Quasicrystal and approximant crystal structures

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Quasicrystals (or quasi-periodic crystals) is one type of aperiodic crystals [1]. Other types of aperiodic crystals include incommensurately modulated structures and incommensurately composite crystals [2]. The structure of aperiodic crystals is best understood based on the higher-dimensional crystallography, initiated by P. de Wolf, A. Janner, and T. Janssen [2]. What makes high dimensionality intrinsic to quasicrystals is the absence of a three-dimensional (3D) average structure, unlike the other two aperiodic crystal members. An approximant crystal, whose structure is considered as a structure obtained by applying a shear strain along the orthogonal complementary space to the 3D physical space to a quasicrystal, is an ordinary crystal with a composition and a local structure similar to that of the quasicrystal. Quasicrystals and approximant crystals form a major part of hypermaterials.

In this lecture, I will explain how structure model of quasicrystals can be constructed based on the higher-dimensional crystallography [3]. An icosahedral quasicrystal, for example, is represented as a 6D periodic crystal. When the 6D crystal is cut with the 3D physical space, atoms appear at the intersection of this 3D physical space and what corresponds to atoms (so-called occupation domains, atomic surfaces, or windows, which extend along the complementary space) in higher dimensions, and finally a quasi-periodic atomic arrangement is obtained in the 3D physical space. The section method used here shows that nD crystals can be regarded as a natural extension of crystals into higher dimensions [4]. Thus, the structure determination of quasicrystals comes down to revealing the location, shape, and size of occupation domains, as well as which elements they contain, in a higher dimensional unit cell. The most successful approach for this purpose is structure analysis based on cluster models. As a typical example, I will show a case of Tsai-type icosahedral quasicrystal in some details [5].

References:

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