MS29-O4 Quasiperiodic canonical-cell tiling with cubic symmetry

Nobuhisa Fujita[1]

1. Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan

email: nobuhisa@tagen.tohoku.ac.jp

In canonical-cell tiling models [1] for icosahedral quasicrystals and their approximants, the atomic structure is presented as a packing of icosahedral clusters sitting on the vertices of a tiling composed of four standard polyhedra (A, B, C, and D), called the canonical cells. The canonical-cell geometry has indeed been observed in many approximants to icosahedral quasicrystals in different alloy systems. It is hence naturally expected that the same geometry holds also for icosahedral quasicrystals, and if so the canonical cells should be able to tile the space in a quasiperiodic manner so that icosahedral symmetry is globally retained. However, the existence of a tiling like the latter one has never been proved. In this work, an inflation rule for the canonical cells is worked out, and the existence of a quasiperiodic canonical-cell tiling has been confirmed for the first time. In the present inflation step, each canonical cell is expanded by a factor of τ^3 (τ: golden mean), and it is then divided into cells of the original sizes. Importantly, there are several different ways to divide expanded cells of the same shape (e.g. A) depending on their surrounding environment, still the division rules are determined locally. The atomic surface of this quasiperiodic canonical-cell tiling is studied by taking the perp-space images of the vertices. Interestingly, the atomic surface exhibits cubic symmetry rather than icosahedral symmetry.

[1] C. L. Henley, Phys. Rev. B 43, 993-1020 (1991).

MS29-O5 Unit-cell twinning in quasicrystals

Erik Zupanič[1], Albert Prodan[1], Herman J.P. Van Midden[1]

1. Jožef Stefan Institute, Ljubljana, Slovenia

email: erik.zupanic@ijs.si

The discovery of quasicrystals [1] rose questions about some basic concepts of crystallography [2,3]. Their structure and the corresponding electron diffraction patterns are explained by means of unit-cell twinning. The twinning operation is applied onto primitive golden rhombohedra, obtained by a small deformation of a parent cubic close-packed structure. The deformation accounts for the required space filling and for the five-fold point symmetry. Stacking of the multiply twinned star polyhedra ("stellae dodecangulae") keeps the golden rhombohedra of adjacent nano-domains in-phase, regardless of their actual separation. The golden rhombohedra form a kind of an intergrown multiply twinned structure, with no obvious boundaries between individual twins.

By taking into account only low-index first order reflections it is shown that unit cell twinning enables a complete reconstruction of the quasicrystalline reciprocal space, with all remaining reflections being accounted for by strong dynamical scattering or belonging to weak higher-order reflections at the outskirts of the zero-Laue zone (Fig.1). Simulated diffraction patterns are in good accord with the published experimental ones of $MnAl_6$ [4].

Twinning and tiling are two fully compatible approaches and quasicrystals do not violate any of the existing crystallographic concepts. The golden rhombohedra, which represent the basic building elements, are small in comparison with the huge cubic cells, suggested in the past. No atoms, and the close packed ones in particular, can be ordered at distances of the order of a few nanometers, because there are no natural forces acting at such distances. When structures with huge unit cells indeed appear, they can only be a result of at least two competing periodicities, which lock-in after relatively large distances. That is also the case in quasicrystals, where the star polyhedra are a result and not the origin of multiple twinning, whose driving force is obviously the need to fill the space exactly with the slightly collapsed parent structure.

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