

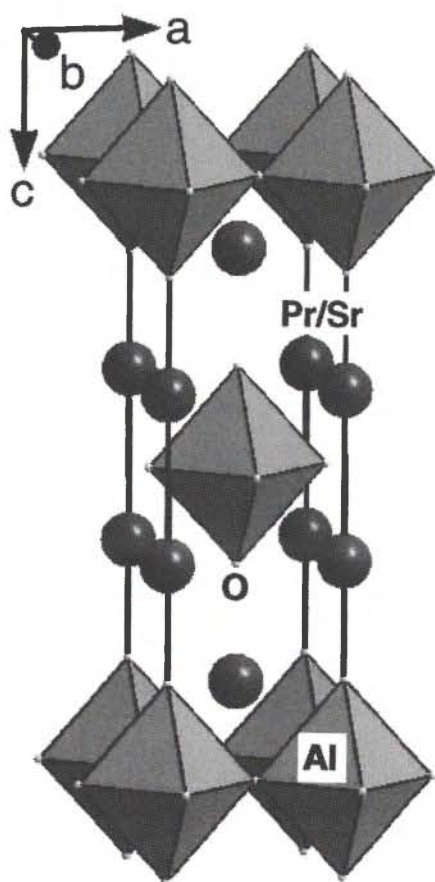
# Crystal structure of strontium praseodym aluminate, $\text{SrPrAlO}_4$

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## Abstract

$\text{AlO}_4\text{PrSr}$ , tetragonal,  $I4/mmm$  (No. 139),  $a = 3.736(1)$  Å,  $c = 12.532(3)$  Å,  $V = 174.9$  Å<sup>3</sup>,  $Z = 2$ ,  $R_{\text{gt}}(F) = 0.010$ ,  $wR(F^2) = 0.021$ ,  $T = 293$  K.

**Table 2.** Atomic coordinates and displacement parameters (in Å<sup>4</sup>).

| Atom  | Site | Occ. | x | y   | z          | $U_{11}$  | $U_{22}$ | $U_{33}$  | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|-------|------|------|---|-----|------------|-----------|----------|-----------|----------|----------|----------|
| Pr(1) | 4e   | 0.5  | 0 | 0   | 0.35845(5) | 0.0043(2) | $U_{11}$ | 0.0037(3) | 0        | 0        | 0        |
| Sr(1) | 4e   | 0.5  | 0 | 0   | 0.35845    | 0.0043    | $U_{11}$ | 0.0037    | 0        | 0        | 0        |
| Al(1) | 2a   |      | 0 | 0   | 0          | 0.0041(7) | $U_{11}$ | 0.007(2)  | 0        | 0        | 0        |
| O(1)  | 4c   |      | 0 | 1/2 | 0          | 0.004(2)  | 0.003(2) | 0.008(3)  | 0        | 0        | 0        |
| O(2)  | 4e   |      | 0 | 0   | 0.1640(4)  | 0.011(1)  | $U_{11}$ | 0.008(4)  | 0        | 0        | 0        |

## Source of material

The single crystal of  $\text{SrPrAlO}_4$  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  $\text{SrPr}_{1.066}\text{Al}_{0.97}\text{O}_4$ . The resulting single crystal was of very good perfection and had green color.

## Discussion

$\text{SrPrAlO}_4$  crystal belongs to the  $\text{ABCO}_4$  group of oxide crystals ( $A = \text{Ca}, \text{Sr}$ ;  $B = \text{rare earth elements and Al, Ga}$ ) with  $\text{K}_2\text{NiF}_4$ -structure which are very promising substrates for high- $T_c$  superconductors. These substrates are favoured for  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  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 $0.1 \times 0.1 \times 0.1$ mm |
| Wavelength:                                          | Mo $K_\alpha$ radiation (0.71073 Å)                   |
| $\mu$ :                                              | $291.10 \text{ cm}^{-1}$                              |
| Diffractionmeter, scan mode:                         | Stoe IPDS, 140 exposures, $\Delta\phi = 1.7^\circ$    |
| $2\theta_{\text{max}}$ :                             | $55.8^\circ$                                          |
| $N(hkl)_{\text{measured}}, N(hkl)_{\text{unique}}$ : | 932, 85                                               |
| Criterion for $I_{\text{obs}}, N(hkl)_{\text{gt}}$ : | $I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$ , 76      |
| $N(\text{param})_{\text{refined}}$ :                 | 13                                                    |
| Program:                                             | SHELXL-93 [2]                                         |

## References

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

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