Crystal structure of strontium praseodym aluminate, $SrPrAlO_4$

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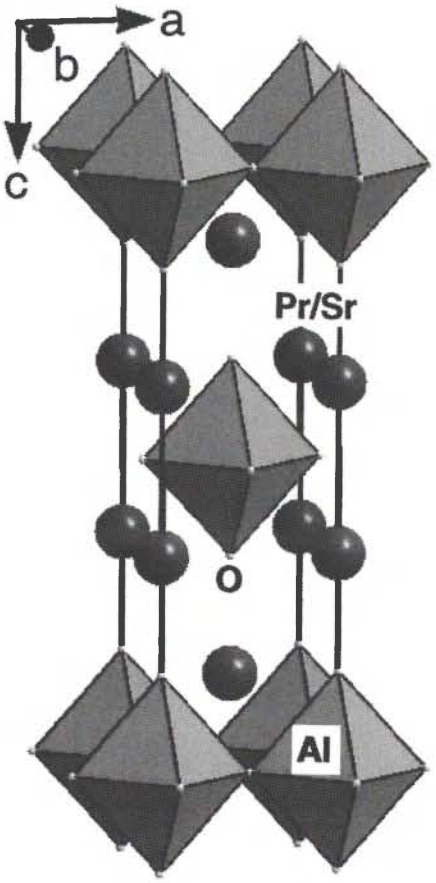

Abstract

AlO_4PrSr, tetragonal, *I4/mmm* (No. 139), $a = 3.736(1)$ Å, $c = 12.532(3)$ Å, $V = 174.9$ Å^3, $Z = 2$, $R_{gt}(F) = 0.010$, $wR(F^2) = 0.021$, $T = 293$ K.

Source of material

The single crystal of $SrPrAlO_4$ was grown by the Czochralski method in slightly reducing atmosphere with a growth rate of 1 mm/h. The starting materials were mixed in a non-stoichiometric ratio according to the formula $SrPr_{1.066}Al_{0.97}O_4$. The resulting single crystal was of very good perfection and had green color.

Discussion

$SrPrAlO_4$ crystal belongs to the $ABCO_4$ group of oxide crystals (A = Ca, Sr; B = rare earth elements and 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 isostructure with the superconductor and their good lattice matching 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:	291.10 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS, 140 exposures, $\Delta\varphi = 1.7°$
$2\theta_{max}$:	55.8°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	932, 85
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 76
$N(param)_{refined}$:	13
Program:	SHELXL-93 [2]

References

1. Uecker, R.; Reiche, P.; Ganschow, S.: Conf. Proc. of the Eastern Regional Conference on Crystal Growth and Epitaxie, 28.9.-1.10.1997, Atlantic City, USA.
2. Sheldrick, G. M.: SHELXS-93. Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1993.

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	0.35845(5)	0.0043(2)	U_{11}	0.0037(3)	0	0	0
Sr(1)	4*e*	0.5	0	0	0.35845	0.0043	U_{11}	0.0037	0	0	0
Al(1)	2*a*		0	0	0	0.0041(7)	U_{11}	0.007(2)	0	0	0
O(1)	4*c*		0	1/2	0	0.004(2)	0.003(2)	0.008(3)	0	0	0
O(2)	4*e*		0	0	0.1640(4)	0.011(1)	U_{11}	0.008(4)	0	0	0

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