

The direct derivation (DD) method for quantitative phase analysis: a practical approach using the observed diffraction patterns for profile modeling

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Weight of a solid cube can simply be derived by dividing the volume of the cube by the volume per unit weight of the same material. In the same manner, the weight proportion of the k th component material in a K -component mixture can be calculated by dividing the total scattered intensity from that material (S_k) by the total scattered intensity per unit weight (a_k^{-1}). The magnitude of a_k^{-1} can be calculated from the numbers of electrons belonging to the atoms in the chemical formula and the chemical formula weight, and therefore, if we know the chemical composition of each component material. The formula for calculating the a_k^{-1} was first derived by using the relationship between the height and integrated value of the peak at the origin of the Patterson function¹⁾. It has recently been derived by assuming a general assemblage of atoms in a space like amorphous materials²⁾. Therefore, we can derive weight fractions of individual components irrespective of their crystalline states if a set of S_k can be obtained as observed datasets. Whole-powder-pattern fitting is a powerful technique for separating the observed diffraction pattern of the mixture into individual component patterns and, therefore, for deriving the S_k ³⁾. For a purpose of decomposing the observed pattern, we can arbitrarily combine three kinds of the fitting functions, which have been used in Pawley pattern decomposition, Rietveld structure refinement, and the full-pattern-fitting method using the background-subtracted observed patterns⁴⁾. Recently, we have introduced the background-included observed diffraction pattern of a single phase as the 4th fitting function⁵⁾. This approach requires to prepare the single-phase observed diffraction patterns measured under the same experimental condition as that applied to the target mixture samples, but it is unnecessary to subtract the background intensities. Therefore, it is particularly advantages for the quantification of samples containing low crystallinity materials like hydrates, amorphous component materials, low symmetry materials with many weak peaks in middle and high angle regions *etc.* Some examples of applications, including pharmaceutical materials, will be presented in this report.

References

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