

DDM, the new RIR?

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At the end of the year 2016 Hideo Toraya published a paper [1] describing a new method for QPA using just the sum of the net peak areas and the chemical formula of each phase in a mixture as input. This is called the “Direct Derivation” method, in short DDM.

This finding closes a gap in the current theory and tooling. Without the “Direct Derivation” method, 3-dimensional structures (atomic coordinates) are required to fit relative scale factors using the Rietveld method [2]. These refined scale factors are then used for QPA [3].

The “Direct Derivation” method has one drawback however, which is related to peak overlap. Net peak areas are typically determined via a Pawley or a profile fit. Net areas of overlapping peaks are distributed equally between phases, because until now there has been no way to do any better. In the original paper an iterative correction based on (preliminary) QPA results is used to improve the partitioning of overlapping net peak areas between the phases.

Here we describe an enhancement for the partitioning of overlapped peaks. This improvement allows to perform QPA with any database of reference patterns containing a chemical formula. Finally, this could replace the traditional RIR [4] method used for QPA with reference patterns. The new methodology will be available in one of the next HighScore(Plus) [5] releases.

[1] Hideo Toraya, *A new method for quantitative phase analysis using X-ray powder diffraction: Direct derivation of weight fractions from observed integrated intensities and chemical compositions of individual phases*, J. Appl.Cryst. (2016), **49**, 1508-1516.

[2] H.M. Rietveld, *A profile refinement method for nuclear and magnetic structures*, J. Appl. Cryst. (1969), **2**, 65 - 71.

[3] R.J. Hill and C.J. Howard, *Quantitative Phase Analysis from Powder Diffraction Data using the Rietveld Method*, J. Appl.Cryst. (1987), **20**, 467.

[4] F.H. Chung, *Quantitative interpretation of X-ray diffraction patterns, I. Matrix-flushing method of quantitative multicomponent analysis*, J. Appl.Cryst. (1974a), **7**, 513 - 519.

[5] T. Degen, M. Sadki, E. Bron, U. König, G. Nénert, *The HighScore suite*, Powder Diffraction (2014), **29**, 13-18.