Crystal structure of strontium praseodym trigallium heptaoxide, $(Sr_{0.5}Pr_{0.5})_2Ga_3O_7$

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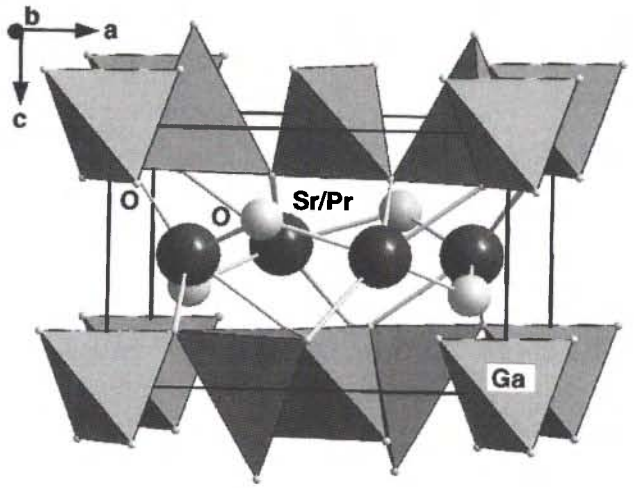

Abstract

Ga_3O_7PrSr, tetragonal, $P\bar{4}2_1m$ (No. 113), a = 8.0198(2) Å, c = 5.2991(1) Å, V = 340.8 Å^3, Z = 2, $R(P)$ = 0.026, $wR(P)$ = 0.040, $R(I)$ = 0.025, T = 295 K.

Source of material

$SrPrGa_3O_7$ was synthesized by melting a mixture of the oxides and carbonates (4N and 5N quality) under flowing nitrogen in an Ir crucible. A mixture containing SrO, Pr_2O_3 and Ga_2O_3 in a molar ratio of 2:1:3 was used. The solidified melt was homogeneous and of green color. Because of the incongruent melting of $SrPrGaO_4$ - one of the most favoured candidates for substrates for high-T_c superconductors - a shift in the melt composition during the growth process takes place. In consequence, $SrPrGa_3O_7$ is formed in the multiphase residual melt [1].

Starting atomic coordinates for the refinement were taken from $SrLaCa_3O_7$ [2]. The displacement parameters of all atoms were fixed to reliable values.

Table 1. Data collection and handling.

Powder:	green
Wavelength:	Cu K_α radiation (1.54059 Å)
μ:	771.1 cm^{-1}
Diffractometer:	Stoe Stadi P
Scan mode:	transmission Debye-Scherrer mode
$2\theta_{max}$, stepwidth:	89.98°, 0.02
$N(points)_{measured}$	3750
$N(hkl)_{measured}$	104
$N(param)_{refined}$:	39
Program:	RIETAN-97 [3]

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

Atom	Site	Occ.	x	y	z	U_{iso}
Sr(1)	4*e*	0.5	0.1621(9)	*x*+1/2	0.509(3)	0.006
Pr(1)	4*e*	0.5	0.1621	*x*+1/2	0.509	0.006
Ga(1)	4*e*		0.644(1)	*x*+1/2	0.975(5)	0.009
Ga(2)	2*a*		0	0	0	0.009
O(1)	8*f*		0.084(5)	0.160(6)	0.212(7)	0.012
O(2)	4*e*		0.634(7)	*x*+1/2	0.356(8)	0.012
O(3)	2*c*		0	1/2	0.193(7)	0.012

References

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