

Web of Science

Search

Search Results

My Tools ▾

Search History

Marked List

Add to Marked List

57 of 723

gamma-Brass Polyhedral Core in Intermetallics: The Nanocluster Model

By: [Pankova, AA](#) (Pankova, Arina A.)^[1]; [Blatov, VA](#) (Blatov, Vladislav A.)^[1,2]; [Ilyushin, GD](#) (Ilyushin, Gregory D.)^[3]; [Proserpio, DM](#) (Proserpio, Davide M.)^[1,4]

[View ResearcherID and ORCID](#)

INORGANIC CHEMISTRY

Volume: 52 Issue: 22 Pages: 13094-13107

DOI: 10.1021/ic4019713

Published: NOV 18 2013

[View Journal Impact](#)

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

Author Information

Reprint Address: Blatov, VA (reprint author)

+ Samara State Univ, SCTMS, Ac Pavlov St 1, Samara 443011, Russia.

Addresses:

+ [1] Samara State Univ, SCTMS, Samara 443011, Russia

- [2] King Abdulaziz Univ, Fac Sci, Dept Chem, Jeddah 21589, Saudi Arabia

Organization-Enhanced Name(s)

King Abdulaziz University

+ [3] Russian Acad Sci, Inst Crystallog, Moscow 117333, Russia

+ [4] Univ Milan, Dipartimento Chim, I-20133 Milan, Italy

E-mail Addresses: blatov@samsu.ru; davide.proserpio@unimi.it

Funding

Funding Agency	Grant Number
Russian government	14.B25.31.0005
Russian Foundation for Basic Research	12-02-00493 13-07-00001

Citation Network

14 Times Cited

57 Cited References

[View Related Records](#)



Create Citation Alert

(data from Web of Science Core Collection)

All Times Cited Counts

14 in All Databases

14 in Web of Science Core Collection

0 in BIOSIS Citation Index

0 in Chinese Science Citation Database

0 in Data Citation Index

0 in Russian Science Citation Index

0 in SciELO Citation Index

Usage Count

Last 180 Days: 0

Since 2013: 11

[Learn more](#)

Most Recent Citation

Shevchenko, V. Ya. [Modeling of self-organization in crystal-forming systems: Symmetry and topology codes of cluster self-assembly of icosahedral structure Sc12B185C9 \(P6/mmm, hP212\)](#). GLASS PHYSICS AND CHEMISTRY, MAR 2017.

[View All](#)

This record is from:

Web of Science Core Collection
- Science Citation Index Expanded

Suggest a correction

If you would like to improve the quality of the data in this record, please [suggest a correction](#).

Cariplo Foundation	
Landau Network-Centro Volta (Como-Italy)	

[View funding text](#)

Publisher

AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036 USA

Categories / Classification

Research Areas: Chemistry

Web of Science Categories: Chemistry, Inorganic & Nuclear

Document Information

Document Type: Article

Language: English

Accession Number: WOS:000327225900032

PubMed ID: 24083847

ISSN: 0020-1669

eISSN: 1520-510X

Other Information

IDS Number: 255FX

Cited References in Web of Science Core Collection: [57](#)

Times Cited in Web of Science Core Collection: [14](#)