Contr. Mineral. and Petrol. 39, 171—174 (1973)

Natural Boehmite Single Crystals from Ceylon

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Received January 16, 1973

Abstract. Single crystals of boehmite, up to 0.1 mm in size, were found in open cavities inside a corundum crystal from the Ratnapura area gem gravels in Ceylon. The unit cell parameters are (X-ray powder pattern): $a_0 = 3.695$ Å $b_0 = 12.212$ Å, $c_0 = 2.867$ Å. The crystallographic orientation is based on X-ray single-crystal precession photographs. The crystals show the faces *(010)*, *(001)*, *(101)*, and *(221)*. Systematic extinctions agree with the space group Amam. Optical orientation: $a \| \gamma$, $b \| \beta$, $c \| \alpha$. Refractive indices are given. The mineral is optically positive with a large optic axial angle.

Introduction

The form of natural AlO(OH) discovered and originally called "bauxite" by Böhm (1925) was renamed boehmite by de Lapparent (1927). The mineral represents a common constituent in the bauxites proper and is mainly found in microscopic or submicroscopic crystals not suitable for crystallographic single-crystal studies. Therefore, the crystal-structure determination (Reichertz and Yost, 1946; Milligan and McAtee, 1956) was made on the X-ray powder pattern of the synthetic mineral, assuming that the mineral is isostructural with lepidocrocite (Ewing, 1935). This assumption is justified because the X-ray powder patterns of boehmite and lepidocrocite are analogous to each other (Böhm, 1925; Goldsztaub, 1936).

During a study of the inclusions contained in the corundum from the Ratnapura area gem gravels, Ceylon, a corundum crystal approximately 6 cm in length was crushed. A couple of open cavities were found inside the crystal. The walls of these cavities, 1 mm wide and 3 mm long, were lined with crystals of a slightly yellowish mineral. The X-ray powder pattern recorded of this mineral matched that of boehmite (Swanson and Fuyat, 1953). Besides aluminum, a microprobe test proved the crystals to contain only iron (0.2–0.3% Fe_2O_3). Such an iron content lies well within the limit of solid solution between boehmite and lepidocrocite (Maurel, 1966). The boehmite crystals (Fig. 1) range up to almost 0.1 mm in size and are suitable for study of the crystal form and the X-ray crystallography of the natural mineral.

Because the mode of occurrence of boehmite as a cavity mineral in corundum is previously unknown and, further, because X-ray single-crystal data combined with crystal morphology of natural boehmite are not available in literature, the results obtained on the Ceylon boehmite are presented in this paper.

Crystal Morphology

The characteristic crystal habit of the Ceylon boehmite is platy or stout prismatic (Fig. 1) with a perfect cleavage parallel to the plate. A cross-section parallel to the cleavage plane displays a lenticular shape.

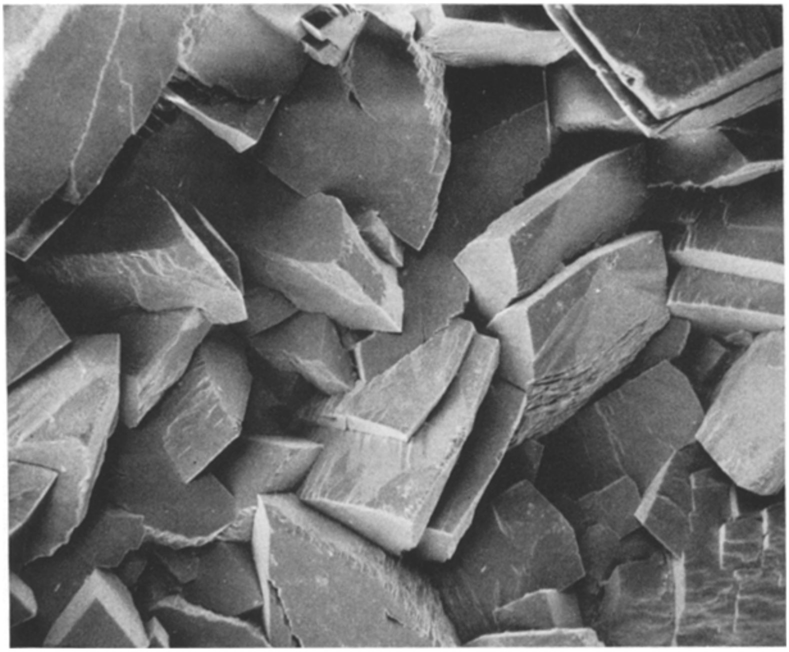

Fig. 1. Boehmite crystals from open cavity in a corundum crystal. Ratnapura area, Ceylon. Scanning electron micrograph. ×500

Table 1. Crystallographic axes of boehmite

	Author	Long axis of the cleavage plane	Perpendicular to the cleavage plane	Short axis of the cleavage plane
I	de Lapparent (1927, 1930); Hocart and de Lapparent (1929)	b	c	a
II	Bohnstedt-Kupletskaya (1947)	c	b/2	a
III	Bosmans and Michel (1959)	a	b	c

There is some confusion in the literature regarding the choice of crystallographic axes of boehmite (Table 1). The cleavage plane was taken as (*001*) in the early microscopic descriptions (I in the table). Later (II), *b*- and *c*-axes were interchanged and the cleavage plane was interpreted as (*010*). Such a setting was based only on the morphology of the crystals without support from single-crystal X-ray data. Recalculation of the values for the φ- and ϱ-angles given by Bohnstedt-Kupletskaya (1947, Table 3 on p. 245) indicates, however, that the *b*-parameter used to assign the indices to the crystal faces (*op. cit.*, Fig. 10) is one half its true value. In addition, *a*- and *c*-axes also appear to be interchanged with respect to the conventional setting. Electron diffraction study of synthetic material (III in Table 1) established a setting which is in accordance with the conventional choice of the axes of the mineral, *i.e.*, with $b_0 > a_0 > c_0$.

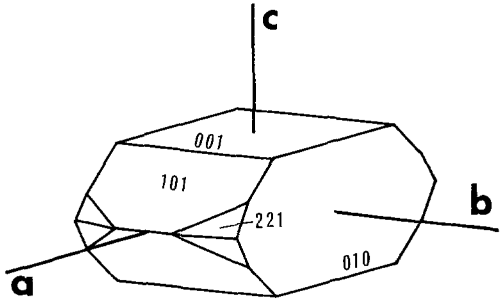

Fig. 2. Crystal habit of boehmite from the Ratnapura area, Ceylon

Fig. 2 presents the ideal crystal habit of the Ceylon boehmite. The choice of the axes corresponds to the setting III in Table 1 and is based on single-crystal X-ray data. The crystals were too small for optical goniometry. Therefore, the angles between the various faces were measured under the microscope and the indices were assigned to suit the angles obtained. The Ceylon boehmite differs from the platy synthetic mineral described by Wyart *et al.* (1963) in not showing face (*100*) but, instead, (*001*). No trace of cleavage parallel to (*100*), reported by de Lapparent (1930, (*010*) in his setting), is visible.

Crystal Geometry

The X-ray powder pattern of the Ceylon boehmite was recorded with a Philips wide-angle goniometer using corundum (ASTM card No. 10-173) as an internal standard. The unit-cell parameters obtained are: $a_0 = 3.695 \pm 0.003$ Å $b_0 = 12.212 \pm 0.006$ Å $c_0 = 2.867 \pm 0.003$ Å. A series of *b*- and *c*-axis precession photographs were taken of a crystal approximately 0.08 mm long. The systematic extinctions found agree with the orthorhombic space group *Amam* adopted for boehmite. The hydrogen bond is asymmetric in the boehmite structure and the true space group might not be centrosymmetric (Holm *et al.*, 1958).

Optical Properties

The data for the optical orientation of boehmite given in literature are uniform in two points (Hocart and de Lapparent, 1929; de Lapparent, 1930; Bohnstedt-Kupletskaya and Vlodavets, 1945; Bohnstedt-Kupletskaya, 1947; Rengarten, 1949): First, the optic axial plane is parallel to the perfect cleavage direction. Second, the optical γ-direction is parallel to the long axis of the cleavage plane. The optical orientation of the Ceylon boehmite was found to agree with these previous observations. Using the axial choice of this paper (III in Table 1) the optical orientation is: $a \| \gamma$, $b \| \beta$, $c \| \alpha$.

The refractive indices given in the literature vary only slightly. The following values were found for the Ceylon mineral (immersion method): $\alpha = 1.648$, $\beta = 1.657$, $\gamma = 1.668$ (all ± 0.002). The birefringence being fairly low, a calculation of the optic axial angle from these refractive indices is inaccurate. Therefore, the birefringence was measured with a Berek compensator on crystals lying on (*010*) and (*001*). Subsequently, the crystals were turned in a vertical position and the thickness was measured with a micrometer eye piece. The following values were obtained: $\gamma - \alpha = 0.020$, $\gamma - \beta = 0.012$. These values are considered more reliable than those calculated from the refractive indices. Because the face (*100*) is not developed in the Ceylon boehmite, the value for $\beta - \alpha$ could not be measured. From the values for the birefringence the optic axial angle is calculated to $2\,V_\gamma =$ 79° ±. Accordingly, the mineral is optically positive. Qualitative conoscopic observations support this conclusion. The large value for $2\,V$ and the particular shape of the crystals did not allow a direct measurement with a universal stage.

Acknowledgements. The authors are indebted to Dr. J. Siivola (microprobe test) and to Mr. B. Saltikoff (translation of Russian papers), both of the Geological Survey of Finland.

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