Algorithms for Solving Crystal Structure using Texture

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Abstract
Texture is generally considered a nightmare for crystal structure solving and refinement. Well-established [1] have demonstrated that texture can be used successfully to help the extraction of reliable structure factors from powder data to enable single crystal like structure solution methods. The methodology has been extended to other structure factors and some new algorithms will be presented to simplify the procedure in a unique improved step. Using an approach derived from Reitveld Texture Analysis [2] the simultaneous texture determination and structure 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 highly overlayered patterns 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 are 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.

Experiment: only one experiment for everything. powdered spectra must be collected at different tilts and rotation angles such that the sample should be sufficient to ensure the ODF (Orientation Distribution Function) determination. The texture images of 

In a MD simulation performed once every refinement cycle at the end of each iteration step of the minimizing procedure, the electron density map is computed for the new structure resulting from the previous iteration, and the second for the new structure factors using the structure factors computed from the last ODF. The procedure is based on the fact that the texture and structure correlation can be easily resolved if the number of data (spectra) is sufficient to cover the entire ODF. Comparison of some structure factors extracted by this procedure with generating values for the example in Panel 2 and one of the spectra fitted by the method.

MEM-Le Bail F₀ extraction:
To calculate the X-ray diffraction intensities from a PDF (Maximum Entropy Electron Map) method can be used after the Le Bail extraction described before. The steps are:
1. the Rₓₓ extracted by EWIMV (derived from WIMV) can then be used to compute an electron map (normalized to the nominal electron density) for the MEM approach.
2. Rₓₓ, or the new structure extraction/ODF computation is then used.

The electron density map enforce a compatibility of the F-o values for highly overlapping reflections. The MEM algorithm has been derived from the algorithm of REED [4] applying some extra constrains to minimize the number of maxima and the background of the map.

Standard functions in the ODF

In Maud there are two type of standard functions: a fiber component and a spherical component (linear combination of a Gauss and Lorentz standard function). The Gauss spherical component is defined as:

where $\sigma$ is a modified Bessel function.

The Lorentz spherical component is instead:

$$I_0(\gamma) = \frac{1}{2\pi} \left(1 + \frac{\sin(\gamma)}{\gamma}\right)$$

$g_\gamma$ and g are the orientational coordinates in the ODF space, the first being the position of the spherical component.

A fiber component is obtained integrating a Gauss spherical component around the fiber axis $\mathbf{a}$:

$$r_a(\mathbf{r}) = \iint_F r_a(\mathbf{r}) \, d\gamma \, dg$$

Advantages of the use of standard function in a Reitveld fitting:
- the texture is described by refraction parameters
- very sharp textures
- very smooth textures, easy to interpret.
- number and locations of components must be manually defined at the beginning.
- complex textures require several components, thus several parameters.

A Genetic Algorithm approach can be used in Maud to avoid the manual location of the component structure factors. It does not compete with the EWIMV block mode of operation (the prior advantage is to be marked).