Systematic absences are consistent with space groups $P2_1$ and $P2_1/m$. The latter was adopted leading to a satisfactory refinement. No higher lattice symmetry was found with *LEPAGE* (Spek, 1988). General reflections with $k + l = 2n + 1$ are systematically weaker but not extinct [the largest exceptions have an observed intensity of $100\sigma(I)$], corresponding to pseudo *A*-centring of the structure. Inspection of the refined structure reveals that the major deviation from *A*-centring is caused by the position of the O atoms. An analytical method (Alcock, 1970) for absorption correction was applied as implemented in *PLATON* (Spek, 1990). The transmission-factor range is consistent with the range 0.13–1.00 as observed in 360° ψ scans. One lower-order reflection (012) was omitted from the final refinement cycles. A final difference density map did not show features other than residual absorption artifacts near Cs. The structure contains no residual solvent-accessible voids (Spek, 1994). Calculations were carried out on a DEC5000 cluster.

Data collection: locally modified *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *SET*4 (de Boer & Duisenberg, 1984). Data reduction: *HELENA* (Spek, 1993). Program(s) used to solve structure: *SIR92* (Altomare, Cascarano, Giacovazzo & Guagliardi, 1993). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *PLATON* (Spek, 1990). Software used to prepare material for publication: *PLATON*.

This work was supported in part (ALS and NV) by the Netherlands Foundation of Chemical Research (SON) with financial aid from the Netherlands Organization for Scientific Research (NWO).

Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: BR1107). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1995). C**51**, 1975–1977

Czochralski-Grown $SrLaGaO_4$

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(*Received* 15 *June* 1994; *accepted* 17 *October* 1994)

Abstract

The structure of Czochralski-grown lanthanum strontium tetraoxogallate, $LaSrGaO_4$, a $K_2Ni_2F_4$-type compound, has been redetermined by X-ray diffraction. The improved quality of the crystals resulted in a higher precision in the determination of the geometric parameters than reported previously [Rüter & Müller-Buschbaum (1990). *Z. Anorg. Allg. Chem.* **584**, 119–124]. La and Sr atoms are equally distributed on a nine-coordinate site, and Ga is in a distorted octahedral site stretched along [001]. PIXE analysis gives excellent quantitative results.

Comment

Single crystals of $SrLaGaO_4$ have been structurally characterized. They are applicable as substrates for high-temperature superconducting thin films (McConnell *et al.*, 1994). The refined structure is in agreement with that published by Rüter & Müller-Buschbaum (1990) for submillimeter single crystals obtained by solid-state reaction; however, the improved quality and size of the crystals results in higher resolution data. There is about one order of magnitude improvement in the standard deviations of the bond lengths. For example, La—O1 is 2.428 (3) *versus* 2.42 (3) Å (Rüter & Müller-Buschbaum, 1990). A 50:50 distribution of La and Sr in the nine-coordinate site was assumed and confirmed by PIXE analyses (Johansson & Campbell, 1989). Ga occupies a distorted octahedral site. The O1 atom shows a higher U_{eq} value than atom O2 as a result of the significantly longer Ga—O1 distance.

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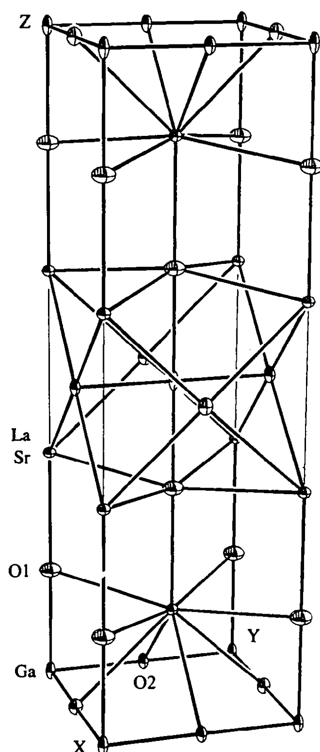

Fig. 1. Structure of $SrLaGaO_4$ in the tetragonal cell showing atom labelling and 50% probability displacement ellipsoids.

Experimental

Single crystals (up to 35 g) of the title material were grown by the Czochralski method using an iridium crucible. 5 *N* purity reagents were used (La_2O_3 from Aldrich, and $SrCO_3$ and Ga_2O_3 from Cerac). High-quality crystals were obtained on (100) oriented seeds with the melt Ga_2O_3 and La_2O_3 rich. PIXE analyses (Johansson & Campbell, 1989) were conducted at five 80 µm spots per specimen, using $LaGaO_3$, $LaAlO_3$ and the NIST steel reference material SRM1155 as standards. The measured concentrations, with precision approximately 1%, indicated that the material was stoichiometric. The experimental details concerning crystal growth and characterization were reported recently by Dabkowski, Dabkowska & Greedan (1993). A sample for the X-ray structure determination was cut from a large single crystal and ground with a pneumatic device on 600 grid sand paper. It was then polished with 1200 and 4000 grid sand paper. The average diameter of the sphere was 0.304 (7) mm. The crystal quality was confirmed by observation under a polarizing microscope and by determination of the rocking curve (FWHM 1′ 30″). The density D_m was measured by displacement.

Crystal data

$LaSrGaO_4$
$M_r = 360.25$
Tetragonal
$I4/mmm$
$a = 3.8437$ (3) Å
$c = 12.6880$ (15) Å
$V = 188.45$ (3) Å^3
$Z = 2$
$D_x = 6.383$ Mg m^{-3}
$D_m = 6.388$ (9) Mg m^{-3}

Ag $K\alpha$ radiation
$\lambda = 0.56086$ Å
Cell parameters from 23 reflections
$\theta = 43.6$–$55.1°$
$\mu = 17.255$ mm^{-1}
$T = 296$ (2) K
Ground sphere
0.152 (4) mm (radius)
Yellow

Data collection

Siemens *R3m/V* diffractometer
$2\theta-\theta$ scans
Absorption correction: spherical
$T_{min} = 0.038$, $T_{max} = 0.104$
1868 measured reflections
781 independent reflections
706 observed reflections [$I > 2\sigma(I)$]

$R_{int} = 0.0281$
$\theta_{max} = 55.29°$
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 11$
$l = 0 \rightarrow 37$
3 standard reflections monitored every 97 reflections intensity decay: none

Refinement

Refinement on F^2
$R(F) = 0.0272$
$wR(F^2) = 0.0679$
$S = 1.156$
780 reflections
13 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0317P)^2 + 0.2075P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 4.982$ e Å^{-3}
$\Delta\rho_{min} = -3.994$ e Å^{-3}
Extinction correction: *SHELXL* (Sheldrick, 1993)
Extinction coefficient: 0.1322 (64)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
La†	0	0	0.358673 (14)	0.00557 (4)
Sr†	0	0	0.358673 (14)	0.00557 (4)
Ga	0	0	0	0.00710 (6)
O1	0	0	0.1673 (2)	0.0144 (5)
O2	0	1/2	0	0.0072 (2)

† Site occupancy = 0.5.

Table 2. *Selected geometric parameters* (Å, °)

La—O1	2.428 (3)	Ga—O2	1.9218 (2)
La—O2^{i}	2.6285 (2)	Ga—O1	2.122 (3)
La—O1^{ii}	2.7378 (4)		
O1—La—O2^{i}	133.016 (5)	O1^{ii}—La—O1^{vi}	89.171 (14)
O2^{i}—La—O2^{iii}	62.264 (6)	Ga—O1—La^{ii}	83.09 (6)
O1—La—O2^{iv}	133.016 (5)	La—O1—La^{ii}	96.91 (6)
O2^{i}—La—O2^{iv}	93.968 (10)	La^{ii}—O1—La^{v}	166.18 (12)
O1—La—O1^{ii}	83.09 (6)	La^{ii}—O1—La^{vi}	89.171 (14)
O2^{i}—La—O1^{ii}	126.53 (5)	La^{vii}—O2—La^{viii}	93.968 (10)
O2^{iv}—La—O1^{ii}	64.46 (5)	La^{v}—O2—La^{viii}	86.032 (10)
O1^{ii}—La—O1^{v}	166.18 (12)		

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

For the X-ray intensity measurements, a profile analysis was used in the data reduction step (Siemens, 1989). The wavelength used to calculate the unit-cell dimensions was Ag $K\alpha_1$ ($\lambda = 0.55941$ Å).

Data collection: *R3m/V Crystallographic Research System* (Siemens, 1989). Cell refinement: *R3m/V Crystallographic Research System* using $K\alpha_1$. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1992). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL/PC* (Sheldrick, 1992). Software used to prepare material for publication: *SHELXL*93.

This work was supported by the National Science and Engineering Research Council of Canada and the Ontario Center of Materials Research.

Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: JZ1003). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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