Characterization of the End of Smectite-to-Illite Transformation: Decomposition of X-ray Patterns

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Abstract: Complex X-ray diffraction (XRD) profiles are described crystallographically by simulating XRD peaks for each phase, and adding the various elementary patterns to fit the experimental X-ray pattern. X-ray patterns of a ground muscovite and three polyphasic diagenetic I/S samples are fitted with this powerful, but time-consuming, technique. In the $6° - 10° 2\theta$ CuKα range, the asymmetry of the muscovite peak is related to a very broad coherent scattering domain size (CSDS) distribution; for the I/S samples the even greater asymmetry is due to the presence of several phases with close, but distinct crystallographic characteristics (I/S, illite, and detrital mica).

A simulation-decomposition approach for modelling XRD patterns is introduced to describe quickly and accurately the various clay minerals (essentially mixed-layer illite/smectite and illite) present in a sedimentary series, and to follow their individual evolution during diagenesis. The theory for these simulations is described briefly. The influence of mixed-layer heterogeneity (the distribution of CSDS, and the distribution of smectite content) on the shape of X-ray peaks is shown theoretically to be minimal. Indeed, for both CSDS and smectite content, the important parameter for peak shape appears to be the mean value of the distribution and not its width and/or its shape. The theoretical limitations of the decomposition method are presented. Minor experimental limitations (reproducibility, experimental peak shape, discrimination) make this method a powerful and reliable tool to describe X-ray patterns. The method is used to show the simultaneous occurrence of three "illitic" phases in a sedimentary series from the Paris Basin. The respective evolution of the three phases is clearly evidenced by using this decomposition method. However, the precise identification of these different phases remains difficult to determine because of the difference in peak width between simulated and experimental X-ray patterns.

Key Words: Decomposition • Diagenesis • Illite • Illite/Smectite • Mixed-layer • Simulation • Smectite • X-ray diffraction

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