Charge Densities of Periodic and Aperiodic Crystals as Studied by the Maximum Entropy Method, Sander van Smaalen[a*] and Lukas Palatinus[b], [a]*Laboratory of Crystallography, University of Bayreuth, 95440 Bayreuth, Germany, and* [b]*Institute of Physics of the Academy of Sciences, Prag, Czech Republic.* E-mail: smash@uni-bayreuth.de

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One of the applications of the Maximum Entropy Method (MEM) in crystallography is the construction of the electron density in the unit cell from phased structure factors [1]. The resulting electron density map (ρ^{MEM}) may provide information about disorder and anharmonic temperature movements or about the electron density in the chemical bond. This information is independent of structural models. 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]. ρ^{MEM} in superspace then provides a model-independent determination of the shapes of the modulation functions of incommensurately modulated crystals and incommensurate composite crystals. Features of the MEM include the facts, that the result is independent of a structural model, and that ρ^{MEM} is a strictly positive function, making MEM densities superior to Fourier maps. Nevertheless ρ^{MEM} contains noise as well as artefacts due to series termination effects in the diffraction data. In this contribution solutions to these problems will be discussed. 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. Selected applications of BAYMEM will be presented, that display the power of the MEM in addressing the full range of crystallographic problems. Applications of BayMEM to aperiodic crystals form the basis for a discussion about the question of the true shapes of modulation functions, and about the information on the modulation functions that is contained in diffraction data.

[1] Gilmore, C. J. (1996). *Acta Cryst.* A**52**, 561-589.
[2] van Smaalen, S., Palatinus, L. and Schneider, M. (2003) Acta Cryst. A **59**, 459-469.