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Ternary rare earth alloys: RAuGe compounds

D. Rossi, R. Marazza and R. Ferro
Istituto di Chimica Generale ed Inorganica, Università di Genova, Viale Benedetto XV, 3-16132 Genoa (Italy)

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Abstract

Ternary line compounds of rare earths with gold and germanium in the stoichiometric ratio 1:1:1 have been identified and studied by means of X-ray and metallographic analyses. Their structures proved to be related to the hP6 LiGaGe type.

1. Introduction

Many intermetallic 1:1:1 RTX ternary phases formed by the rare earths (R) with a transition metal (T) and an element of the p block (X) of the periodic table and their crystal structures have been discussed in several papers [1–3].

We have previously described a few series of rare earth intermetallic compounds [4, 5] having the hP6 $CaIn_2$ or cF12 MgAgAs structural types.

We now report the data obtained in the study of RAuGe compounds (R = rare earth).

2. Experimental details

The metal used had a purity of around 99.9 mass% for the rare earths and 99.99 mass% for gold and germanium. The samples (each of mass about 1–2 g) were prepared by melting the metals (enclosed in an argon atmosphere in a tantalum vessel) in an induction furnace.

They were then generally annealed at 800 °C for 1 week. In general the alloys so obtained appeared as well-melted compact ingots. They were brittle and stable in the air. The different samples were examined under a metallographic microscope (after etching in a dilute ethanol solution of triiodide) and a scanning electron microscope. In some cases, electron probe microanalysis was also carried out. All the samples were examined by X-ray diffraction (the powder method using Fe Kα radiation). The lattice parameters were refined by a least-squares method using the Nelson–Riley function. The diffraction intensities, visually scaled on the films, were compared with the values calculated with the program PULVERIX [6].

3. Results

The majority of the RAuGe samples were homogeneous around the nominal 1:1:1 composition (as an example see Fig. 1). The powder photographs of the alloys were indexed on the basis of an hexagonal unit cell (Table 1). No indication was obtained of a lattice parameter change as a function of the composition. In the specific case of the Dy–Au–Ge alloys a number of

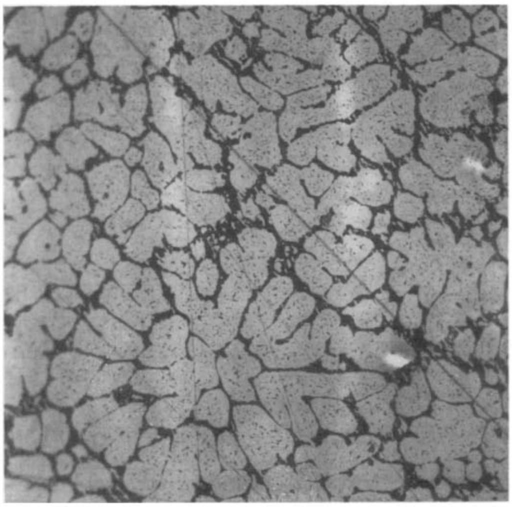

Fig. 1. Nd–Au–Ge alloy having the 1:1:1 nominal composition. (Magnification, 375×.)

TABLE 1

Crystal data for ternary RAuGe of the hP6 LiGaGe type

Compound	a (±0.3 pm)	c (±0.3 pm)	$\bar{V}$[a] ($\times 10^{-6}$ pm^3)	ΔV[b] (%)
LaAuGe[c]	446.3	816.9	23.5	−2.6
CeAuGe[c]	446.4	791.0	22.8	−1.7
PrAuGe	445.7	780.3	22.4	−3.5
NdAuGe	444.7	770.2	22.0	−4.6
SmAuGe	443.4	753.3	21.4	−5.8
GdAuGe	443.2	741.8	21.0	−7.2
TbAuGe	441.6	733.5	20.7	−7.5
DyAuGe	441.1	728.7	20.5	−7.8
HoAuGe	440.5	723.9	20.3	−8.0
ErAuGe	439.7	720.3	20.1	−8.2
YbAuGe	447.5	716.3	20.7	−18.5
YAuGe	440.8	730.7	20.5	−10.1

[a] Average atomic volume $\bar{V} = V_{cell}/6$.

[b] Volume contraction $\Delta V\% = [(V_{cell} - \Sigma V_{at})/\Sigma V_{at}]100$ (atomic volumes for a coordination number of 12 as reported in ref. 7).

[c] These values have been obtained from heterogeneous samples (two phase).

samples were prepared having the following compositions: $DyAuGe_{0.8}$, $DyAuGe_{1.2}$, $DyAu_{1.2}Ge$, $DyAu_{0.8}Ge$, $Dy_{1.2}AuGe$ and $Dy_{0.8}AuGe$. From their powder photographs no significant difference was observed in the constants.

A preliminary evaluation of the diffraction intensities, carried out for different alternative structures and atomic positions, suggested an ordered structure of the LiGaGe type (ordered variant of the $CaIn_2$ type), corresponding to the following atomic positions in the space group $P6_3mc$ (No. 186): two R atoms in 2a (0, 0, z with $z = 0.250$); two gold atoms in 2b(1) ($\frac{1}{3}$, $\frac{2}{3}$, z with $z = 0.046$); two germanium atoms in 2b(2) ($\frac{1}{3}$, $\frac{2}{3}$, z with $z = 0.480$).

4. Final remarks

As a conclusion a few comments can be made considering the volume data. We may first remember that for several RTX 1:1:1 alloys of the rare earths a clear subdivision of some structural types (MgAgAs, $CaIn_2$ and AlB_2 types) may be obtained in a plot of the atomic volume ratios V_R/V_T *vs.* V_X/V_T [5]. The $CaIn_2$-type structure and its variants for the RAuGe alloys fit well in the above-mentioned plot.

Figure 2, on the contrary, gives a compact representation of a group of selected 1:1:1 alloys all having the nominal $\frac{8}{3}$ value for the valence electron concentration. The effect of the dimensional factor on the relative stability of the MgAgAs and $CaIn_2$ type structures is evident. The particular behaviour of ytterbium in several alloys should be noted. The sharp characteristic

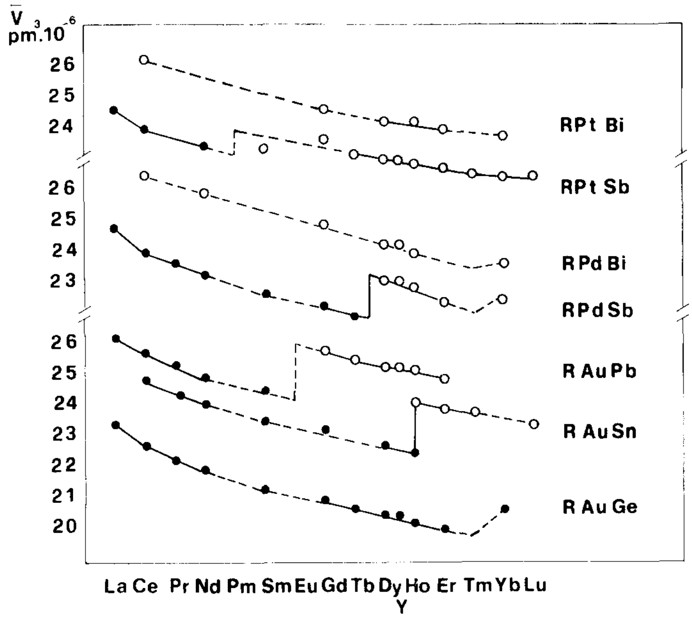

Fig. 2. Average atomic volumes of R–(Pt, Pd, Au)–(Bi, Sb, Pb, Sn, Ge), 1:1:1 phases: ●, hP6 $CaIn_2$ or hP6 LiGaGe structure type; ○, cF12 MgAgAs structure type.

deviation of the atomic volume of the YbAuGe compound from that of the trivalent-R RAuGe alloys is evident. It is in agreement with the general trends observed in several binary and ternary ytterbium alloys [8].

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