Decomposition of Experimental X-ray Diffraction Patterns (Profile Fitting): A Convenient Way to Study Clay Minerals

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Abstract: This paper thoroughly describes the decomposition procedure, using the example of DECOMPXR (Lanson 1990). The steps of the decomposition procedure are: 1) preliminary data processing; 2) decomposition; 3) validation of results; and 4) use of the results. The use of decomposition is restricted to the separation of contributions from various phases. The effect of preliminary data processing steps (data smoothing, background stripping) on profile shape is shown to be limited and their implementation is detailed. Potential experimental limitations such as peak symmetry, experimental reproducibility or discrimination are equally minor. A logical decomposition process starts from the definition of the angular range to be fitted, proceeds with the determination of the number of elementary peaks to be fitted and ends with the check for results consistency.

Numerical data processing is a powerful tool for the accurate identification of monophases, because of the additional parameters available to constrain XRD profile simulation. Ultimately, however, the match over the whole angular range of both the experimental and the simulated patterns remains the only valid way to characterize the phases present in the sample. Additionally, the decomposition procedure permits both the identification of complex clay mineral assemblages and the characterization of their evolution. This step constrains, and may help to determine, the reaction mechanisms of a transformation; and, as a consequence, to characterize and to model the kinetics of this transformation.

Key Words: Clay Minerals • Decomposition • Mixed Layering • Simulation • X-ray Powder Diffraction

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