

RIETVELD REFINEMENT OF POWDER DATA FROM MULTILAYER AND POLYCAPILLARY OPTICS

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An empirical study of the feasibility of using the standard Rietveld codes to refine data from parallel beam optics is presented. A sealed tube diffractometer was used and equipped as follows:

1. Polycapillary optic for parallel beam on the incident beam side with soller collimator on the receiving side and no diffracted beam monochromator.
2. Polycapillary optic for parallel beam on the incident beam side with soller collimator and LiF diffracted beam monochromator.
3. Parabolic multilayer optic on the incident beam side and soller collimator on the receiving side.
4. Parabolic multilayer optic on the incident beam side and flat multilayer optic on the receiving side.

The quality of the data will be discussed and related to the beam divergence provided by the various optical configurations. The diffraction line shape and FWHM as a function of angle will be presented for comparison to Bragg-Brentano geometry.

Rietveld refinements of powder patterns for NIST standards, including LaB₆ and Si, will be presented. The results demonstrate that the data are fully applicable for Rietveld analysis. The difference between coupled theta-two theta measurements and asymmetric diffraction at fixed incident angle will be covered.