MS23-2-2 Dual nature of CdYb quasicrystal: the structure with Bergman or Tsai clusters?
#MS23-2-2

I. Buganski [1], R. Strzalka [1], J. Wolny [1]
[1]AGH - Krakow (Poland)

Abstract
The atomic structure model of CdYb [1] quasicrystal became a universal standard for all icosahedral quasicrystals with Tsai clusters. The model is praised for its geometrical simplicity and chemical order. Atoms cluster in simple shapes like icosahedron, triacontehedron, etc. Clusters are linked via rhombic faces of triacontahedron along 2-fold axis (b-linkage) and interpenetrate along 3-fold axis (c-lnkage). The unaviodable gaps between clusters are filled with rhombohedral units decorated according to the simple-decoration scheme derived based on identity to existing approximiant periodic strucutres with cubic unit cell.
Recently, a structural model of ZnMgTm icosahedral quasicrystal was developed [2]. The model was founded on different principia than the CdYb model. The unique decoration of rhombohedra in Amman-Kramer-Neri tiling was found and exploited for strucutral study. When the model was interpreted for atomic clusters, the linkage along 5-fold axis was found, that does not exist in periodic approximant crystals. Not only that. The additional linkage discards the neccessity of having interstitial atoms occupying positions outside of clusters making the model interpretable as a covering of triaconsthedral clusters with Bergman inner shells.
Due to the fact that the principia standing behind the model of ZnMgTm are not reserved exclusively to Bergman quasicrystals, we decided to apply the model to CdYb icosahedral quasicrystal. We found out the model can be successfully solved in the tiling-and-decoration scheme with Tsai clusters as a covering. The crystallographic R-factor of the model reached 11.5% for over 5000 symmetry-independent diffraction amplitudes. Not only that. The model can be equally well interpreted as the covering with Bergman clusters what is also evident in the electron density maps recovered based on the experimental diffraction aplitudes phased with charge flipping algorithm. Both models will be discussed during the presentation.

References
[1] Takakura, H., et al., Nature Mat. 6 (2007), 58-63
[2] Buganski, I., et al., Acta Cryst. A76 (2020), 180-196