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Sc_2MgGa_2 and Y_2MgGa_2

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Scandium magnesium gallide, Sc_2MgGa_2, and yttrium magnesium gallide, Y_2MgGa_2, were synthesized from the corresponding elements by heating under an argon atmosphere in an induction furnace. These intermetallic compounds crystallize in the tetragonal Mo_2FeB_2-type structure. All three crystallographically unique atoms occupy special positions and the site symmetries of (Sc/Y, Ga) and Mg are *m*2*m* and 4/*m*, respectively. The coordinations around Sc/Y, Mg and Ga are pentagonal (Sc/Y), tetragonal (Mg) and triangular (Ga) prisms, with four (Mg) or three (Ga) additional capping atoms leading to the coordination numbers [10], [8+4] and [6+3], respectively. The crystal structure of Sc_2MgGa_2 was determined from single-crystal diffraction intensities and the isostructural Y_2MgGa_2 was identified from powder diffraction data.

Comment

The potential use of magnesium alloys as storage materials for hydrogen has led to a large number of investigations on different magnesium alloys (Selvam *et al.*, 1986; Sahlberg & Andersson, 2007; Sahlberg *et al.*, 2007; Zlotea *et al.*, 2008). Different compositions in the ternary Sc–Mg–Ga and Y–Mg–Ga systems have been synthesized in order to investigate the hydrogen absorption properties of these compounds, and several intermediate phases have been found. There are numerous RE_2T_2X compounds (where RE is a rare earth metal, *T* is a transition metal and *X* is a p-block metal) which often crystallize in the W_2CoB_2-type (Rieger *et al.*, 1966) or Mo_2FeB_2-type structures (Rieger *et al.*, 1964). These types of compounds were reviewed by Lukachuk & Pöttgen (2003). The Mo_2FeB_2-type structure is a ternary ordered version of the U_3Si_2-type structure (Zachariasen, 1949), where the two uranium sites are occupied by different atoms.

We have synthesized single crystals of Sc_2MgGa_2, determined the crystal structure and found it to have the Mo_2FeB_2-type structure. Prior to this investigation, there were no ternary gallide phases reported with the Mo_2FeB_2-type structure, only for the binary Ce_3Ga_2 and Gd_3Ga_2 structures. It should also be noted that in the Sc–Mg–Ga ternary system this is, to our knowledge, the first reported ternary phase.

The Mo_2FeB_2-type structure, space group *P*4/*mbm*, can be described as two intergrown slabs of CsCl and AlB_2 types, as shown in Fig. 1. The compositions in the CsCl and AlB_2 slabs are ScMg and $ScGa_2$, respectively. The structure is layered in the *z* direction, and in Sc_2MgGa_2 the Mg and Ga atoms form a Ga_2Mg layer at $z = 0$ and the Sc atoms form a layer at $z = 0.5$.

The coordination around Mg is approximately a tetragonal prism of eight Sc atoms with four additional Ga atoms capping

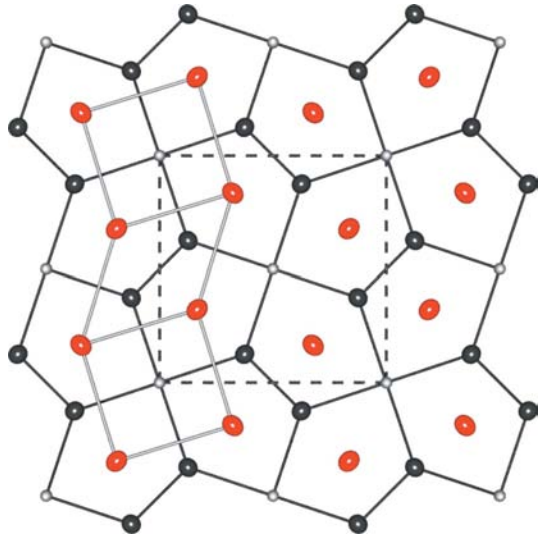

Figure 1
The crystal structure of Sc_2MgGa_2, viewed down the *c* axis, showing the Ga_2Mg and Sc layers. The two slabs of 'CsCl' and 'AlB_2' are emphasized. Key: Mg white, Ga black and Sc light grey (red in the electronic version of the paper). Displacement ellipsoids are drawn at the 95% probability level.

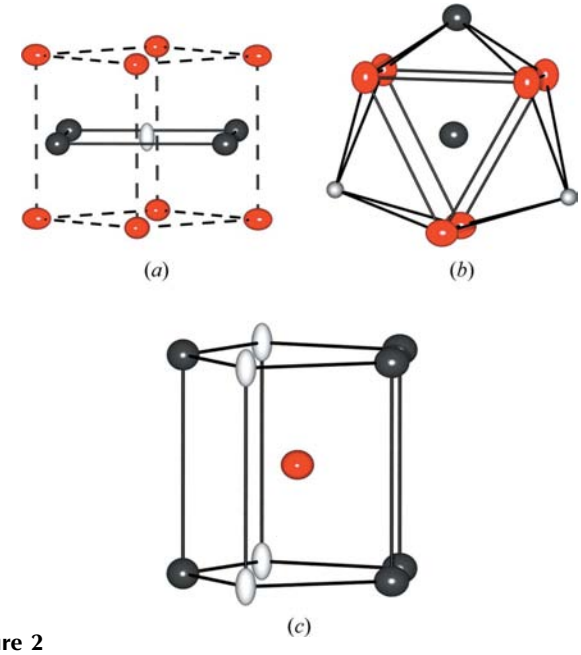

Figure 2
Coordination around (*a*) the Mg atom, (*b*) the Ga atom and (*c*) the Sc atom. Displacement ellipsoids are drawn at the 95% probability level.

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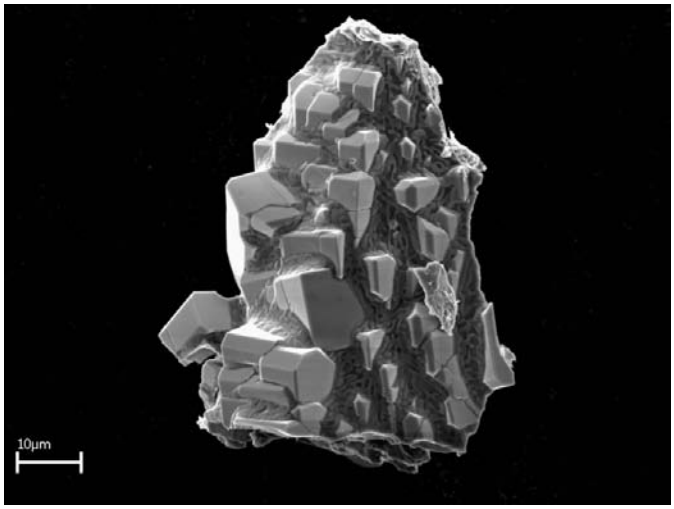

Figure 3
SEM image of a sample with the overall composition $ScMg_4Ga$. The Sc_2MgGa_2 crystals are shown in the matrix.

the rectangular faces (Fig. 2*a*). Ga is coordinated by nine atoms in a capped triangular prismatic arangement, *viz.* six Sc atoms in the prism plus two Mg and one Ga atom outside the rectangular faces (Fig. 2*b*). Sc is surrounded by two $[Ga_3Mg_2]$ rings, forming a distorted pentagonal prism (Fig. 2*c*).

The interatomic distances are in agreement with the corresponding binary compounds. The shortest interatomic distance is the Ga···Ga distance [2.535 (2) Å], which is slightly longer than the interatomic distance (2.48 Å) in orthorhombic α-Ga. The bonding in the compound is believed to be metallic.

The unit cell for the isostructural Y_2MgGa_2 compound was determined to be a = 7.428 (2) Å and c = 4.2537 (2) Å.

Experimental

Appropriate amounts of the elements (Mg 99.99%, Sc 99.95%, Ga 99%) were melted inside a tantalum tube sealed under an argon atmosphere, using a high-frequency induction furnace. The tubes were heated to ∼1373 K for 10 min, and then cooled to room temperature. Large single crystals of Sc_2MgGa_2 were obtained on the surface of magnesium-rich samples. The mm-sized single crystals were cut into smaller pieces. The bulk samples were characterized by X-ray powder diffraction. The chemical composition of the single crystals was also analysed with SEM–EDS (scanning electron microscopy–energy-dispersive X-ray spectroscopy). The image in Fig. 3 is taken from a sample with the nominal composition ScMgGa. The composition from EDS was found to be $Sc_{0.37}Mg_{0.20}Ga_{0.43}$ after correction by the ZAF method, which corrects for atomic number (Z), absorption (A) and fluorescence (F). Y_2MgGa_2 was synthesized using the same method as for Sc_2MgGa_2. The phase was found in a multiphase sample with the overall composition YMgGa. Attempts to synthesize large single crystals were not successful, probably due to the high stability of YMgGa and YGa_2. The crystal structure was indexed from powder X-ray diffraction data. The unit cell was determined using the *CHECKCELL* program (Laguier & Bochu, 2004).

Table 1
Selected bond lengths (Å).

Sc1—Ga1^{i}	2.8286 (15)	Ga1—Ga1^{iii}	2.535 (2)
Sc1—Mg1^{i}	3.2931 (6)	Ga1—Mg1^{iv}	2.8283 (6)
Sc1—Sc1^{ii}	3.505 (4)		

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

Crystal data

Sc_2MgGa_2
M_r = 253.67
Tetragonal, $P4/mbm$
a = 7.1577 (10) Å
c = 3.9166 (8) Å
V = 200.66 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 16.43 mm^{-1}
T = 293 (2) K
0.14 × 0.09 × 0.04 mm

Data collection

Bruker APEX-I diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.20, T_{max} = 0.52
2538 measured reflections
154 independent reflections
135 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.069
S = 1.16
154 reflections
11 parameters
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2007); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *publCIF* (Westrip, 2009).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: BD3001). Services for accessing these data are described at the back of the journal.

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