MS098.O01

Canonical-cell approach to icosahedral quasicrystals and their approximants

Nobuhisa Fujita[1]

[1]*Institute Of Multidisciplinary Research For Advanced Materials, Tohoku Univ., Sendai, Japan*
E-mail: nobuhisa@tagen.tohoku.ac.jp

Recent studies (e.g., [1][2]) have shown that the arrangement of atomic clusters in various approximants to icosahedral quasicrystals can be well described using the so-called canonical-cell geometry, which was first introduced by C. L. Henley in 1991 [3]. The latter geometry allows us to capture a number of complex intermetallic compounds in a unified manner as a packing of icosahedral clusters centered at the vertices of a tiling composed of four fundamental polyhedra, called the canonical cells. In this paper, we illustrate some of the recent developments in the foundation of this concept and demonstrate its ability to describe a variety of complex structures and related structural transformations. In particular, we take up the question whether there exists any quasiperiodic canonical-cell tiling or not. Although this would be a critical issue in order for us to apply the present approach to icosahedral quasicrystals, the possible existence of such a tiling has been controversial for almost a quarter of a century. We settle this issue by proving that there exists a certain inflation rule for the canonical cells with a scaling factor of τ^3 (τ is the golden mean). It turns out that the quasiperiodic tiling obtained using this inflation rule exhibits a super-lattice ordering associated with a decomposition of the standard P-type icosahedral lattice into four equivalent sub-lattices. Each of the sub-lattices is identified as the coincidence site lattice of order 4 associated with a 4-fold rotation about a 2-fold axis. This implies that our quasiperiodic canonical-cell tiling does not maintain icosahedral symmetry in a strict sense, although the breaking of symmetry is weak. We also consider the relevance of `phason flips' in the canonical-cell approach to the structural understanding of related compounds. Whereas unlimited kinds of phason flips can generally take place in canonical-cell tilings, we show that a simple mode of local flips is responsible for a microscopic merohedral twinning which we have recently observed in an approximant phase in Al-Pd-Ru. A Monte Carlo study predicts that there exists a peculiar kind of order-disorder phase transition in close connection with the twinning.

[1] Kreiner, G. (2002). J. Alloys Compd. 338, 261-273.
[2] Fujita, N. et al. (2013). Acta Cryst. A69, 322-340.
[3] Henley, C. L. (1991). Phys. Rev. B43, 993-1020.

Keywords: icosahedral quasicrystal, canonical-cell tiling, cluster