NEW TERNARY LAVES PHASES FROM THE Mg-Ni-Ga SYSTEM

Pavlyuk N. V.[1], Kowalczyk G.[2], Krzyczmonik M.[2], Balińska A.[2], Dmytriv G. S.[1], Pavlyuk V. V.[1,2]

[1]Department of Inorganic Chemistry, Ivan Franko National University of Lviv, 6 Kyryla i Mefodiya St., 79005 Lviv, Ukraine

[2]Institute of Chemistry, Enviroment Pprotection and Biotechnology, Jan Dlugosz University of Częstochowa, Poland

nazar.pavlyuk@gmail.com

New ternary Laves phases were prepared from pure elements which were melted in induction furnace under continuous argon flow. Metallic grey lamine-like crystals were found using a conventional light microscope. Single crystal data were collected by using a four-circle diffractometer (*Xcalibur Oxford Diffraction diffractometer*) with CCD detector. Scans were taken in the ω mode, the empirical absorption corrections were made by CrysalisRed. The crystal structure of $MgNi_{1.11}Ga_{0.89}$, MgNiGa and Mg_2NiGa_3 compounds were successfully solved by direct methods. The $MgNi_{1.11}Ga_{0.89}$ is cubic ($MgCu_2$-type), space group *Fd-3m* and refined lattice parameters are: a = 7.0781 (8) Å. The MgNiGa is hexagonal ($MgZn_2$-type), *P6₃/mmc* and refined lattice parameters are: a = 5.0781(3) Å, c = 8.194(1) Å. The Mg_2NiGa_3 is orthorhombic (Mg_2MnGa_3-type), *Cmcm* and refined lattice parameters are: a = 5.4152 (10) Å, b = 8.6512(13) Å, c = 8.5621 (15) Å. The starting atomic parameters were taken from an automatic interpretation of direct methods followed by difference Fourier syntheses using SHELX-97 package programs. Atomic coordinates and thermal displacement parameters are listed in the Table 1. Finally, all parameters for $MgNi_{1.11}Ga_{0.89}$ phase are refined to $R[F^2 > 2s(F^2)] = 0.0173$, for MgNiGa phase are refined to $R[F^2 > 2s(F^2)] = 0.0143$, for Mg_2NiGa_3 are refined to $R[F^2 > 2s(F^2)] = 0.0599$. The unit cell of Mg_2NiGa_3 and atomic nets is presented in Fig.

Table. Crystalographic data for Laves phases of the Mg-Ni-Ga system

Atom	Wyck.	x/a	y/b	z/c	$B_{eqv.}$
Mg_2NiGa_3					
Ga1	4a	0	0	1/2	1.48(7)
Ni1	4c	0	0.15806	1/4	2.09(8)
Ga2	8g	-0.26372	-0.09114	1/4	1.39(6)
Mg3	8f	0	0.32705	0.56468	1.6(1)
$MgNi_{1.11}Ga_{0.89}$					
Mg	8a	1/8	1/8	1/8	0.8(1)
Ni+Ga	16d	0	1/2	0	1.12(5)
MgNiGa					
(Ga+Ni)1	6h	0.17017	0.34033	1/4	1.38(3)
(Ni+Ga)2	2a	0	0	0	1.75(3)
Mg	4f	2/3	1/3	1/16	1.25(6)

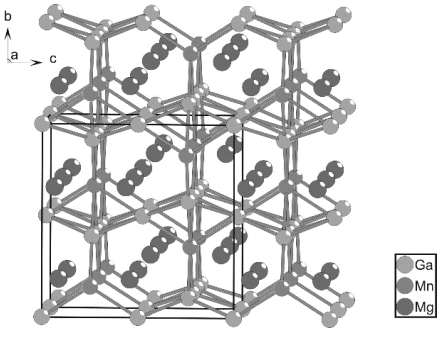

Fig. Atomic nets in the Mg_2NiGa_3 structure

Funding for this research was provided by National Science Centre, Poland (award No. 2017/25/B/ST8/02179).