The interstitial structure of icosahedral quasicrystals

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Although the atomic structure of icosahedral quasicrystals (iQCs) is considered as a quasiperiodic arrangement of atomic clusters, gaps need to be filled remain in-between the atomic clusters for the complete space-filling description. The Tsai-type i-QCs are described by means of an atomic decoration of the three building units, namely, rhombic triacontahedron (RTH), acute rhombohedron (AR) and obtuse rhombohedron (OR) [1-4]. Two types of short connection between adjacent RTHs are allowed: *b*-linkage sharing a rhombus face along a two-fold axis and *c*-linkage sharing an OR along a three-fold axis. As the underlying geometry, this successful structural description of iQCs relies on Ammann-Kramer-Neri (AKN) tiling composed of AR and OR units with the same edge length [5]. Since a RTH is considered as consisting of ten ARs and ten ORs, the gaps existing in-between RTHs can be characterized fully by AR and OR units, whose atomic decorations can be given uniquely in this case.

A similar structural description with the three building units is also possible to other iQCs characterized by Bergman-type and/or Mackay-type atomic clusters [6,7]. The atomic decorations of the AR and OR units in this case may depend on their local environments. It is thus individual interstice that appears as a multiple combinations of the AR and OR units needs to be considered. In this contribution, I identify the set of nine possible gap structures, provided that the cluster centers are generated by the occupation domain of twelvefold packing vertices of an AKN tiling, i.e. Henley's polyhedron [8]. As an application of this approach to the structure description of iQCs, I discuss the atomic structure of F-type Al-based iQCs whose structure is characterized by pseudo-Mackay type and mini-Bergman-type clusters [9].

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