Crystal structure of distrontium praseodym gallium pentaoxide, Sr_2PrGaO_5

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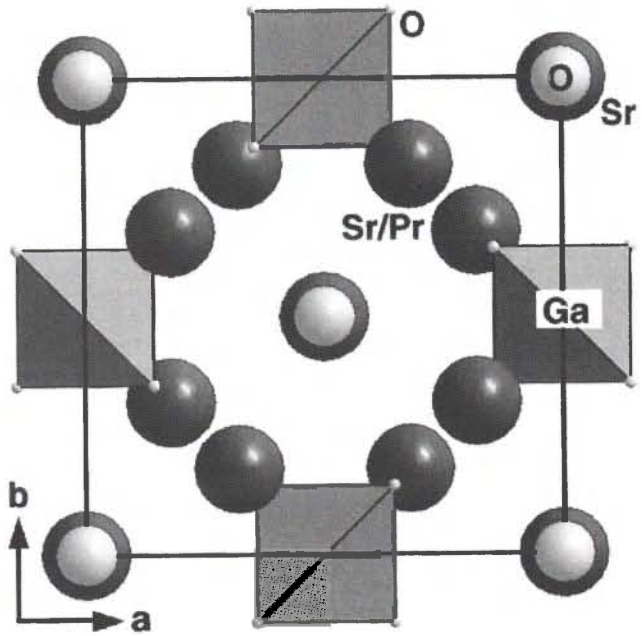

Abstract

GaO_5PrSr_2, tetragonal, *I4/mcm* (No. 140), $a = 6.8441(2)$ Å, $c = 11.2534(4)$ Å, $V = 527.1$ Å^3, $Z = 4$, $R(P) = 0.035$, $wR(P) = 0.052$, $R(I) = 0.038$, $T = 295$ K.

Source of material

Sr_2PrGaO_5 was synthesized by solid state reaction of the oxides and carbonates (4N and 5N quality). A mixture containing SrO, Pr_2O_3 and Ga_2O_3 in a molar ratio of 4:1:1 was used. The sample was sintered in air in a closed Pt crucible up to 1573 K for 56 h. This reaction led to a homogeneous brown product [1]. Because of the incongruent melting of $SrPrGaO_4$ - one of the most favoured candidates for substrates for high-T_c superconductors - primary crystallization of Sr_2PrGaO_5 takes place when starting the crystal growth from the stoichiometric melt composition $SrPrGaO_4$.

Starting atomic coordinates for the refinement were taken from Sr_2GdGaO_5 [2]. The displacement parameters of all atoms were fixed to reliable values.

Table 1. Data collection and handling.

Powder:	brown
Wavelength:	Cu K_α radiation (1.54059 Å)
μ:	1008.6 cm^{-1}
Diffractometer:	Stoe Stadi P
Scan mode:	transmission Debye-Scherrer mode
$2\theta_{max}$, stepwidth:	89.98°, 0.02
$N(points)_{measured}$	3500
$N(hkl)_{measured}$	67
$N(param)_{refined}$:	30
Program:	RIETAN-97 [3]

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

Atom	Site	Occ.	x	y	z	U_{iso}
Sr(1)	8*h*	0.5	0.180(2)	x+1/2	0	0.006
Pr(1)	8*h*	0.5	0.180	x+1/2	0	0.006
Sr(2)	4*a*		0	0	1/4	0.006
Ga(1)	4*b*		0	1/2	1/4	0.009
O(1)	4*c*		0	0	0	0.012
O(2)	16*l*		0.143(8)	x+1/2	0.642(5)	0.012

References

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