The Direct Derivation Method: Quantitative Phase Analysis from Observed Intensities and Chemical Composition Data

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We can measure the weight (W) of a solid cube by dividing its volume (V) by the specific volume (d^{-1}) of the same material as that of the cube, and the W can be calculated by $W = V/d^{-1} = Vd$, where d is the density. In the same manner as that of weighing the cube, we can measure the weight of a material by dividing the total sum of scattered X-ray intensities (S) from that material by the scattered intensity per unit weight (a^{-1}) of the same material, that is, $W = S/a^{-1} = Sa$. In quantitative phase analysis (QPA) using the RIR (reference intensity ratio) method, the parameter a^{-1} is obtained experimentally by using the standard reference material. In Rietveld QPA, it is calculated by using a crystal structure model for each component material in a mixture. Atomic parameters are required when we need to calculate the intensity of a reflection or the diffraction pattern. The intensity can, however, be calculated only from the chemical composition data if it is not of individual reflections but of a total sum of diffracted/scattered intensities from the material [1 – 2]. The direct derivation (DD) method, based on this idea, can, therefore, be applied to QPA of any types of mixtures, consisting of components materials in various crystalline states, including amorphous materials. A technical problem, remained to be solved, is how to separate the diffraction pattern of the mixture into individual component patterns for obtaining the S for individual phases. Various whole-powder-pattern fitting (WPPF) techniques are powerful tools for solving the problem: the Pawley method for the pattern decomposition, the full-pattern fitting (FPF) method using observed single-phase diffraction patterns with the background being subtracted, the FPF method without subtracting the background as in a software suite FULLPAT. For a purpose of just separating the diffraction pattern of the mixture into individual component patterns, the fitting functions used in these WPPF techniques can arbitrarily be combined and then fitted simultaneously [3 – 4]. As a recent development of the DD method, the normalization has been introduced to these fitting functions. Then we can shorten the 2θ-range used for WPPF to the target mixture pattern, and thus we can save the time required for intensity data collection without losing the accuracy in QPA. In this report, a brief review of the theoretical background and various examples of applications will be given.

References

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