Incommensurately modulated crystal structures

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Three classes of aperiodic crystals have been described in the literature [1]: incommensurately modulated crystals, incommensurate composite crystals and quasicrystals. Aperiodic crystals are crystals: their atomic structures are perfectly ordered, they form facets on their surfaces and their diffraction patterns comprise sharp Bragg reflections. They differ from ordinary crystals through the lack of translational symmetry. The latter is restored by the superspace theory developed by De Wolff, Janner & Janssen in the years 1974–1981 [1, 2]. Superspace is a (3+d)-dimensional [(3+d)D] space that is created by the introduction of *d* additional dimensions perpendicular to our 3-dimensional (3D) physical space (d = 1, 2,...). The superspace model for crystal structures is periodic in superspace but not in physical space. For quasicrystals, physical space is often called parallel space and the additional dimensions then form perpendicular space.

Crystal structures of incommensurately modulated crystals are described by a basic structure with translational symmetry in 3D space and modulation functions. The superspace approach restores or generalizes many concepts known for periodic crystals. It allows for a visualisation of the modulation functions in Fourier maps, it provides the symmetry of these materials through so-called superspace groups and it allows for crystal-chemical interpretation of crystal structures with the aid of *t*-plots.

In this lecture I will present the fundamentals of the superspace model for incommensurately modulated crystal structures. I will briefly introduce the concept of symmetry of modulated crystals. Finally, recent examples will be discussed of *t*-plots and the interpretation of crystal structures towards understanding physical properties [3] and chemical properties [4].

References:

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