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Lanthanum dimagnesium

Besma Belgacem,[a] Samia Yahyaoui,[a] P. Yu. Demchenko,[b] O. I. Bodak,[b] Michal Dusek[c] and Rached Ben Hassen[a]*

[a]Département de Chimie, Unité de Chimie des Matériaux, Faculté des Sciences de Sfax BP 802, Sfax 3018, Tunisia, [b]Department of Inorganic Chemistry, Ivan Franko National University of Lviv, Kyryla i Mefodiya Str. 6, 79005 Lviv, Ukraine, and [c]Institute of Physics, Na Slovance 2, Praha 8, Czech Republic

Correspondence e-mail: rached.benhassen@fss.rnu.tn

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(La–Mg) = 0.0008 Å
R factor = 0.008
wR factor = 0.024
Data-to-parameter ratio = 12.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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Single crystals of the $LaMg_2$ cubic Laves phase were synthesized by arc melting. The binary $LaMg_2$ compound has been shown to adopt the $MgCu_2$-type structure. The coordination sphere of the rare earth metal, adopting a site symmetry of $\bar{1}$, consists only of 12 Mg atoms. The site symmetry of the alkaline earth metal is $\bar{3}m$, giving rise to superimposed distorted $MgLa_6$ and $MgMg_6$ octahedra.

Comment

Binary intermetallics with the general formula RM_2 (where R is a rare earth and M an alkaline earth metal) have been studied extensively in the past because of their interesting magnetic properties (Leisure *et al.*, 2003). These compounds can adopt a wide variety of crystal structures with different geometrical arrangements for the rare earth atoms and with, therefore, different $R-R$ and $R-M$ interatomic distances (Klaus, 2000). A new family with the general formula LaM_2 crystallizes in different structure types (cubic and tetragonal; Liang *et al.*, 2003). AB_2-type intermetallic compounds have been of interest because of their possible use in high-temperature structural applications (Leisure *et al.*, 2003).

The C_{15} Laves phase compounds have received special attention for their elastic and magnetic properties and ability to absorb hydrogen (Leisure *et al.*, 2003). Moreover, many investigations have been carried out on MH electrode alloys

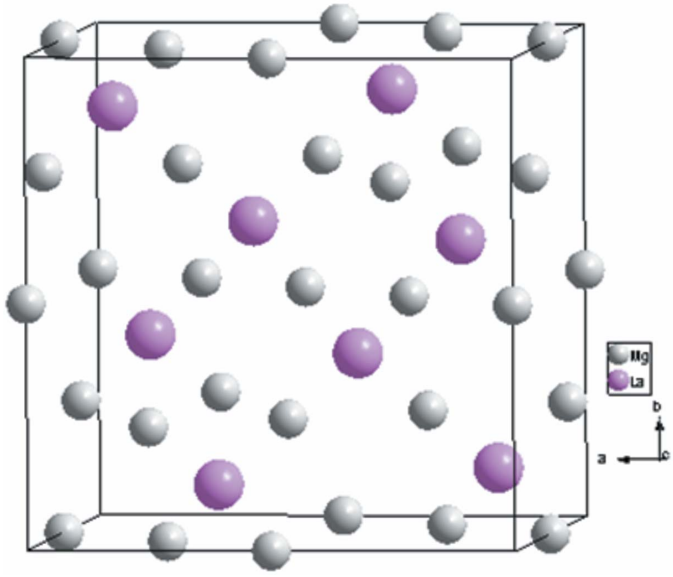

Figure 1
Clinographic projection of the unit cell of the cubic structure of the Laves phase $LaMg_2$.

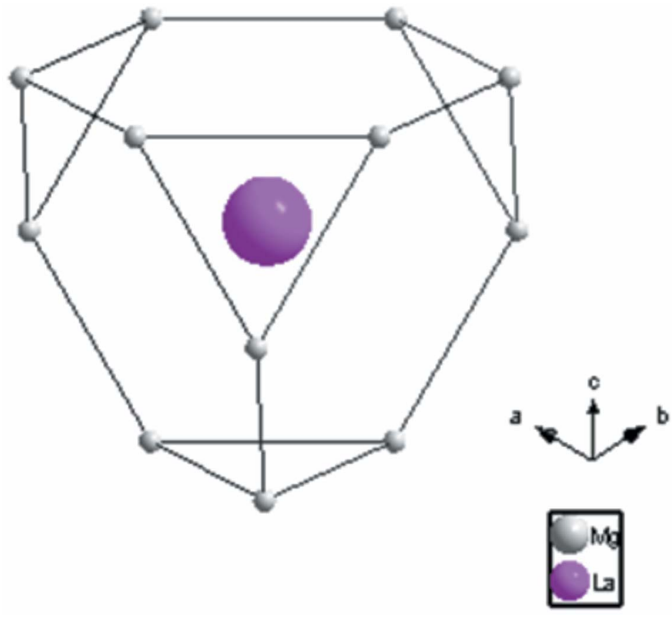

Figure 2
Coordination sphere of the La atom in the $LaMg_2$ structure.

with higher energy density, such as AB_2-type Laves phase alloys (Liao *et al.*,2004).

The La–Mg system was critically assessed by means of the calculation of phase diagram (CALPHAD) technique. The solution phases were modeled with the Redlich–Kister equation (Cuiping & Zhenmin, 2004). The intermetallic compounds LaMg, $LaMg_2$ and La_2Mg_{17} were treated as stoichiometric, while $LaMg_3$ and $LaMg_{12}$, which have a homogeneity range, were treated as $(La,Mg)Mg_3$ and $(La,Mg)(La,Mg)_{12}$, respectively (Cuiping & Zhenmin, 2004). Only X-ray powder diffraction analysis has previously been undertaken for $LaMg_2$ (Kost *et al.*,1987) and no single-crystal structural investigation has been carried out.

In the present work, we are interested in the synthesis and determination of the structural arrangement of $LaMg_2$ by X-ray single-crystal diffraction. The single crystals obtained are not very sensitive to air and moisture.

The structural arrangement of $LaMg_2$ at room temperature seems to be the same as that of the Laves phase structure type of $MgCu_2$. If we consider the arrangement of Mg atoms one can see that they are disposed at the corners of tetrahedra and that these tetrahedra are linked into a three-dimensional framework by sharing each Mg atom with an adjacent tetrahedron (Fig. 1); the disposition of the Mg atoms is therefore geometrically the same as that of O atoms in β-cristobalite (Evans 1964). The cavities in this framework of Mg atoms are occupied by the larger La atoms, arranged in the same way as the C atoms in diamond.

The structure of the title compound contains different coordination polyhedra around the La and Mg atoms. The coordination sphere of lanthanum (site symmetry $\overline{1}$; Fig. 2) consists only of 12 Mg atoms with equal La–Mg distances (Table 1). The polyhedron around lanthanum can be described with four regular triangular faces and four hexagonal faces.

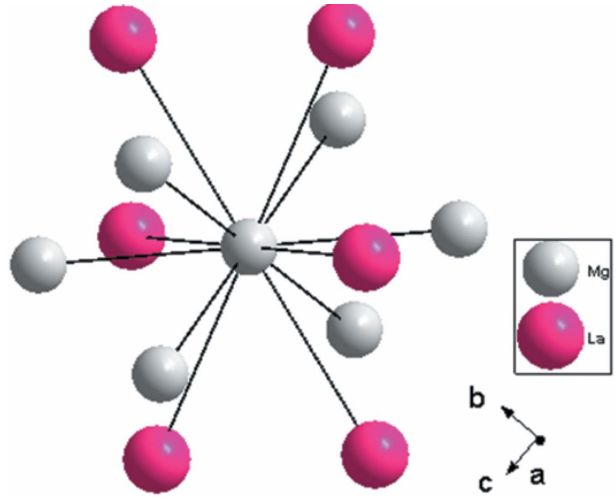

Figure 3
Coordination sphere of the Mg atom in the $LaMg_2$ structure.

Magnesium (site symmetry $\overline{3}m$) is bonded to six lanthanum and six other magnesium neighbors (Fig. 3), with La—Mg and Mg—Mg distances of 3.6524 (8) and 3.1148 (7) Å, respectively, giving rise to distorted $MgLa_6$ and $MgMg_6$ octahedra. The $LaMg_{12}$ polyhedra are connected together by sharing triangular faces.

Experimental

During the preparation of alkali/rare earth metal alloys, difficulties arise from the relatively low boiling points of the alkali metals compared with the high melting temperatures of the rare earth metals (Range *et al.*,1989). Essentially, a conventional melting process based on powder metallurgy cannot produce magnesium-based intermetallics with a specific chemical composition, because magnesium evaporates easily as a result of its high vapor pressure. Thus, a repeated melting process with an additional supply of magnesium is needed to prepare an intermetallic (Liquan *et al.*, 2004). Single crystals were extracted from alloys obtained by arc melting of the initial components (purity better than 99.9%) in an electric arc furnace in an argon atmosphere. A preliminary crystal investigation was performed using Laue and rotation methods (RKV-86 and RGNS-2 chambers, Mo $K\alpha$ radiation).

Crystal data

$LaMg_2$
M_r = 187.53
Cubic, $Fd\overline{3}m$
a = 8.810 (2) Å
V = 683.8 (3) Å^3
Z = 8
D_x = 3.642 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 2.2–27°
μ = 12.55 mm^{-1}
T = 295 K
Elongated tablet, colorless
0.36 × 0.1 × 0.07 mm

Data collection

Oxford Diffraction Xcalibur point-detector diffractometer
$\omega/2\theta$ scans
Absorption correction: Gaussian (*JANA2000*; Petricek *et al.*, 2000)
T_{min} = 0.323, T_{max} = 0.550
648 measured reflections
50 independent reflections
46 reflections with $I > 3\sigma(I)$
R_{int} = 0.031
θ_{max} = 26.6°
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = 0 \rightarrow 11$
3 standard reflections
every 100 reflections
intensity decay: 1.1%

Refinement

Refinement on F^2	4 parameters
$R[F^2 > 2\sigma(F^2)] = 0.008$	$w = 1/[\sigma^2(I) + 0.0004I^2]$
$wR(F^2) = 0.025$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.14$	$\Delta\rho_{max} = 0.11$ e Å^{-3}
50 reflections	$\Delta\rho_{min} = -0.09$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

La1—Mg1^{i}	3.6524 (8)	Mg1—Mg1^{ii}	3.1148 (7)
Mg1^{i}—La1—Mg1^{iii}	117.036	La1^{vi}—Mg1—La1	62.964
Mg1^{i}—La1—Mg1^{iv}	95.216	La1^{vi}—Mg1—Mg1^{ii}	115.239
Mg1^{i}—La1—Mg1	50.479	La1^{vi}—Mg1—Mg1	64.761
Mg1^{i}—La1—Mg1^{v}	144.903	Mg1^{ii}—Mg1—Mg1	180
La1^{vi}—Mg1—La1^{vii}	117.036	Mg1^{ii}—Mg1—Mg1^{v}	120
La1^{vi}—Mg1—La1^{viii}	180	Mg1^{ii}—Mg1—Mg1	60

Symmetry codes: (i) $x+1, y, z$; (ii) $-y+\frac{1}{2}, +x+\frac{1}{4}, +z-\frac{1}{4}$; (iii) $+x+\frac{1}{2}, y, +z+\frac{1}{2}$; (iv) $-y+1, +x+\frac{1}{4}, +z+\frac{1}{4}$; (v) $-x+\frac{1}{4}, -y+\frac{5}{4}, z$; (vi) $x-1, y, z$; (vii) $+x-\frac{1}{2}, y, +z-\frac{1}{2}$; (viii) $-x+1, -y+1, -z$.

Data collection: *KM4B8* (Galdecki *et al.*, 1996); cell refinement: *KM4B8*; data reduction: *JANA2000* (Petricek *et al.*, 2000); program(s) used to solve structure: *JANA2000*; program(s) used to refine structure: *JANA2000*; molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *JANA2000*.

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