VALIDATION OF FUNDAMENTAL PARAMETERS APPROACH SOFTWARE FOR USE IN NIST SRM CERTIFICATION

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The line profile shapes observed in X-ray powder diffraction measurements consist of a convolution of the source emission spectrum, optical aberrations of the diffractometer, and the sample broadening function. The optical aberrations, referred to collectively as the geometric instrument profile function, are the largest source of the asymmetry in the line profiles. Their effect means that the position of maximum intensity in an observed peak cannot be used to directly infer the true *hkl* lattice spacing in the sample. To obtain accurate estimates for lattice spacings, as needed to certify powder diffraction NIST Standard Reference Materials (SRMs) for lattice parameter, the effect of the geometric instrument response function on the line profile must be correctly characterized. The fundamental parameters approach (FPA) provides a complete description of the geometric instrument response. All parameters in FPA models are physically based, with parameters that map directly onto the geometry of the diffractometer. This facilitates the interpretation and evaluation of the line profile model fit. FPA models are used in the certification of SRMs for lattice parameter via the closed-source software program TOPAS (Bruker AXS GmbH, 2010). To validate the FPA models and fits output by this program ('de-black-boxing' this component of the SRM certification process) the FPA models described in Cheary and Coelho (1992, 1998) have been implemented in the R language and environment for statistical computing (R Development Core Team, 2011) and used to perform a suite of comparison studies. The results demonstrate an accurate correspondence between the description of FPA models in the literature and the implementation in TOPAS for all cases thus far investigated.

References

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