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Crystal structure of strontium praseodum gallium oxide, $SrPrGaO_4$

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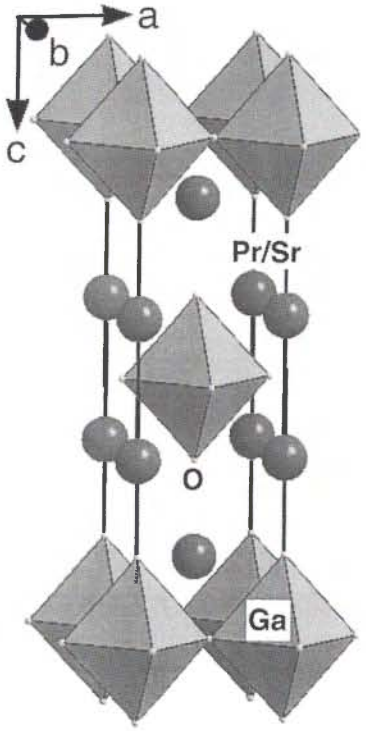

Abstract

GaO_4PrSr, tetragonal, *I4/mmm* (No. 139), $a = 3.822(1)$ Å, $c = 12.622(2)$ Å, $V = 184.4$ Å^3, $Z = 2$, $R_{gt}(F) = 0.028$, $wR(F^2) = 0.082$, $T = 293$ K.

Source of material

$SrPrGaO_4$ is an incongruent melting material which was synthesized as single crystal by the Czochralski method in flowing nitrogen atmosphere with a growth rate of 0.7 mm/h [1]. The starting materials were mixed in a non-stoichiometric ratio according to the formula $Sr_1Pr_{1.066}Ga_{1.091}O_{4.236}$. The resulting single crystal was of very good perfection and green color.

Discussion

$SrPrGaO_4$ crystal belongs to the $ABCO_4$ group of oxide crystals (A = Ca, Sr; B = rare earth elements and C = Al, Ga) with K_2NiF_4 structure which are very promising substrates for high-T_c superconductors. These substrates are favoured for $YBa_2Cu_3O_{7-x}$ epitaxy, mainly because of their isotype with the superconductor and their good lattice matching, their chemical stability in LPE process and well suited dielectric properties.

Table 1. Data collection and handling.

Crystal:	green, irregular, size 0.1 × 0.1 × 0.1 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	345.27 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS, 140 exposures, $\Delta\varphi = 1.7°$
$2\theta_{max}$:	56.16°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1094, 90
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 84
$N(param)_{refined}$:	13
Program:	SHELXL-93 [2]

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

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pr(1)	4*e*	0.5	0	0	0.35793(9)	0.0066(9)	U_{11}	0.004(1)	0	0	0
Sr(1)	4*e*	0.5	0	0	0.35793	0.0066	U_{11}	0.004	0	0	0
Ga(1)	2*a*		0	0	0	0.003(1)	U_{11}	0.012(2)	0	0	0
O(1)	4*c*		0	1/2	0	0.008(7)	0.001(6)	0.015(7)	0	0	0
O(2)	4*e*		0	0	0.168(2)	0.012(6)	U_{11}	0.029(9)	0	0	0

References

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