Crystal structure of praseodym gallate, $Pr_4Ga_2O_9$

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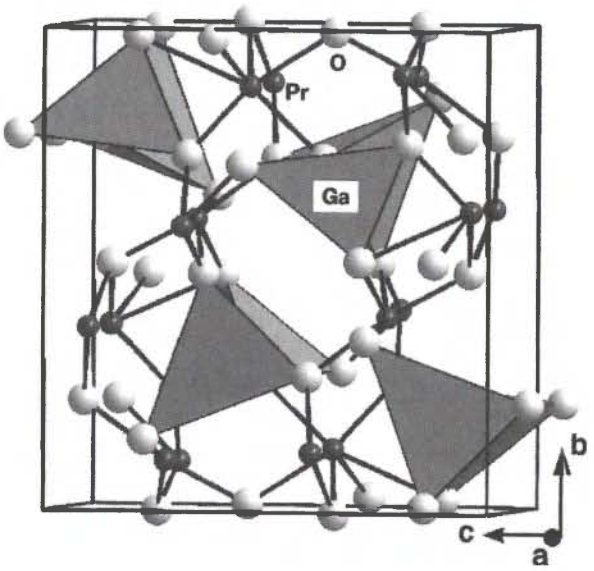

Abstract

$Ga_2O_9Pr_4$, monoclinic, $P12_1/c1$ (No. 14), $a = 7.8256(4)$ Å, $b = 11.0322(5)$ Å, $c = 11.4959(7)$ Å, $\beta = 109.187(3)°$, $V = 937.4$ Å^3, $Z = 4$, $R(P) = 0.026$, $wR(P) = 0.034$, $R(I) = 0.033$, $T = 295$ K.

Source of material

$Pr_4Ga_2O_9$ was synthesized by solid state reaction of the oxides of 4N and 5N quality containing Pr_2O_3 and Ga_2O_3 in a molar ratio of 2:1. The sample was sintered in air in a closed Pt crucible up to 1753 K for 20 h. This reaction led to a homogeneous product which was of light green color after grinding. 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, $Pr_4Ga_2O_9$ is formed in the multiphase residual melt [1]. Starting atomic coordinates for the refinement were taken from $Eu_4Al_2O_9$ [2]. The displacement parameters of all atoms were fixed to reliable values.

Table 1. Data collection and handling.

Powder:	light-green
Wavelength:	Cu K_α radiation (1.54059 Å)
μ:	1629.9 cm^{-1}
Diffractometer:	Stoe Stadi P
Scan mode:	transmission Debye-Scherrer mode
$2\theta_{max}$, stepwidth:	89.98°, 0.02
$N(points)_{measured}$	4000
$N(hkl)_{measured}$	765
$N(param)_{refined}$:	79
Program:	RIETAN-97 [3]

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

Atom	Site	x	y	z	U_{iso}
Pr(1)	4*e*	0.520(2)	0.100(2)	0.782(1)	0.006
Pr(2)	4*e*	0.027(2)	0.091(2)	0.806(1)	0.006
Pr(3)	4*e*	0.332(3)	0.122(2)	0.424(2)	0.006
Pr(4)	4*e*	0.834(3)	0.121(2)	0.419(2)	0.006
Ga(1)	4*e*	0.215(5)	0.190(3)	0.137(3)	0.009
Ga(2)	4*e*	0.660(4)	0.184(3)	0.117(3)	0.009
O(1)	4*e*	0.761(9)	0.146(5)	0.804(5)	0.012
O(2)	4*e*	0.202(7)	0.236(4)	0.797(4)	0.012
O(3)	4*e*	0.176(9)	0.018(7)	0.190(7)	0.012
O(4)	4*e*	0.030(9)	0.219(7)	0.940(7)	0.012
O(5)	4*e*	0.404(8)	0.226(4)	0.083(5)	0.012
O(6)	4*e*	0.64(1)	0.224(8)	0.950(8)	0.012
O(7)	4*e*	0.737(7)	0.009(5)	0.173(4)	0.012
O(8)	4*e*	0.03(1)	0.020(5)	0.374(5)	0.012
O(9)	4*e*	0.613(9)	0.991(6)	0.390(6)	0.012

References

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