

CONVOLUTION BASED PROFILE FITTING

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In convolution based profile fitting profiles are generated by convoluting functions together to form the observed profile shape. For a convolution of n functions this process can be written as

$$Y(2\theta) = F_1(2\theta) \otimes F_2(2\theta) \otimes \dots \otimes F_i(2\theta) \otimes \dots \otimes F_n(2\theta) \quad (1)$$

In powder diffractometry the functions $F_i(2\theta)$ can be interpreted as the aberration functions of the diffractometer [1], leading to the so-called Fundamental Parameters Approach FPA, but in general any combination of appropriate functions for $F_i(2\theta)$ may be used in this context. Most direct convolution fitting methods are restricted to combinations of $F_i(2\theta)$ that can be convoluted analytically (e.g. GSAS) such as Lorentzians, Gaussians, the hat (impulse) function and the exponential function. However, software such as TOPAS [2] is now available that can accurately convolute and refine a wide variety of profile shapes numerically, including user defined profiles, without the need to convolute analytically.

In the literature, convolution based profile fitting is normally associated with microstructure analysis where the sample contribution needs to be separated from the instrument contribution in an observed profile. This is no longer the case. Convolution based profile fitting can be also performed on a fully empirical basis to provide better fits to data and a greater variety of profile shapes.

References:

- [1] H.P. Klug & L.E. Alexander (1954), X-ray Diffraction Procedures, John Wiley & Sons, Inc., New York.
- [2] Bruker AXS (2000): TOPAS V2.0: General profile and structure analysis software for powder diffraction data. Bruker AXS, Karlsruhe, Germany.