the basal reflections (e.g., 001, 002) are symmetrical, whereas other peaks show a more or less pronounced asymmetry. The effect of turbostratic disorder in diffraction is better understood by visualizing the effects in reciprocal space: the scattering intensity parallel to the stacking direction is not affected and there are sharp reciprocal lattice points in the a*-b* plane. The