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Refinement of the crystal structure of praseodymium orthoscandate, $PrScO_3$

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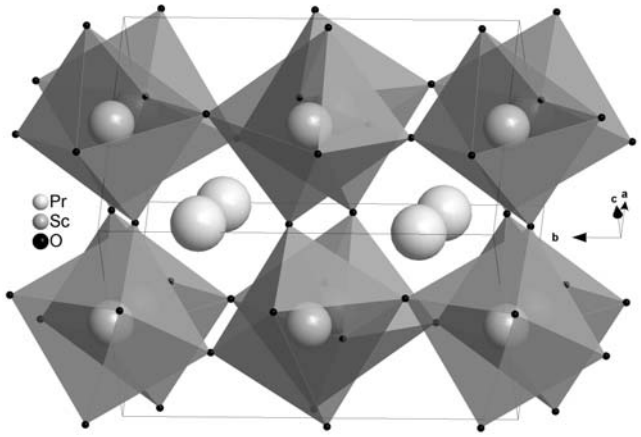

Abstract

O_3PrSc, *Pnma* (no. 62), $a = 5.780(1)$ Å, $b = 8.025(2)$ Å, $c = 5.608(1)$ Å, $V = 260.1$ Å^3, $Z = 4$, $R_{gt}(F) = 0.025$, $wR_{ref}(F^2) = 0.060$, $T = 298$ K.

Source of material

A $PrScO_3$ single crystal of 30 mm in length and 15 mm in diameter was grown by the Czochralski technique with RF heating and automatic diameter control. The starting oxides Pr_6O_{11} and Sc_2O_3 were of 99.999 % and 99.99 % purity, respectively. Due to its very high melting temperature about 2200 °C $PrScO_3$ was grown from an Ir crucible under flowing nitrogen. The pulling rate was 1 mm/h and the rotation 10 rpm. The occurrence of Pr^{4+} ions caused a dark-brown colour of the as-grown crystal. Subsequent annealing under reducing atmosphere (5 % H_2 + 95 % N_2) led to green colour of the crystal which is characteristic for Pr^{3+} ions.

Discussion

Rare-earth scandates with larger RE ions (La-Dy) have a perovskite-type crystal structure with pseudo-cubic lattice parameter between 395 and 405 pm. Those compounds which can be grown as large single crystals are suitable substrates for the growth of high-quality films of a variety of ferroelectric, multiferroic, and superconducting perovskites. Uniform strain can be achieved in sufficiently thin commensurate epitaxial films on these rare-earth scandates which allows their ferroelectric properties to be tuned. For example unstrained $SrTiO_3$ which is not ferroelectric at any temperature, has been made ferroelectric at room temperature *via* biaxial strain imposed by commensurate growth on rare-earth scandate substrates [1].

Liverovich and Mitchell have published the crystal structure of $PrScO_3$ obtained by solid state reaction which were refined from powder X-ray data using the Rietveld method [2]. Using the Czochralski technique we have grown large single crystals which were used for a single crystal structure refinement. This refinement was carried out in the standard setting space group *Pnma* instead of the non standard configuration *Pbam* as used by Liverovich and Mitchell. The positional parameters reported for *Pbam* can be transfered to *Pnma* using the symmetry operation ½+*y*,*z*,½–*x*. Doing so, the positional parameters reported here are comparable to the former one but more precized. Additionally, we have refined all atomic positions with anisotropic displacement parameters showing a slight ellipsoidal movement of the oxygen atoms perpenticular to the metal-oxygen bonds. All metal atoms are found with a nearly isotropic displacement. The scandium atoms are octahedral coordinated by oxygen atoms with an offset of 17.50(1)° along [010] and 16.87(8)° parallel to the [1 0 1] direction of the oxygen atoms away from a linear Sc—O—Sc bond as observed in the $Pm\bar{3}m$ aristotype ABO_3 perowskites. The praseodymium atoms are 8-fold coordinated by oxygen atoms with distances between 234.1(5) pm and 285.2(3) pm.

Table 1. Data collection and handling.

Crystal:	green triangle, size 0.11 × 0.15 × 0.18 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	208.47 cm^{-1}
Diffractometer, scan mode:	STOE IPDS I, dynamic profile intergration
$2\theta_{max}$:	60.64°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5144, 409
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 395
$N(param)_{refined}$:	29
Programs:	SHELXL-93 [3], DIAMOND [4]

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

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pr(1)	4*c*	0.44930(6)	¼	0.48788(6)	0.0092(3)	0.0097(3)	0.0091(3)	0	0.00065(9)	0
Sc(1)	4*b*	0	0	½	0.0077(5)	0.0075(6)	0.0074(6)	0.0001(5)	0.0003(3)	0.0004(3)
O(1)	4*c*	0.0395(7)	¼	0.6052(8)	0.012(2)	0.009(2)	0.011(2)	0	0.001(1)	0
O(2)	8*d*	0.1992(5)	0.0555(4)	0.1977(5)	0.010(1)	0.014(2)	0.010(1)	0.002(1)	0.003(1)	0.001(1)

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