

CRYSTAL STRUCTURES OF INTERMETALLIC COMPOUNDS WITH CORE-SHELL CLUSTERS. NEW POINT OF VIEW.

Dmytriv G.¹, Pavlyuk N.^{1,2}, Pavlyuk V.^{1,2}, Ehrenberg H.³

¹Department of Inorganic Chemistry, Ivan Franko National University of Lviv,
Kyryla & Mefodia str. 6, 79005 Lviv, Ukraine,

²Częstochowa Jan Długosz University, Institute of Chemistry,
al. Armii Krajowej 13/15, 42200 Częstochowa, Poland

³Institute for Applied Materials (IAM), Karlsruhe Institute of Technology (KIT),
Hermann-von-Helmholtz-Platz 1 D-76344 Eggenstein-Leopoldshafen Germany
gr_dmytriv@yahoo.com

There are many different concepts that describe the crystal structure of intermetallic compounds because there are numerous types of them. In our presentation, we will focus on some intermetallic compounds with core-shell clusters and will try to show how the interpretation of their structure can be connected with an unusual point of view, namely some works of art.

First of all we are presented crystal structures of $\text{Li}_{20}\text{Mg}_6\text{Cu}_{13}\text{Al}_{42}$ (sp. gr. *Im-3*, $a = 13.8451(2)$ Å), $\text{Mg}_9\text{Ni}_6\text{Ga}_{14}$ (sp. gr. *Fd-3m*, $a = 19.8621(1)$ Å), $\text{Mg}_3\text{Ni}_2\text{Ga}$ (sp. gr. *Fd-3m*, $a = 11.4886$ (17) Å) and $\text{MgMn}_4\text{Ga}_{18}$ (sp. gr. *P4/mmm*, $a = 6.3116(9)$ Å, $c = 9.944(2)$ Å). The crystal structures of all these intermetallic compounds were studied by single crystal method and confirmed by X-ray powder diffraction. The results of electronic structure calculations for all these compounds confirm the three-shell clusters.

In the literature such type of structure was described as “matryoshka clusters” [1] and we will show that this definition is not fully correct and must be changed. First of all this definition is completely wrong from point of view of symmetry of such type of compounds. In historical concept there are at least three another concepts for describing compounds with core-shell clusters. The first concept is ivory puzzle balls, the second is “contrefait Kugeln” and the third is Johannes Kepler’s Platonic Solids model of the Solar system from *Mysterium Cosmographicum*.

References:

1. Xiaoming Huang, Jijun Zhao, Yan Su, Zhongfang Chen, R. Bruce King. Design of Three-shell Icosahedral Matryoshka Clusters $\text{A@B}_{12}\text{@A}_{20}$ ($\text{A} = \text{Sn, Pb}$; $\text{B} = \text{Mg, Zn, Cd, Mn}$) // Scientific Reports. – 2014. – Vol. 4. – P. 6915