An empirical study of the performance of capillary and reflection geometry parallel beam instruments in the context of profile shapes has been completed by using the fundamental parameters approach. Multiple measurements of NIST standards with different instrumental configurations were performed. The beam width, height, and axial divergence were varied for samples in flat plate reflection geometry and in capillary transmission mode. The instrument was equipped with a parabolic multilayer on the incident beam side and a flat multilayer on the diffracted beam side in a + - - configuration.

The use of FP profile fitting allows a full definition of the instrumental parameters necessary to describe the peak shapes. Additional convolutions beyond those defined for a divergent-beam system were investigated. The software TOPAS® from Bruker Analytical X-Ray Systems was used to allow convolution of gaussian and hat functions to describe the transmission profiles of the optics.

The empirical results indicate that the optics provide excellent reproducibility in peak location and that the peak shapes can be modeled with exceptionally low residuals when additional convolutions are included. A discussion of the reliability and applicability of the FP approach for data from a standard commercial diffractometer will be provided.
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OK to put on DXC website  
Oral presentation preferred, but poster OK (XRD session)  
Session: Parallel beam diffraction