

Simple decoration model for icosahedral quasicrystals based on AUC approach

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The structure solution and refinement of icosahedral quasicrystals remains still very difficult task for crystallographers. The most problematic is to find an appropriate model corresponding to atomic structure. Models used for structural solution of such systems like *i*-AlCuFe, *i*-AlPdMn or *i*-CdYb are based on higher-dimensional description (atomic surface modeling) and cluster approach (see, e.g. [1]). Within this approach the shell-like cluster shape is known from corresponding approximant crystal structure. Such models use the Ammann Tiling (called also 3D Penrose Tiling) as a framework structure for cluster centers in internal (perpendicular) space.

In this presentation, another approach is proposed as a way of structure modeling of icosahedral quasicrystals. The so-called statistical description as a method complementary to higher dimensional description uses the idea of Average Unit Cell (AUC). This approach allows modeling quasicrystals in real (parallel) space only with no need of introducing the mathematical 6D description. Every atom position in a given building unit corresponds to a distribution in Average Unit Cell. Such a distribution is formed by projections of atomic positions onto the reference grid, which is periodic. The distribution is dense and uniform and it follows the so-called TAU2-scaling rule. The statistical approach has been recently successfully applied for refining number of decagonal quasicrystals by Kuczera *et al.*

As the structural units for icosahedral quasicrystals two Ammann rhombohedra (prolate and oblate) are considered. The simple decoration scheme means that atoms are placed on vertices and mid-edge positions of both rhombohedra and on a long diagonal of the prolate rhombohedron. This scheme has been used for structure modeling of *i*-CdYb within higher dimensional approach. First application of statistical approach to icosahedral model structure was successfully proposed for non-decorated Ammann Tiling [2,3]. The structure factor for arbitrarily decorated Ammann Tiling within statistical description was recently obtained. The details about the model of icosahedral quasicrystals based on Ammann Tiling with simple decoration scheme within statistical approach will be presented.

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