

MS25 Quasicrystal and approximant: structure and properties

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MS25-P1 Two-shell nanoclusters in intermetallic compounds: beyond the icosahedral core

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In this work, we apply the nanocluster method [1] to analyze all known intermetallic compounds containing two-shell nanoclusters with icosahedral core. Using the ToposPro program package [2] we have found all intermetallics with two-shell nanoclusters as primary nanoclusters or local configurations., we have analyzed in more details Mackay, Bergman, Bergman-based and two types of icosahedral-based 63-atom nanoclusters, which have been discovered for the first time using the nanoclustering procedure [3]. With the TTN collection [4] we have found that the four isomeric 63-atom clusters occur in 60 topological types of intermetallic compounds, and only two models of these clusters contain icosahedral inner polyhedron. We have also studied all kinds of isomeric Bergman-type 0@12@32 and 1@12@32 nanoclusters, which occur in intermetallics. Simplification of the nanocluster representations to their underlying nets revealed widespread topologies such as body-centered cubic (**bcc-x**), face-centered cubic (**fcc**), and hexagonal primitive (**hex**). We have performed topological analysis of these intermetallics in terms of local and overall binding of clusters. The statistical data on chemical composition of the nanoclusters and their topological descriptors are presented. We have found 23 and 3 different topologies for binding of the intermetallics composed of the Bergman clusters and 63-atom clusters, respectively. As a result, the correlations between topological parameters and chemical composition of the nanoclusters were found. For instance, if the inner icosahedron of a Mackay nanocluster consists of the same atoms and composition of the second shell is 30A+12B, the topology of underlying net is **bcc-x** in 82% cases. The results of our analysis are included to the set of the ToposPro topological collections.

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