

MS23-P02 | THE REAL SPACE REFINEMENT OF THE ICOSAHEDRAL QUASICRYSTAL

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The icosahedral quasicrystal (i-QC) is an aperiodic crystal exhibiting an icosahedral symmetry. The state-of-art of the i-QC structure solution is the Takakura's model, vastly used for numerous quasicrystals with Tsai cluster and recently, Mackay cluster. The model, proposed for the i-CdYb is set in a 6D space, where atoms are grouped in three domains, called occupation domains, extended along the 3D perpendicular space. In addition to the occupation domain of the cluster atoms, there are the interstitial atoms to be modelled. The third known type, the Bergman-type, frequently found in ZnMg alloys, was never successfully refined with the cluster approach.

To find the structure of i-ZnMgTm, we have chosen a different approach. We have resigned from the cluster-based model and focus on a real space structure refinement based on the decoration of the Ammann-Kramer-Neri tiling. With the *Supeflip* software we obtained an *ab initio* structure solution which served to find a unique decoration of two golden rhombohedra with an edge length of 24.1 Å. To reduce the number of parameters during a refinement, the asymmetric part of each rhombohedron was used. The refinement concluded with $R=9.7\%$, which is one of the best results among obtained for an icosahedral quasicrystal.

After the model was refined, we were able to confirm the existence of three occupation domains by lifting the structure to a 6D space. The similarity to the simple decoration model is found.