MS13-1-3 $MgMn_4Ga_{18}$: new structural type with three core-shell cluster packing
#MS13-1-3

N. Pavlyuk [1], V. Pavlyuk [1], G. Dmytriv [1], H. Ehrenberg [2], S. Indris [2], B. Schwarz [2]
[1]The Ivan Franko National University of Lviv - Lviv (Ukraine), [2]Institute of Applied Materials- Energy Storage Systems (IAM-ESS) of Karlsruhe Institut für Technologie (KIT) - Karlsruhe (Germany)

Abstract. The new ternary gallide $MgMn_4Ga_{18}$ was synthesized by induction melting from the pure elements in a sealed tantalum crucible. The crystal structure was studied both by single crystal and powder X-ray diffraction. Single crystal diffraction data were collected at 20 degrees C on an Xcalibur™3 CCD diffractometer with graphite-monochromatized Mo- or Cu-Ka radiation. Scans were taken in the u-mode, the analytical absorption corrections were made by CrysalisRed [1]. Crystal structures of the compounds were solved by direct methods and refined using the SHELX-97 software package [2]. The $MgMn_4Ga_{18}$ structure (tP23, *P4/mmm*, *a* = 6.3116 (9) Å, *c* = 9.944 (2) Å) can be described as a three-core-shell cluster compound. The Mg atoms are surrounded by 16 adjacent Ga atoms [$MgGa_{16}$] in the form of an octadecahedron. The [$MgGa_{16}$] octadecahedron is encapsulated within the [Ga_{32}] icohexahedron, which is again encapsulated within a [Ga_{40}] pentacontaoctahedron, forming as a result three core–shell cluster [$MgGa_{16}$@Ga_{32}@Ga_{40}].The electronic structure calculations were performed by means of the TB-LMTO-ASA program and they confirm the core–shell packing of these clusters.

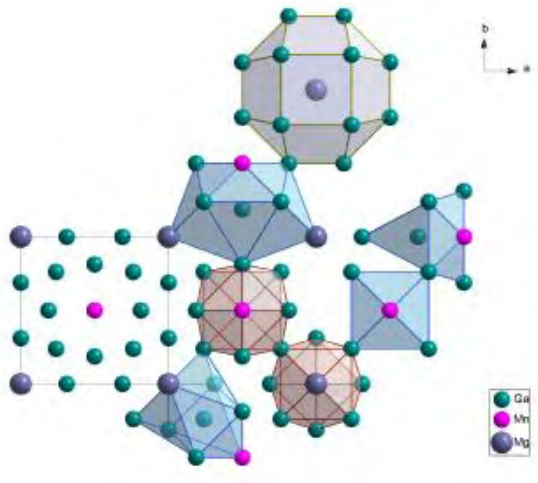
Table 1. Fractional atomic coordinates and isotropic displacement parameters (Å^2) for $MgMn_4Ga_{18}$

Atoms	*x*	*y*	*z*	U_{iso}/ U_{eq}
Ga1	0.23869(17)	0.23869(17)	0.23605(15)	0.0172 (5)
Ga2	0.5	0.5	0.3872(4)	0.0558 (17)
Ga3	0	0.3110(4)	0.5	0.0232 (7)
Ga4	-0.1870(4)	0.5	0	0.0183 (6)
Mn5	0	0	0.3433(4)	0.0059 (9)
Mn6	0.5	0.5	0.1526(4)	0.0077 (9)
Mg7	0	0	0	0.033 (4)

References

1. CrysAlis PRO, UK Ltd., Agilent Technologies, Yarnton, Oxfordshire, England, 2011.
2. G.M. Sheldrick, A short history of SHELX, Acta Cryst. A 64 (2008) 112e122.

Unit cell and coord. polyhedr. in MgMn4Ga18



Cluster core shell packing in MgMn4Ga18