Single Crystal Quality Structures from Polycrystalline Samples

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We have recently demonstrated [1,2] a method whereby single crystal quality data can be extracted from polycrystalline samples comprising up to 1000 crystals. The method works by focusing the X-ray beam on the sample such that a sufficiently small active area is illuminated such that the diffraction from the individual crystallites is sufficiently distinct that a some individual spots may be extracted. With these data we simultaneously determine, via a novel algorithm [3], the orientation matrices of the crystallites which constitute the powder specimen.

Given these orientation matrices, the intensities of the contributions from the different crystallites may then be deconvoluted, scaled, and filtered/reweighted by a variety of methods. In this way we determine not only the average structure of a powder specimen, with single crystal precision, but also the distribution of structural properties within the sample.

We have now attempted to apply this technique to progressively more complicated systems; the latest results will be presented.

[1] Schmidt S., Poulsen H.F., Vaughan G.B.M., *J. Appl. Cryst.,* 2003, **36**, 326. [2] Vaughan G.B.M., Schmidt S., Poulsen H.F., *Z. Kristallogr.*, 2004, **219**, 813. [3] Lauridsen E.M., Schmidt S., Suter R.M., Poulsen. H.F., *J. Appl. Cryst.*, 2001, **34**, 744.

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