The atomic structure of Bergman-type icosahedral ZnMgTm quasicrystal

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The icosahedral quasicrystal (i-QC) is a quasiperiodic crystal having an icosahedral symmetry. The state-of-art of the i-QC structure solution is the cluster-based model. The model, proposed for the i-CdYb, resulted in an excellent agreement with the X-ray diffraction pattern [1]. It is set in a 6D space, where atoms are grouped in three domains, called occupation domains, extended along the 3D perpendicular space. The model was successfully used to describe Tsai-type and Mackay-type i-QCs. The third known type, the Bergman-type, frequently found in ZnMg alloys, was never successfully refined with the cluster approach. ZnMg alloys are extensively studied for their mechanical properties and potential medical applications. Recently, the superconductivity in i-AlZnMg was observed [2]. That discovery signifies the importance of understanding the structure of QCs in ZnMg-based alloys. Without it, further advences in the research can be ceased .

The existing hurdle for the structure solution of the ZnMg-based Bergman-type i-QC in a cluster approach is that it does not uniquely determine the atomic decoration of the interstitial part of the structure (decoration of golden rhombohedra outside of atomic clusters) [3]. A local-environment-dependent decoration, contrary to a unique decoration of rhombohedra in the i-CdYb, makes difficult to give a definite shape of each occupation domain, which are indispensable for a 6D structure refinement.

To find the structure of i-ZnMgTm, we have chosen a different approach. In this work 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. By the use of *Supeflip* software we were able to obtain an *ab initio* structure solution with an R-factor≅ 14% for unique 3010 Bragg reflections that helped to find a unique decoration of two golden rhombohedra with an edge length of 24.1 Å (Fig. 1). To reduce the number of parameters during a refinement, the asymmetric part of each rhombohedron was used. Bergman-type cluster, as a motif, still exists in the structure but is no longer a fundamental building unit of the present model. The refinement concluded with $R(F)$=9.7%.

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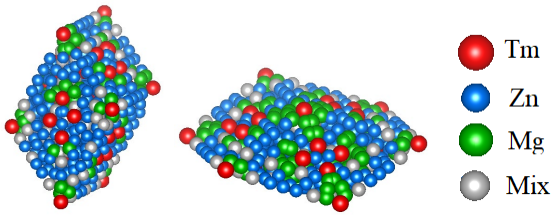

Fig. 1: The atomic decoration of the prolate (left) and the oblate (right) rhombohedra forming the structure of the i-ZnMgTm QC. “Mix” atomic position is not assigned to a particular element but is a mixture of components.