gamma-Brass Polyhedral Core in Intermetallics: The Nanocluster Model

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Abstract

Using the TOPOS program package, 26-atom nanoclusters of the gamma-brass (Cu5Zn8) type (0@4@22 or 0@8@18) were found in 5918 crystal structures of cubic intermetallics. The nanocluster models were built for all the intermetallics using a recently developed algorithm implemented into TOPOS. The relations of the structures based on the 0@4@22 core are explored as a result of migration of atoms between different shells of the nanoclusters. It is shown that the 0@4@22 nanoclusters frequently occur as building units of intermetallics of different composition and structure type. Regularities in chemical composition of 702 gamma-brass-type nanoclusters were found within both the nanoclusters approach (multishell structure) and the nested-polyhedra model. A database containing all topological types of gamma-brass nanoclusters is created with which one can search for the corresponding atomic configuration in any intermetallics.

Keywords

KeyWords Plus: CUBIC A6B COMPOUNDS; CRYSTAL-STRUCTURE; UNIT CELLS; PHASE; COMPOUND; SYSTEM; SUPERSTRUCTURE; CHEMISTRY; CLUSTERS; DATABASE

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