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Growth, structure and morphology study of monoclinic $RbGd(WO_4)_2$ crystals

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Abstract

The undoped rubidium gadolinium bis(tungstate) crystals, $RbGd(WO_4)_2$ (RGW), have been grown by the spontaneous nucleation from high-temperature solutions. The crystal structure has been refined at room temperature by using single-crystal X-ray diffraction data. The unit-cell parameters are $a = 10.6953(12)$ Å, $b = 10.5017(11)$ Å, $c = 7.6064(11)$ Å, $\beta = 130.504(7)^\circ$, with $Z = 4$ in space group C2/c, which is a little difference with $KGd(WO_4)_2$. Crystal habits were predicted by the attachment energy model of Hartman and Perdok and we compared predictions to experimentally grown crystal shapes.

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1. Introduction

Monoclinic double tungstate single crystals, with chemical formula $KRE(WO_4)_2$, RE being the rare earths, are currently receiving attention as hosts for self-induced frequency shifting [1–3]. The low-temperature phase of the potassium gadolinium tungstate, $KGd(WO_4)_2$, is a promising laser material and has been extensively studied [4–6]. On the other hand, $RbGd(WO_4)_2$, which has $KGd(WO_4)_2$-related structure, is, to our knowledge, rarely studied up to now [7,8]. Similar to $KGd(WO_4)_2$, $RbGd(WO_4)_2$ has polymorph transitions under the melting point, so it is impossible to grow this crystal directly from melt, and we grew the crystal by spontaneous crystallization from high-temperature solution. In this paper, we present the growth and structural determination

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of the $RbGd(WO_4)_2$ crystals. And we compared predictions to experimentally grown crystal shapes.

2. RGW single-crystal growth and X-ray photoelectron spectrograph analyze

$RbGd(WO_4)_2$ single crystals were grown by spontaneous nucleation technique from high-temperature solutions, using $Rb_2W_2O_7$ as solvent. The solution composition of 20 mol% of solute and 80% of solvent was chosen. The solutions used in the crystal growth experiments, weighing about 180 g, were prepared in a cylindrical Pt crucible, 50 mm in diameter, by melting and decomposing the appropriated quantities of Gd_2O_3, Rb_2O_3, and WO_3. The homogenization of the solutions was achieved by maintaining them at about 50 °C above the expected saturation temperature for 24 h. Then the solution temperature was decreased at a rate of 2–5 °C/day. RGW crystals with dimensions $\sim 3 \times 1.5 \times 1\ mm^3$ along **c**, **b** and **a*** directions, respectively, were taken out after the room temperature was reached. The representational grown crystal is shown in Fig. 1a. We powdered some single crystals in an agate mortar and made elementary analysis on PERKIN ELEMER PHI-1600 ESCA System. The X-ray photoelectron spectrograph (shown in Fig. 2) showed that the atomic ratios in the powder are 38.5%(O), 10.5%(W), 6.3%(Rb), 4.4%(Gd) and 40.3%(C). The existance of carbon in RGW crystals is due to the absorption of the CO_2 on the sample surface and the contamination of carbon oil on the instrument. Without taking into account the carbon the atomic ratios will be 64.5%(O), 17.6%(W), 10.6%(Rb), 7.4%(Gd), yielding the actual ratio of Rb:Gd:O:W equal to 1:1:8:2 within the experimental errors.

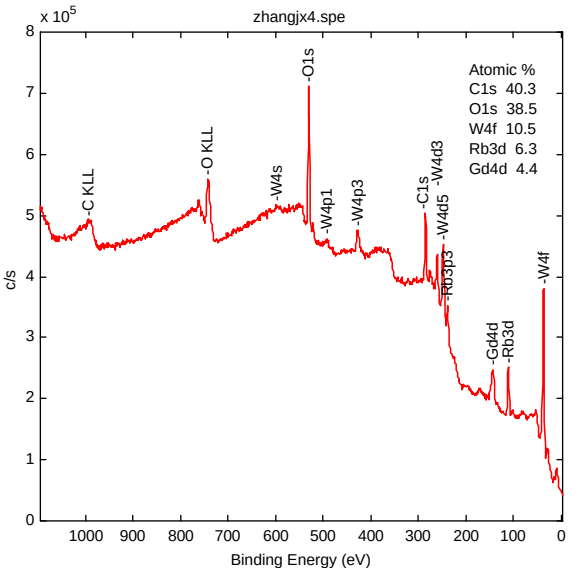

Fig. 2. X-ray photoelectron spectrograph.

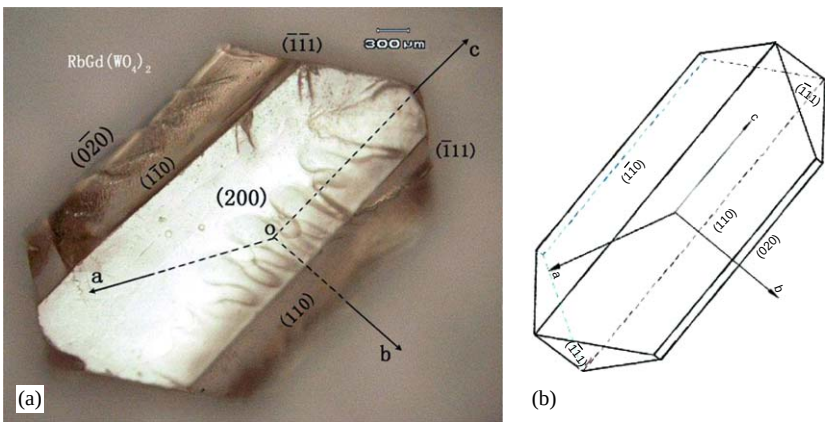

Fig. 1. (a) The as-grown representational RGW crystal with sizes $\sim 3 \times 1.5 \times 1\ mm^3$. (b) The crystal habit generated using a Wulff plot from the list of faces and center-to-face distances shown in Table 4.