s4.m13.o3 **3D reconstruction of quasicrystal approximant structures by electron crystallography.** Xiaodong Zou[a], Zhimin Mo[a], Sven Hovmöller[a], Xingzhong Li[b] and Kehsin Kuo[c], [a]*Structural Chemistry, Stockholm University, SE-106 91 Stockholm, Sweden,* [b]*Center for Materials Research & Analysis, Univ. of Nebraska-Lincoln, Lincoln, NE 68588-0656,* [c]*Beijing Laboratory of Electron Microscopy, P.O. Box 2724, 100080 Beijing, China. Email: zou@struc.su.se*

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Electron crystallography can be applied for solving structures of crystals too small for X-ray diffraction. The advantage of electron crystallography over X-ray crystallography is that the phases of the crystallographic structure factors, which are lost in X-ray diffraction, are present in HREM images. Electron crystallography has been demonstrated on many structures with one short axis[1]. However, for crystals lacking of short axes, atoms may overlap in all directions so several images from different directions must be combined in order to solve the 3D structure. We have reconstructed the 3D structure of a complex quasicrystal approximant ν-AlCrFe ($P6_3/m$, a = 40.687 and c = 12.546 Å). Due to the huge unit cell, it was necessary to combine crystallographic data from 13 projections to resolve the atoms. Electron microscopy images containing both amplitude and phase information were combined with amplitudes from electron diffraction patterns. 124 of the 129 unique atoms (1176 in the unit cell) were found in the remarkably clean calculated potential maps (Fig. 1) [2]. This investigation demonstrates that inorganic crystals of any complexity can be solved by electron crystallography. A method to deduce the structures of several other related approximants is presented.

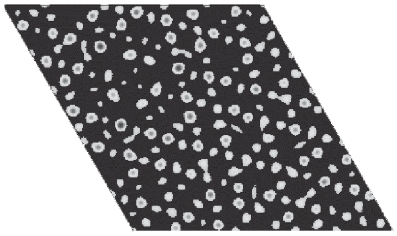

Fig.1. A section of the 3D potential map of ν-AlCrFe obtained by electron crystallography. All atoms are clearly resolved and it is possible to distinguish transition metals (Fe, Cr, strong peaks) from Al (weak peaks).

References

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s4.m13.o4 **Charge Density Studies on Hematite by Convergent Beam Electron Diffraction.** Ralf Theissmann, Helmut Ehrenberg, Hartmut Fuess, Kenji Tsuda, Masami Terauchi, *TU Darmstadt, Materials Sceince, Structure Research, Petersenstr. 23, Darmstadt, GERMANY, Email: zottel@st.tu-darmstadt.de*

Keywords: Charge Density; Electron Diffraction; Hematite

Hematite (α-Fe_2O_3) crystallizes in the corundum type structure (spacegroup R-3c) with the magnetic ions on the threefold axis. Antiferromagnetic ordering takes place at 950 K, a magnetic phase transition occurs at ≈ 250 K, the so called Morin transition. Below the Morin transition the magnetic moments are ordered antiferromagneticaly parallel to [111]. Above, a slightly canted antiferromagnetic arrangement with the spins perpendicular to the [111] direction is observed, which leads to a weak ferromagnetic component (Morin phase). The magnetic ordering of the Morin phase is not in agreement with the crystal symmetry, since the magnetic moments are perpendicular to the threefold axis. This break of symmetry should either result in an orthorhombic distortion of the lattice, a shift of the magnetic ions off the axis (implying static disorder) or an orbital ordering of the valence electrons. None has been reported in the literature.

To investigate the points in question, electron density studies are carried out on a natural hematite. Convergent beam electron diffraction patterns were taken from the three symmetry zone axes [001], [100] and [210] (hex. setting) with the corresponding whole- and bright-pattern symmetries of 3m, 2 and m. The patterns were each measured at room temperature and 90K using a JEOL2010FEF microscope equipped with a Schottky-type field emission gun and a Wollnik-type Ω-Filter [1]. Distortion and background corrections were applied. A maximum of 91 reflections per pattern was fitted using the software package MBFIT, which provides a multi beam nonlinear least squares algorithm for zeroth order and higher order Laue zone (ZOLZ, HOLZ) reflections, fully based on dynamical diffraction theory [2]. The set of fitting parameters contains full structural information (atomic positions, anisotropic Debye-Waller-factors and low order structure factors). Precise lattice parameters and starting parameters for the structural data were taken from Rietveld refinement based on synchrotron powder diffraction data measured at the beamline BL20B2 at SPring8 / Japan [3] at the above mentioned temperatures. The charge density distribution is calculated from the refined low order structure factors.

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