Quantitative Phase Analysis of Industrial Materials Using Newly Developed Direct Derivation Method

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Industrial Materials have played a central role to the development of human civilization from the time unknown. Existing materials are consistently improved by atomic substitutions, admixing and new syntheses. The existing, improved and newly developed materials must then be verified by various analytical tools of their desired composition. Quantitative phase analysis (QPA) of X-ray diffraction data is one such central technique for an accurate compositional analysis of materials.[1)]

A new method of QPA called the Direct Derivation Method (DDM) developed by Hideo Toraya[2)] is discussed in relation to various industrial materials. DDM offers advantage in cases where structural information is not available and only chemical composition is known. Four different types of fitting functions (type A, B, C and C_2) can be arbitrarily chosen and combined in accordance with analysis condition.[3)] The presentation will discuss these different function types in relation to sample types then proposes possible application, where DDM provides better and stable results compared to the existing techniques.

1. Alexander, L. E. & Klug, H. P. (1948). *Anal. Chem.* **20**, 886-889.
2. H. Toraya (2016). *J. Appl. Cryst*., **49**, 1508–1516.
3. H. Toraya (2018). *J. Appl. Cryst*., **51**, 446–455.