Algorithms for Solving Crystal Structure using Texture

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Texture is generally considered a nightmare for crystal structure solving or refinement. Wessels et al. [1] have demonstrated as texture can be used successfully to help the extraction of reliable structure factors from powder data to employ single crystal like structure solution methods.

The methodology has been extended a little further and some new algorithms will be presented to simplify the procedure in a unique improved step. Using an approach derived from Rietveld Texture Analysis [2] the simultaneous texture determination and structure factors extraction can be done. This was possible by introducing a new texture algorithm (EWIMV) and a texture aware extraction algorithm to combine the two procedures. By this method it is possible to extract structure factors from really highly overlapped pattern and use only one single experiment. An alternative method uses instead a Maximum Entropy Electron Map fitting approach to apply some constraints to the structure factors extraction.

The algorithms were implemented in the software Maud [3] along with other ab-initio structure solution routines for peak finding and indexing (through evolutionary algorithms), space group sorting and refinement constraints (energy computation, fragments etc.). Some examples of application of the methodology will be presented as well.

[1] Wessels T., Baerlocher Ch., McCusker L.B., *Science,* 1999, **284**, 477. [2] Lutterotti L., Matthies S., Wenk H.-R., Schultz A.S., Richardson J. W. Jr, *J. Appl. Phys.*, 1997, **81**, 594. [3] http://www.ing.unitn.it/~luttero/maud

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