Crystal structure of samarium nickel tetraaluminide, $SmNiAl_4$

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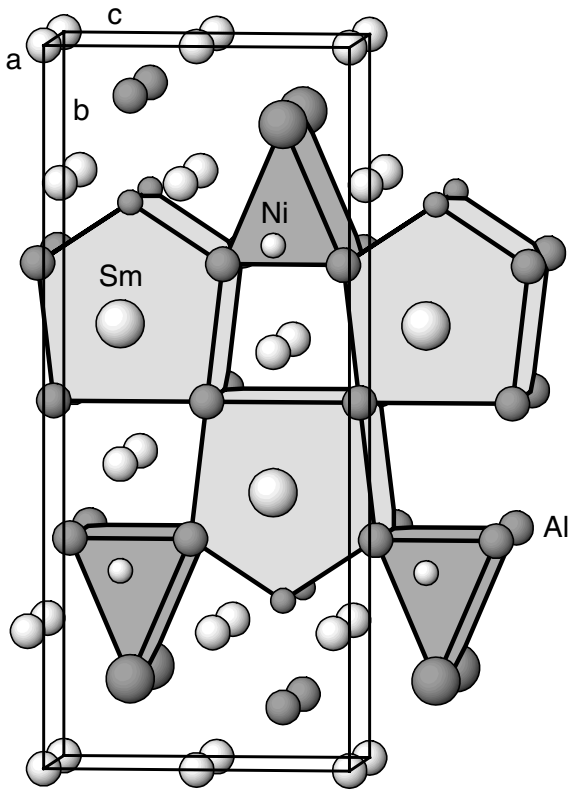

Abstract
Al_4NiSm, orthorhombic, *Cmcm* (no. 63), $a = 4.0948(6)$ Å, $b = 15.582(3)$ Å, $c = 6.610(1)$ Å, $V = 421.8$ Å^3, $Z = 4$, $R_{gt}(F) = 0.028$, $wR_{obs}(F^2) = 0.074$, $T = 293$ K.

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 under 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 $SmNiAl_4$, $Sm_4Ni_6Al_{23}$, $SmNiAl_3$ and $SmNi_2Al_3$. The compound $SmNiAl_4$ (Pearson code *oS*24) 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 *CN*12 [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 × 0.12 × 0.13 mm
Wavelength:	Mo K_α radiation (0.71070 Å)
μ:	188.60 cm^{-1}
Diffractometer, scan mode:	Bruker-Nonius MACH3, ω-θ
$2\theta_{max}$:	59.8°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	747, 374
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 354
$N(param)_{refined}$:	23
Programs:	SHELXL-97 [4], ATOMS [5]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sm	4*c*	0	0.38404(3)	1/4	0.0068(3)	0.0031(3)	0.0070(3)	0	0	0
Ni	4*c*	0	0.72547(8)	1/4	0.0065(6)	0.0045(5)	0.0064(5)	0	0	0
Al(1)	8*f*	0	0.1900(1)	0.0527(3)	0.009(1)	0.0070(9)	0.0049(9)	0	0	0.0001(7)
Al(2)	4*c*	0	0.5780(2)	1/4	0.013(2)	0.005(1)	0.012(1)	0	0	0
Al(3)	4*a*	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 $YNiAl_4$ and $YNiAl_2$. 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.