Modelling of Aperiodic Structures

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Incommensurate structure analysis has come a long way, and many of the specific problems of solving and understanding modulated structures can now be handled with relative ease. Some challenges are however persistent and we are still struggling with how to integrate sparse data with closely spaced reflections etc.

A particular and perhaps unexpected problem is that of modelling. While many modulated systems lend themselves to straight-forward harmonic models and others yield easily once their composite nature is realized there are systems where modelling remains a real challenge.

This contribution will present a number of such cases including one-dimensional systems on the borderline between composite and regular, non-linear composites and 3+2 dimensional systems with strongly non-harmonic occupational modulations.

At the bottom of this is always the problem of limitations in data. Since the fall-of in intensity for high-order satellite reflections is quite sharp, the number of parameters that can be used for modelling is limited and this will always be a challenge for highly non-harmonic modulations. Predefined modulation functions such as saw-tooths and crenel waves help, but for more general shapes the situation is complicated. For 3+2 dimensional cases and even more so for higher dimensional modulations, the problem is even more pronounced.

In the figure (1) below, a section of the electron density for $Ho_{13}Zn_{58}$ shows a behaviour that is particularly difficult to model – A composite structure where the second composite part has a sinusoidal path through the host structure.

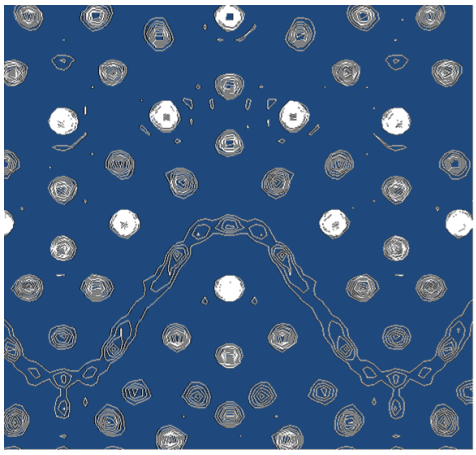

Figure 1. Electron density of a section of the structure of $Ho_{13}Zn_{58}$.

The difficulty here lies in describing the very large amplitude modulations of the Zn positions inside the sinusoidal tube.