

Ytterbium cobalt gallium oxide, YbCoGaO_4 , as grown by the floating zone technique

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Key indicators

Single-crystal X-ray study
 $T = 299 \text{ K}$
 Mean $\sigma(\text{Plane check}) = 0.006 \text{ \AA}$
 R factor = 0.027
 wR factor = 0.062
 Data-to-parameter ratio = 13.4

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Single crystals of YbCoGaO_4 have been grown for the first time by the optical floating zone technique and characterized by X-ray diffraction at room temperature. Atomic parameters were refined in space group $R\bar{3}m$. The structure is isomorphous with that of other materials belonging to the YbFe_2O_4 family. Magnetic measurements suggest spin glass behavior with an ordering temperature around 20 K. The electrical resistivity of the material was measured. The site symmetry of all the atoms is $3m$.

Comment

Single crystals of YbCoGaO_4 have been structurally characterized. The refined structure is similar to that of other materials belonging to the YbFe_2O_4 family (Cava *et al.*, 1998). Yb is bonded to six O atoms and is found in layers of flattened edge-shared octahedra. It is slightly disordered in the c direction. Five-coordinate Co and Ga atoms are statistically distributed in a double layer of face-shared trigonal bipyramids interleaving the Yb layers, as shown in Fig. 1. These alternating Yb and Co,Ga layers exhibit a corner-shared stacking in the direction of the c axis. The electron microprobe chemical analysis (EPMA) confirms the 1:1 distribution of Co and Ga on the Fe site. Magnetic measurements suggest spin glass behavior with an ordering temperature around 20 K. Electrical conductivity was found to be of the order of 10^{-5} A/Vm and anisotropic.

Experimental

Single crystals of YbCoGaO_4 were grown by the floating zone technique for the first time. 99.999% pure reagents were used, preannealed before mixing. The growth rate was 1.7 mm h^{-1} , rotation used was 30 r.p.m. for the feed rod and 25 r.p.m. for the seed rod. The total growth was 41.5 mm. Growth was perpendicular to the c axis in the hexagonal system. The experimental details concerning crystal growth and magnetic characterization will be published elsewhere (Dabkowska *et al.*, 2001). Samples for X-ray structure determination and electron microprobe were cut from the top part of the grown rod. Crushed crystals were examined using a Guinier–Haag camera, with $\text{Cu } K\alpha_1$ radiation and silicon as an internal standard. Intensity and peak positions were determined using a film scanner (LS-20 Keij Instruments, Sweden). The pattern was indexed on the basis of the hexagonal cell. The lattice constant were refined using LSUDF program and the results are in good agreement with both powder diffraction data (Kimizuka & Takayama, 1982) and the single-crystal measurement given in the Crystal Data Table.

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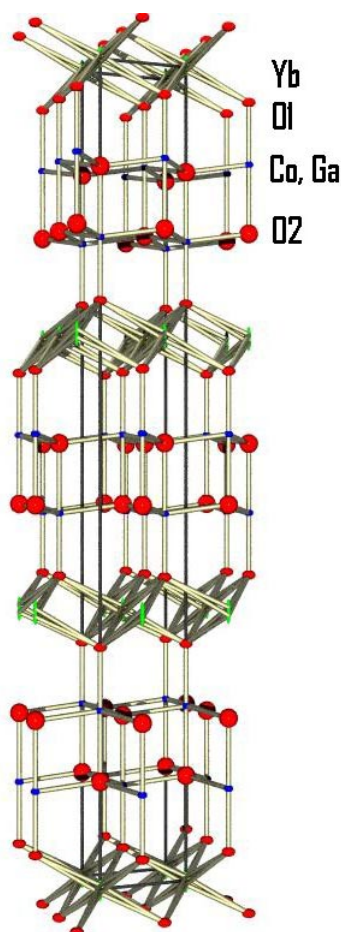


Figure 1
90% displacement ellipsoid plot of the structure as viewed normal to the *c* axis.

Crystal data

YbCoGaO₄
M_r = 365.69
 Rhombohedral, *R* $\bar{3}m$
a = 3.4165 (1) Å
c = 25.122 (1) Å
V = 253.95 (2) Å³
Z = 3
D_x = 7.174 Mg m⁻³

Data collection

Bruker SMART CCD diffractometer
 φ and ω scans
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.023, *T_{max}* = 0.142
 1932 measured reflections

Mo *K* α radiation
 Cell parameters from 1391 reflections
 θ = 2.4–36.2°
 μ = 39.98 mm⁻¹
T = 299 (2) K
 Plate, black
 0.22 × 0.16 × 0.01 mm

187 independent reflections
 178 reflections with *I* > 2 σ (*I*)
R_{int} = 0.047
 θ_{max} = 36.2°
h = -4 → 5
k = -5 → 4
l = -40 → 37

Refinement

Refinement on *F*²
R[*F*² > 2 σ (*F*²)] = 0.027
wR(*F*²) = 0.062
S = 1.16
 187 reflections
 14 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 4.4469P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 2.94 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{min} = -2.88 \text{ e } \text{Å}^{-3}$
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.049 (4)

Table 1

Selected interatomic distances (Å).

Yb1—O1 ⁱ	2.182 (4)	Co1—O2 ⁱ	1.9907 (12)
Yb1—O1 ⁱⁱ	2.296 (6)	Co1—O2	2.144 (9)
Co1—O1	1.926 (7)		

Symmetry codes: (i) $\frac{2}{3} - x, \frac{1}{3} - y, \frac{1}{3} - z$; (ii) $x - \frac{2}{3}, y - \frac{1}{3}, z - \frac{1}{3}$.

Refinement of the structure required a 50:50% distribution of Co and Ga on the same site, with common coordinates and displacement parameters. The Yb *z* coordinate refined slightly off the $\bar{3}m$ site, improving the displacement parameter refinement and residuals. The relatively large anisotropic displacement parameters for O2 are likely a result of the variation in coordination at the Co/Ga site. The sample used for the experiment was a 10 μm flake from the bulk sample. The equatorial edges were not natural faces. An analytical face correction using approximate faces and distances in Sheldrick's *XPREP* (Sheldrick, 1997) did not provide as good a correction (based on *R_{int}*) as did the empirical correction from *SADABS* (Sheldrick, 2000). The volume of the sample could have been reduced, but this would have prevented the collection of high-resolution data. The maximum density peak is 2.03 Å from the Ga1 atom.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Sheldrick, 1997b).

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References

- Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Cava, R. J., Ramirez, A. P., Huang, Q. & Krajewski, J. J. (1998). *J. Solid State Chem.* **140**, 337–344.
 Dabkowska, H. A., Dabkowski, A., Luke, G. M. & Gaulin, B. D. (2001). *J. Cryst. Growth*. In the press.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Kimizuka, N. & Takayama, E. (1982). *J. Solid State Chem.* **41**, 166–173.
 Sheldrick, G. M. (1997a). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997b). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
 Sheldrick, G. M. (2000). *SADABS*. University of Göttingen, Germany.