Modeling the IRF of Synchrotron Powder Diffractometers with focusing Optics

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We extend the theory developed by Caglioti, Paoletti, Ricci [1-3] and Sabine [4,5] that provides an analytical description of the Instrumental Resolution Function (IRF) of single crystal and powder spectrometers consisting of collimators and crystals by including the effect of collimating and refocusing mirrors. Two cases are explicitly considered: the case when both collimating and refocusing mirrors are bent to a parabolic shape and the case when the collimating mirror is bent to a parabolic shape and the refocusing mirror is flat. The effect of isotropic sample size is also considered as a possible additional contribution to the peak width.

Experimental IRFs collected at the Swiss Light Source Materials Science beamline powder diffractometer at different photon energies and in both optical configurations are modeled by our analytical expressions and the agreement found is good. All experimental tests are performed using the $Na_2Ca_3Al_2F_{14}$ (NAC) standard powder.

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