

A Direct Approach towards High Resolution Structure Determination without Fourier Inversion,

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For determining one-dimensional centrosymmetric structures or inspecting structural details in projections of known structures we have developed an approach which is based on a point scatterer model and its “geometrical structure amplitudes“. [1] The method provides higher resolution than a Fourier sum, needs less observations and detects either a unique unambiguous solution or all possible scatterer arrangements that are compatible within the experimental uncertainty.

The significant gain in direct space resolution was successfully tested in a feasibility study concerning a possible pseudosymmetric split ($< 0.1 \text{ \AA}$) of the (La, Sr) position in $(\text{La}_{0.5}\text{Sr}_{1.5})\text{MnO}_4$ [2].

Theoretical progress has been made towards relieving some of the initial restrictions imposed on the structure model, i.e. we can show that:

- special positions can be included,
- point scatterers with unequal scattering powers both positive and negative can be handled,
- two-dimensional point structures can be solved, as proven by test calculations.

Additional details of the method as well as test examples, including a case of quasi-homometry, will be presented.

[1] Fischer, K.F., Kirfel, A., Zimmermann, H. (2004). Annual DGK-meeting, Jena (2004).

[2] Kirfel, A., Fischer, K.F. (2004). Annual DGK-meeting, Jena (2004)..