Crystal structure of samarium nickel tetraaluminide, SmNiAl_4

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Abstract

Al_4NiSm , orthorhombic, $Cmcm$ (no. 63), $a = 4.0948(6)$ Å, $b = 15.582(3)$ Å, $c = 6.610(1)$ Å, $V = 421.8$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.028$, $wR_{\text{obs}}(F^2) = 0.074$, $T = 293$ K.

Source of material

The metals used were Sm (99.9 wt.%), Ni and Al (99.999 wt.%). The samples, each with a total weight of 1–1.5 g, were prepared by induction melting of the components in alumina crucibles un-

der an argon flow. In order to attain proper homogenization the samples were remelted several times under continuous shaking. The alloys were then annealed at 773 K for 15 days and finally water quenched.

Discussion

A recent investigation of the phase relations in the ternary system Sm–Ni–Al at 773 K [1] revealed the formation of four new ternary compounds, namely SmNiAl_4 , $\text{Sm}_4\text{Ni}_6\text{Al}_{23}$, SmNiAl_3 and SmNi_2Al_3 . The compound SmNiAl_4 (Pearson code $oS24$) was found to be isotypic with YNiAl_4 [2]. The Ni atom is surrounded by a trigonal prism formed by 2Sm + 4Al capped on each lateral face by three other Al atoms. The Sm atom is at the centre of a pentagonal prism formed by 8Al + 2Ni with all lateral faces capped by aluminium atoms. These polyhedra are highlighted in the figure. The Ni–Al distances are the shortest ones, reaching with 2.297(4) Å a 14.2 % contraction with respect to the sum of the metallic radii for CN12 [3], while contractions of 8.9 % and 6.5 % are found for 2.608(4) Å Al–Al and 3.023(3) Å Sm–Al contacts, respectively. On the contrary, the Sm–Ni distances are about 5 % greater than the sum of the metallic radii.

Table 1. Data collection and handling.

Crystal:	silver luster prism, size $0.04 \times 0.12 \times 0.13$ mm
Wavelength:	Mo K_α radiation (0.71070 Å)
μ :	188.60 cm ⁻¹
Diffractometer, scan mode:	Bruker-Nonius MACH3, ω - θ
$2\theta_{\text{max}}$:	59.8°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	747, 374
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 354
$N(\text{param})_{\text{refined}}$:	23
Programs:	SHELXL-97 [4], ATOMS [5]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Sm	4c	0	0.38404(3)	1/4	0.0068(3)	0.0031(3)	0.0070(3)	0	0	0
Ni	4c	0	0.72547(8)	1/4	0.0065(6)	0.0045(5)	0.0064(5)	0	0	0
Al(1)	8f	0	0.1900(1)	0.0527(3)	0.009(1)	0.0070(9)	0.0049(9)	0	0	0.0001(7)
Al(2)	4c	0	0.5780(2)	1/4	0.013(2)	0.005(1)	0.012(1)	0	0	0
Al(3)	4a	0	0	0	0.012(1)	0.006(1)	0.013(1)	0	0	0.002(1)

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References

1. Borzone, G.; Raggio, R.; Delsante, S.; Ferro, R.: Phase equilibria in the Sm-Ni-Al alloy system. Submitted to *Intermetallics*.
2. Rykhal', R. M.; Zarechnyuk, O. S.; Yarmolyuk, Ya. P.: Crystal structure of the compounds YNiAl₄ and YNiAl₂. *Sov. Phys. Crystallogr.* **17** (1972) 453-455.
3. Teatum, E.; Gschneidner Jr., K. A.; Waber, J.: Rep. LA-4003. National Technical Information Service, Springfield, VA, USA 1968.
4. Sheldrick, G. M.: SHELXL-97. Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1997.
5. Dowty, E.: ATOMS. Version 5.1 for Windows. Program for Displaying Atomic Structures. Shape Software, Kingsport TN, USA 2000.