

K3 Charge Densities of Periodic and Aperiodic Crystals as Studied by the Maximum Entropy Method. Sander van Smaalen^a and Lukas Palatinus^b, ^aLaboratory of Crystallography, University of Bayreuth, 95440 Bayreuth, Germany, and ^bInstitute of Physics of the Academy of Sciences, Prag, Czech Republic. E-mail: smash@uni-bayreuth.de

Keywords: Maximum Entropy Method; Aperiodic Crystals; Charge Density

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 (nD) 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.

K4 Microfocus Diffraction with X-ray Synchrotron Radiation. Christian Riekkel, *European Synchrotron Radiation Facility, France. E-mail: riekkel@esrf.fr*

Keywords: Microdiffraction; Single Crystal; Powder

Synchrotron radiation microdiffraction methods have been applied since about 10 years to various types of materials including alloys, minerals, polymers and biopolymers at the European Synchrotron Radiation Facility (ESRF).[1] Methods developed at the ID13 beamline span from single crystal diffraction to powder diffraction extending into the small-angle scattering range. Routinely available beam sizes for user experiments have reached the 0.7 μm scale and a number of test experiments have been performed at the 100 nm scale. Smaller beam sizes have been demonstrated and will become eventually available for user experiments.

Methodological developments allow to select single grains of a few microns diameter from a powder batch and to perform full single crystal structural analysis as shown for a number of inorganic and organic materials. Selecting the right powder grain requires the use of scanning diffractometry, which has originally been developed for the mapping of heterogeneous materials such as skin/core structures in polymer fibres or spherulitic materials. The frontier between single crystal and scanning diffractometry is therefore dissolving and future instrumentation will no longer make a distinction between both techniques.

Texture effects often gain in importance when working at the micrometer scale. As a recent example I will show texture induced by microindentation in polymeric materials. This is just one example for the mapping of deformation zones in bulk materials.

[1] C. Riekkel, *Rep. Prog. Phys.* (2000) **63**, 233-262