Exploiting Preferred Orientation to Resolve the Intensities of Overlapping Reflections

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In 1999, Wessels et al.[1] demonstrated the practical viability of the 'texture method' for resolving reflections that overlap in a powder diffraction pattern. By collecting synchrotron data on a textured polycrystalline sample as a function of sample orientation, more information about the relative intensities of overlapping reflections could be obtained. A full texture analysis is used to establish how the crystallites are oriented in the sample, and then a single set of (singlecrystal-like) reflection intensities is extracted via a joint refinement procedure using all diffraction patterns (between 5 and 1296) simultaneously. The data collection and analysis strategies for both reflection and transmission geometries have been described [2]. To develop the method further so that even more complex structures can be accessed, several possibilities are being explored. (1) A new method for preparing textured powder samples using a repetitive pressing procedure has been developed. (2) To optimize the resolution of the data, diagonal displacement of the imaging plate at the maximum sample-to-detector distance has been evaluated. (3) To improve the resolution still further, an experimental setup with a onedimensional Si-microstrip detector, has been devised. (4) A new background and scaling procedure has been implemented in the data analysis software.

[1] Wessels T., Baerlocher Ch., McCusker L.B., *Science*, 1999, **284**, 477. [2] Baerlocher Ch., McCusker L.B., Prokic S., Wessels T., *Z. Kristallogr.*, 2004, **219**, 803.

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