Crystal structure of distrontium lanthanum gallium pentaoxide, Sr_2LaGaO_5

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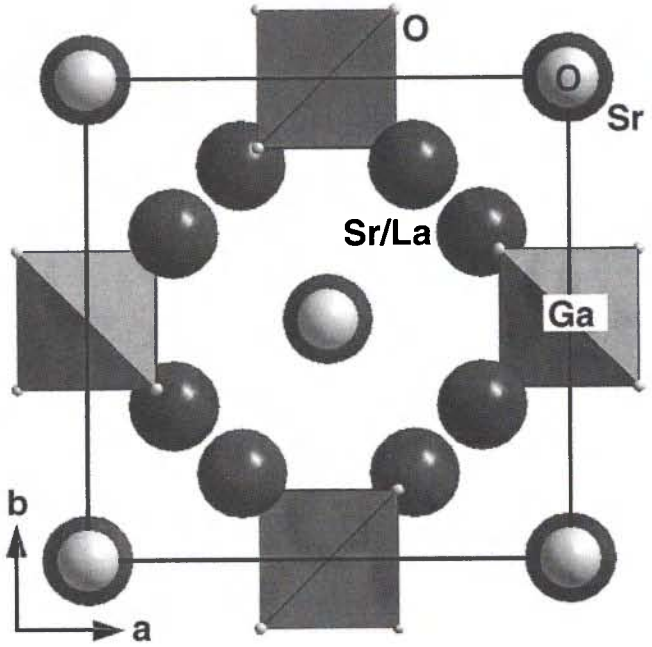

Abstract

$GaLaO_5Sr_2$, tetragonal, *I4/mcm* (No. 140), $a = 6.9339(4)$ Å, $c = 11.2823(8)$ Å, $V = 542.4$ Å^3, $Z = 4$, $R(P) = 0.018$, $wR(P) = 0.027$, $R(I) = 0.031$, $T = 295$ K.

Source of material

Sr_2LaGaO_5 melts incongruently, therefore it was synthesised by solid state reaction of the single oxides and carbonates, respectively. They were of 4N and 5N quality and the mixture of them was prepared containing SrO, La_2O_3 and Ga_2O_3 in a molar ratio of 4:1:1. The sample was sintered in air in a closed Pt crucible up to 1573 K for 20 h. This reaction led to a homogeneous grey product [1]. Because of the incongruent melting of $SrLaGaO_4$ - one of the most favoured candidates for substrates for high-Tc superconductors - primary crystallisation of Sr_2LaGaO_5 takes place when starting the crystal growth from the stoichiometric melt composition $SrLaGaO_4$.

Discussion

Preliminary, lattice parameter of this compound were given by Mansmann [2]. The structure of Sr_2LaGaO_5 is isotypic with Sr_2GdGaO_5 [3] from which the starting atomic coordinates for the refinement were taken.

Table 1. Data collection and handling.

Powder:	grey
Wavelength:	Mo K_α radiation (0.7093 Å)
μ:	321.3 cm^{-1}
Diffractometer:	Stoe STADI P
Scan mode	transmission Debye-Scherrer mode
$2\theta_{max}$, stepwidth:	59.98°, 0.02°
$N(points)_{measured}$:	2850
$N(hkl)_{measured}$:	232
$N(param)_{refined}$:	30
Program:	RIETAN-97 [4]

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

Atom	Site	Occ.	x	y	z	U_{iso}
Sr(1)	8*h*	0.5	0.181(1)	*x*+1/2	0	0.017
La(1)	8*h*	0.5	0.181	*x*+1/2	0	0.017
Sr(2)	4*a*		0	0	1/4	0.015
Ga(1)	4*b*		0	1/2	1/4	0.018
O(1)	4*c*		0	0	0	0.032
O(2)	16*l*		0.143(8)	*x*+1/2	0.642(5)	0.035

References

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