Modulation Functions of Aperiodic Crystals Determined by the Maximum Entropy Method

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The Maximum Entropy Method (MEM) can be used for the reconstruction of the electron density in the unit cell from phased structure factors [1]. The maximum entropy density map (ρ^{MEM}) may provide information about disorder and anharmonic temperature movements. If an informative prior density is employed, ρ^{MEM} may be used to derive the electron density in the chemical bond.

The MEM can also be applied to the electron density in the *n*-dimensional (*n*D) unit cell of the superspace description of aperiodic crystals [2]. We have thus shown that ρ^{MEM} in superspace may provide a model-independent, quantitatively correct determination of the shapes of the modulation functions of incommensurately modulated crystals and incommensurate composite crystals [3]. All procedures have been implemented into a computer program BayMEM, that can be used for a Maximum Entropy analysis of both periodic and aperiodic crystals. In this contribution the features and problems of the MEM will be discussed, and selected applications of BayMEM will be presented [4].

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