Crystal structure of lanthanum silver aluminium, $\text{LaAg}_{0.6}\text{Al}_{3.4}$

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Source of material: The compound was prepared from the elements (purity min. 99.9 mass%) at 1273 K in corundum crucibles in argon atmosphere.

In the crystal structure of $\text{LaAg}_{0.6}\text{Al}_{3.4}$, a new variant of the ThCr_2Si_2 -type, the Al2-atoms form plain 4^4 -nets perpendicular to [001] at $z=0.2498$ and $z=0.7502$. The Ag1/Al1-, the Ag2/Al2- and the Al3-atoms are located alternately above and below the squares of the 4^4 -nets forming layers of edge-sharing TX-pyramids. Thereby the Al3-atoms occupy in an ordered way one fourth of the pyramid-top. The other three fourth of these positions are occupied statistically by Ag/Al-atoms. The pyramid-layers are staggered along [001] in such a distance, that reciprocal actions between the Al3- and Ag/Al-atoms respectively Ag/Al- and Ag/Al-atoms occur (distances 249.6 pm and 269.0 pm). The La-atoms are located between these layers occupying the centers of two tetragonal prisms formed by four Al3-, four Ag2/Al2 and eight Al4-atoms respectively eight Ag2/Al2- and eight Al4-atoms.

$\text{Ag}_{0.6}\text{Al}_{3.4}\text{La}$, tetragonal, $P4/nmm$ (No. 129), $a=6.180(2)$ Å, $c=11.051(4)$ Å, $V=422.1$ Å³, $Z=4$, $R(F)=0.055$, $R_w(F^2)=0.173$.

Table 1. Parameters used for the X-ray data collection

Crystal:	metallic luster, xenomorph, size 0.05 x 0.06 x 0.07 mm
Wavelength:	Mo $K\alpha$ radiation (0.71070 Å)
μ :	133.12 cm ⁻¹
Diffractometer:	Philips PW1100
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	59.9°
$N(hkl)_{\text{unique}}$:	406
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	21
Program:	SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
La(1)	2c		1/4	1/4	0.0016(1)	0.0000(5)	U_{11}	0.0000(7)	0	0	0
La(2)	2b		3/4	1/4	1/2	0.0000(5)	U_{11}	0.0000(7)	0	0	0
Ag(1)	2c	0.50(1)	1/4	1/4	0.3753(2)	0.002(1)	U_{11}	0.003(2)	0	0	0
Al(1)	2c	0.50	1/4	1/4	0.3753(2)	0.002(1)	U_{11}	0.003(2)	0	0	0
Ag(2)	4f	0.298(9)	3/4	1/4	0.1206(2)	-0.001(1)	-0.001(1)	0.004(1)	0	0	0
Al(2)	4f	0.702	3/4	1/4	0.1206(2)	-0.001(1)	-0.001(1)	0.004(1)	0	0	0
Al(3)	2c		1/4	1/4	0.6133(6)	0.000(2)	U_{11}	0.000(3)	0	0	0
Al(4)	8j		0.0030(3)	x	0.7502(2)	0.002(1)	U_{11}	0.000(2)	0	0.001(2)	U_{13}

References

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- Sheldrick, G. M.: SHELXL-93, a program for refining crystal structures. University of Göttingen, Germany 1993.