

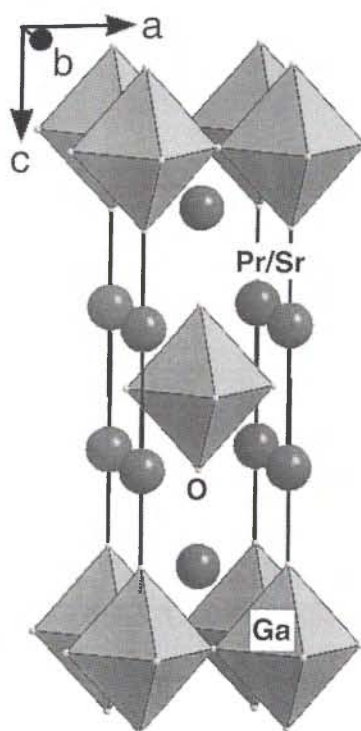
Crystal structure of strontium praseodum gallium oxide, SrPrGaO₄

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Abstract

GaO₄PrSr, tetragonal, *I4/mmm* (No. 139), *a* = 3.822(1) Å, *c* = 12.622(2) Å, *V* = 184.4 Å³, *Z* = 2, *R*_{gt}(*F*) = 0.028, *wR*(*F*²) = 0.082, *T* = 293 K.

Table 2. Atomic coordinates and displacement parameters (in Å²).

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

References

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2. Sheldrick, G. M.: SHELXL-93. Program for the Refinement of Crystal Structures. Universität Göttingen, Germany 1993.

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Source of material

SrPrGaO₄ 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 Sr₁Pr_{1.066}Ga_{1.091}O_{4.236}. The resulting single crystal was of very good perfection and green color.

Discussion

SrPrGaO₄ crystal belongs to the ABCO₄ group of oxide crystals (A = Ca, Sr; B = rare earth elements and C = Al, Ga) with K₂NiF₄ structure which are very promising substrates for high-T_c superconductors. These substrates are favoured for YBa₂Cu₃O_{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, Δφ = 1.7°
2θ _{max} :	56.16°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	1094, 90
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 84
<i>N</i> (<i>param</i>) _{refined} :	13
Program:	SHELXL-93 [2]