

## MAIN HABIT TYPES OF DIAMOND SINGLE CRYSTALS SEED-GROWN IN THE DIAMOND THERMODYNAMIC STABILITY REGION\*

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The morphology and habits of diamond single crystals that were seed-grown in the diamond thermodynamic stability region have been studied. Diamond single crystals were grown by the temperature gradient method in a recessed-anvil type high-pressure apparatus at a pressure of 6 GPa and temperatures from 1350 to 1420 °C. The paper describes the characteristic features of face surfaces of the crystals under study. We have indexed the faces using an optical goniometer. It has been found that there are five main habit types of crystals.

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### 1. Introduction

The crystal morphologies of the majority of substances are governed by the conditions of growth. In this respect, diamond is no exception. It is known that there is a variety of morphological types of natural diamond crystals [1-3]. Many describe the crystalline morphology of synthetic diamond [4-10]. It has been reliably established that depending on p,T-conditions of synthesis, the crystal morphology varies regularly in a series cube-cubooctahedron-octahedron-rhombododecahedron. We have studied the inner morphology of statically synthesized diamond crystals and specific features of their face topography.

The reports on morphology and structure of diamond crystals grown by crystallization onto a seed under the temperature gradient conditions are devoted to individual crystals only [10-12]. In the course of the present investigation we have managed to produce synthetic diamond crystals of a new habit type, which contain faces of tetragontrioctahedron as the main forms [13].

### 2. Experimental

The external morphology of crystals has been studied using a MBS-1 binocular and a Camebax scanning electron microscopes (magnifying power being from 30 to 200). The indexing of crystal faces and determination of their position with respect to the faces of perfect simple forms have been performed employing a GD-1 goniometer that allows to determine the spherical coordinates of faces with an error smaller than 2-3 angular minutes. The crystals were adjusted on the {111} and {001} faces.

### 3. Results

The following single forms: cube (001), octahedron (111), rhombododecahedron (110) and tetragontrioctahedron (113) are responsible for the habits of crystals under study. Earlier we have

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described spherical coordinates of typical crystals [14] and Figs. 1-4 provide their habits. The deviations of faces from their theoretical position vary in the range from several minutes to 1.5-2.0 degrees. If we assume that the extent of the face deviation characterizes the perfection of simple forms that are responsible for the crystal habit, then the most perfect form of a crystal grown by the T-gradient method is octahedron. The deviation of octahedral faces from the theoretical position measures usually several minutes and rarely is as much as 20-30 minutes.

Faces of other forms exhibit much higher deviations of about tens of minutes and often 1-2°. In the first approximation the other forms arranged in the order of lower perfection are cube, rhombododecahedron, tetragontrioctahedron.

All observed habits of crystals could be divided into five main types:

1. Octahedral habit. For crystals of this type, the octahedron is the holohedral and best-developed form. Other forms are not holohedral and of an inferior or weak development. The  $\{110\}$  faces blunt the  $\{111\}:\{111\}$  and  $\{113\}$  edges and truncate the  $\{111\}$  faces at vertices; and the  $\{001\}$  faces truncate vertices of an octahedron. Crystals of this habit type form by growing on the  $\{001\}$  face of a seed crystal. Fig. 1 shows crystals of octahedral habit (samples As-60 and A-84). Among crystals of this habit, one comes across such that do not virtually have faces of any other habit. For instance, a crystal 3-mm in size has cubic faces, whose maximum size is 0.2-0.3 mm (see Fig. 1). These faces are narrow and blunt the pseudo edge at the crystal vertex.

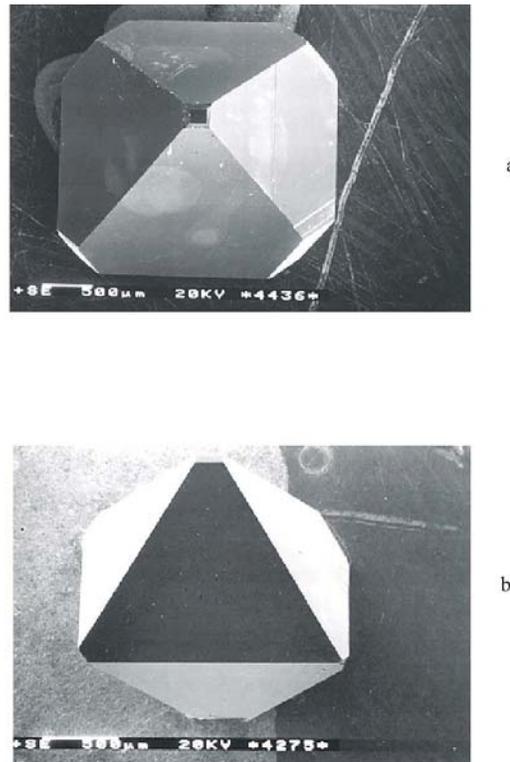


Fig. 1. Octahedral habit type: samples As-60 (a), A-84 (b).

2. *Tetragontrioctahedron-octahedral habit.* This habit is defined by the uniform development of tetragontrioctahedron and octahedron faces. In crystals of this habit, the  $\{111\}$  and  $\{311\}$  simple forms are best developed and virtually always holohedral; other forms are of an inferior development, the  $\{110\}$  faces are less developed than the  $\{100\}$  are. See sample A-62/2 in Fig. 2a.

3. *The habit, which is defined by the uniform development of octahedron, rhombododecahedron and tetragontrioctahedron faces.* See sample KK1/1/5 in Fig. 2b. The forms, which are responsible for this habit, are almost holohedral but the sizes of faces of the same form can be different. Cubic faces are weakly developed, they blunt vertices and the  $\{113\}$  pseudoedges.

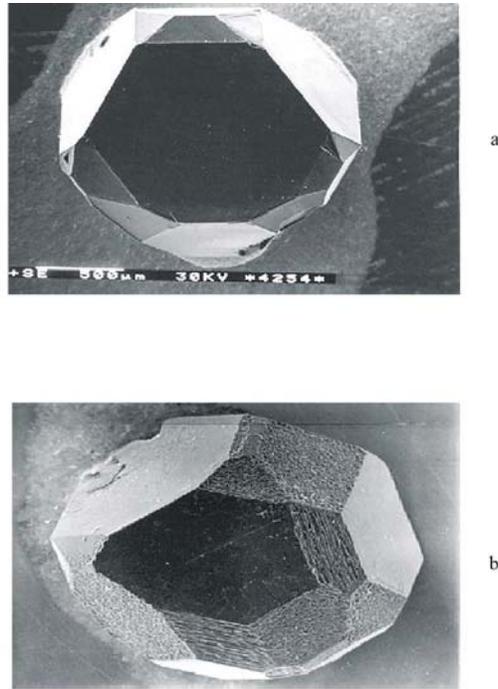


Fig. 2. Diamond single crystals of the tetragontrioctahedron - octahedral (a) and rhombododecahedron-tetragontrioctahedral (b) habits. Samples A62/2 (a) and KK1/1/5 (b).

4. *Cubooctahedral habit.* In addition to habit faces, crystals of this type exhibit also the  $\{110\}$ ,  $\{113\}$  and rarely  $\{115\}$  faces, which blunt edges to a variable degree and are weakly developed. See samples As-62/2 and A-78 in Figs. 3a, b. Crystals of this habit form if a seed is oriented relative to a carbon source either with the  $(111)$  or the  $(001)$  face. In the first case, the as-grown crystals are flattened along the  $L_3$  axis (see Fig. 3a, sample As-62/2). In the second case, the crystals can be either isometric or elongated along the  $L_2$  axis (sample A-78, Fig. 3b).

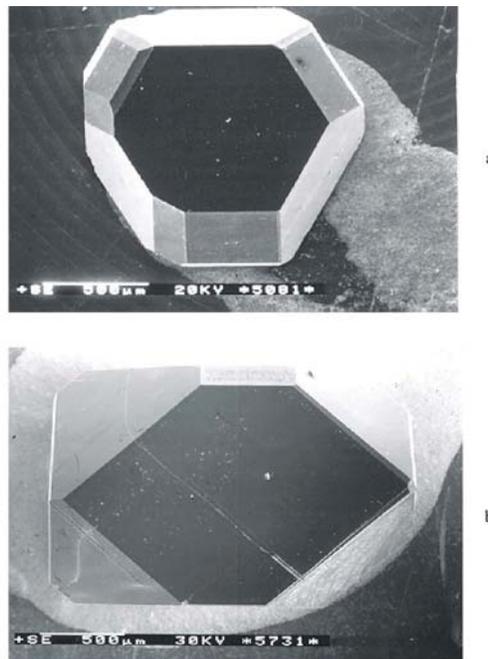


Fig. 3. Crystals of the cubooctahedral habit: samples As-62/2 (a) and A-78 (b).

5. *Cubic habit.* Only two forms are responsible for the cubic habit of crystals. Except for the habit faces  $\{100\}$ , they have only the  $\{111\}$  faces, which truncate vertices of a cube to a variable degree (see samples As-41/1 and As-42/2 in Fig. 4). The elongation of crystals along the  $L_2$  axis is observed; in these cases the crystals acquire pseudoprismatic habit (see Fig. 4b). Crystals of the cubic habit are well developed, have even edges and flat faces. It should be noted that sometimes the  $\{100\}$  faces have dull surfaces. At high magnifications these faces are found to be covered by low isometric or elongated heaps (fractions of a micrometer in height) without any orientation.

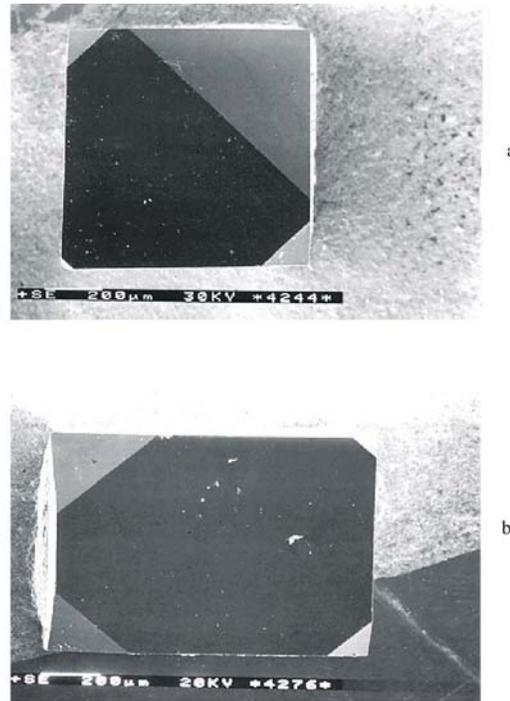


Fig. 4. Diamond single crystals of the cubic habit: samples As-41/1 (a) and As-42/2 (b).

#### 4. Conclusions

Goniometric measurements of single crystals allow for the following conclusions:

1. In addition to the observed earlier simple forms ( $\{111\}$  – the octahedron,  $\{100\}$  – the cube,  $\{110\}$  – the rhombododecahedron and  $\{113\}$  – tetragontrioctahedron), a new form – the  $\{115\}$  tetragontrioctahedron has been established (Fig. 5). Earlier this form has been found on the crystals of spontaneous nucleation [14] and has not been observed on the crystals grown on a seed.

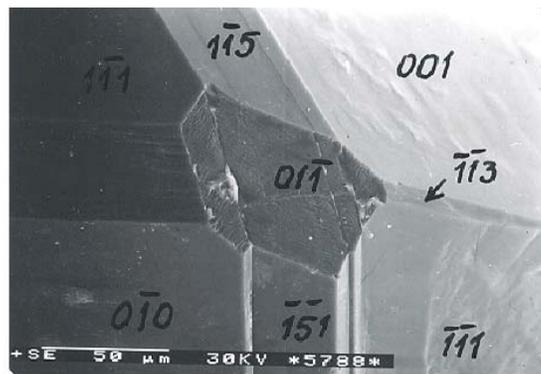


Fig. 5.  $\{115\}$  faces that blunt edges of a crystal. Sample A-78.

2. The crystals under study have rather perfect habits. The position of octahedral faces of all the crystals is the closest to the ideal one. A mean deviation of spherical coordinates of the {111} faces from the theoretical value is 11 angular minutes. 40% of all measured faces deviate from the ideal position by 5' and less and the highest deviation of the {111} faces is as high as 35'. For each of the {100}, {113} and {110} forms, the mean deviation from the ideal position is 17'. Coordinates of 40% of each form differ from the theoretic ones by 10' and less, the highest deviation being 45'. It should be noted that the deviation of the {111} and {110} faces of natural diamonds from the ideal positions might run as much as 1°30' [3].

3. When studied under a binocular microscope, the majority of {111} and {110} faces of the best-developed forms appear perfect and mirror-smooth. Goniometric measurements have, however, shown that faces of all simple forms of the majority of crystals have a block structure. The measurements of the coordinates of clearly isolated light reflections, which correspond to the individual regions of the surface of 0.1 - 0.2 mm in size, have shown that disorientation of blocks within the same face can run to 1°.

Thus, we have found that five habit types are characteristic of diamond single crystals grown by the T-gradient method. They are octahedral, tetragontrioctahedral, rhombododecahedral, cubooctahedral and cubic.

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