Poster

The real space approach to the atomic structure of Tsai-type quasicrystal

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The great breakthrough in understanding the atomic structure of iQCs came with the model of binary $Cd_{5.7}Yb$($Cd_{85.1}Yb_{14.9}$) phase [1] that provided a template for other QC structures in the Tsai-type family. It was the first binary iQC to be discovered together with $Cd_{85}Ca_{15}$. Two periodic approximant crystals (PACs) with cubic symmetry, 1/1 Cd_6Yb and 2/1 $Cd_{5.8}Yb$, were known for i- CdYb and provided information on the local atomic arrangement that was adapted for QC. The novelty of the model was that the structure was understood as interpenetrating rhombic triacontahedral (RTH) clusters with a concentric Tsai-type shell structure.

The solution of the binary $Cd_{5.7}Yb$ phase, which falls under the Tsai-type category of icosahedral quasicrystals, involves assigning a unique atomic arrangement to the rhombohedral units within the Ammann-Kramer-Neri tiling [2]. This distinctive decoration applies specifically to units with an edge length of 24.1 Å and $\bar{3}m$ internal point symmetry. The structural refinement process utilizes two underlying tilings derived from the projection method in a 6D space. The discrepancy lies in the origin point placement: one tiling situates it at the vertex, while the other places it at the center of the 6D unit cell. Consequently, these tilings are mutually dual. The selection of the tiling has a negligible impact on the final structural model, with both converging to an R-factor of approximately 11.5%. The primary disparity involves the treatment of the Cd4 tetrahedral motif, which can be either orientationally ordered and aligned with the 3-fold axis, or disordered and represented as a partially occupied icosahedron. Both models manifest themselves as a coverage of rhombic triacontahedral clusters, with identical cluster positions within rhombohedral units. The shell structure adheres to the Tsai type in one tiling and to the Bergman type in the other.

The 6D approach was utilized solely to analyze interatomic correlations, while the refinement itself took place in real space, employing the average unit cell method. It was demonstrated that the structure can be depicted as covered by either Tsai clusters or Bergman clusters, with a short *a*-linkage evident along the five-fold axis. Bergman clusters show analogous local distortions found in Tsai-type periodic approximant crystals, including vacancies within the outer icosahedral shell (Figure 1.) [3]. The positioning of cluster centers, whether Tsai- or Bergman-type, within the quasicrystal is intricately tied to shifts in electron density along the body diagonal of the 6D unit cell. Regarding the treatment of the tetrahedron within the Tsai cluster, it can either maintain orientationally ordered unity or exist as a partially occupied icosahedron without breaking icosahedral symmetry.

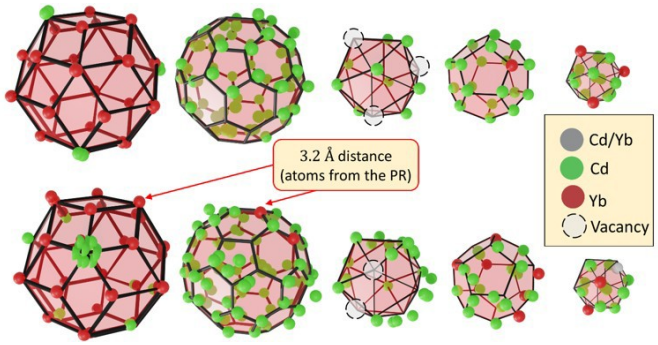

Figure 1. The atomic decoration of Bergman cluster shells in the refined model of i-CdYb. Vacancies and atomic distortions are visible and correspond to known systematic deviations observed in Bergman clusters found in Tsai-type structures.

[1] Takakura, H., Gómez, C. P., Yamamoto, A., de Boissieu, M. & Tsai, A. P. (2007). *Nat. Mater.* **6**, 58–63.

[2] Buganski, I., Strzalka, R., Wolny, J. (2024). *Acta Cryst. B***80**, 84-93.

[3] Buganski, I., Wolny, J. (2023). *J. Alloy. Compd.* **939**, 168823.