Decomposition of X-ray Diffraction Patterns: A Convenient Way to Describe Complex I/S Diagenetic Evolution

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Abstract: Decomposition of complex X-ray diffraction profiles is used on well characterized (image analysis of transmission electron micrographs, X-ray fluorescence chemical analyses) diagenetic samples from the Paris basin. The simultaneous occurrence of three "illitic" phases (mixed-layer illite/smectite or I/S, poorly crystallized illite, and mica-like phase) is shown on the various diffraction peaks of the $2-50$ °2θ CuKα (44-1.8 Å) range. However, because of theoretical and experimental constraints, it is easier to perform the decomposition routine in the $5-11$ °2θ CuKα (17.6-8.0 Å) range. The identification (i.e., illite content and mean coherent scattering domain size) of the various phases is performed by comparing the associated elementary peak characteristics (position, full width at half maximum intensity) with simulated X-ray patterns. When available, the characteristics obtained from the various angular regions are mutually consistent; however, the precise structures of smectite and illite end-members, on the one hand, and the structure of I/S crystallites, on the other hand, are not well known. Consequently, on some angular regions, there is a discrepancy between the characteristics obtained on experimental and calculated X-ray profiles. The definition of more realistic simulation hypotheses for I/S minerals, and for other interstratified clay minerals, would make this powerful and reliable tool to describe X-ray patterns a precise and sensitive identification tool even for complex clay parageneses.

Key Words: Decomposition • Diagenesis • Illite • Illite/smectite • Mixed-layering • Simulation • X-ray powder diffraction

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