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*

Keywords: Electron crystallography, 3D reconstruction, quasicrystal approximants

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.

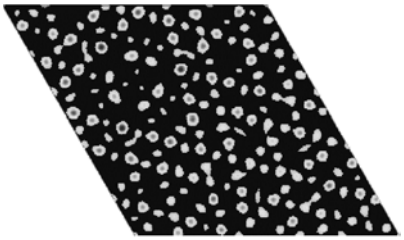

Fig.1. A section of the 3D potential map of ν-AlCrFe obtained by electron crystallography. All atoms are clearly resolved and it is possible to distinguish transition metals (Fe, Cr, strong peaks) from Al (weak peaks).

References

[1] Weirich, T.E., Ramlau, R., Simon, A., Hovmöller, S. & Zou, X.D. (1996) Nature, 382, 144.

[2] Zou, X.D., Z.M. Mo, S. Hovmöller, X.Z. Li & Kuo, K.H. (2003) Acta Cryst.A59, 526.