

Differential Thermal Expansion and Laboratory Capillary X-ray Powder Diffraction: Progress, Practicalities and Performance

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The challenge for experimental XRPD applied to crystal structure determination, is to obtain the best possible estimates of diffracted intensities. The chance of achieving this is enhanced by using (i) low-*T* data collections to decrease thermal vibration and therefore boost the intensities seen at higher diffraction angles and (ii) new PSD detector technologies yielding improved signal-to-noise and count-rates. Importantly, significant improvements to the extracted intensity information available from overlapping peaks may be gained by using multiple low-*T* data collections, thereby exploiting differential thermal expansion (DTE) [1,2]. Here we present the exploitation of DTE to retrieve an immense amount of accurate intensity data from a series of laboratory capillary X-ray powder diffraction data sets collected at several temperatures. We describe a validated method for intensity extraction and include details on the impact of improved PSD detectors and high intensity laboratory X-ray sources on this approach.

[1] David W. I. F., Shankland K., McCusker L. B., Baerlocher Ch. in *Structure Determination from Powder Diffraction Data*, Ch. 1, David et al. (Eds), Oxford University Press, Oxford, 2002. [2] Zachariasen W. H., Ellinger F. H., *Acta Crystallogr.*, 1963, **16**, 369.

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