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On the Twinning and Lattice Type of Polyhalite

By

Tateo UEDA and **Masahisa TATEKAWA**

Geological and Mineralogical Institute, University of Kyoto

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Abstract

The twinning of polyhalite might extend to a submicroscopic scale, and it occurs in two ways, i.e., one is the twinning by [001], the other is that on (100). The cell is triclinic face-centered. The cell-dimensions and interaxial angles are as follows:

$a=11.73\pm0.01$ Å $\quad \alpha=90°51'\pm0.1°$
$b=16.42\pm0.01$ Å $\quad \beta=90°08'\pm0.1°$
$c=7.65\pm0.01$ Å $\quad \gamma=91°08'\pm0.1°$.

The unit cell contains $4[K_2Ca_2Mg(SO_4)_4\cdot2H_2O]$.

Introduction

PEACOCK (1938) made a close investigation on the morphology of polyhalite comparing the mineral with leightonite, a copper homologue of the former. At that time he adopted a pseudo-orthorhombic setting. With reference to the setting polyhalite is commonly elongated in parallel with c-axis and has been described to be usually twinned on (010) and (100), and its axial ratio and interaxial angles have been given as follows:

$$a:b:c=0.7176:1:0.4657;\ \alpha=90°39',\ \beta=90°06\frac{1}{2}',\ \gamma=91°53'.$$

In such a setting the indices of the faces suggest that the nature of the lattice of the mineral might, as PEACOCK pointed out, be face-centered. PEACOCK says in his article that "*if a rigorous röntgenographic determination can be made, in spite of the difficulties which will arise from the complicated twinning, it will be interesting to compare the results with those obtained from the morphology.*"

Recently the authors have examined polyhalite in detail by taking Weissenberg photographs and clarified the problem in question. Results will be given below.

Experimental

Specimens used for taking Weissenberg photographs are from Salzburg, Austria. They are elongated in parallel with c-axis, colourless and transparent. Specimen stuck to the crystal holder was so minute, about 1 *mm* in length and about 0.1 *mm* in diameter, that no trace of twinning could be observed even under the microscope. The rotation photograph was taken about c-axis. The reflexions are all arranged perfectly on the layer lines. (Fig. 1) The reflexions on the zero layer Weissenberg

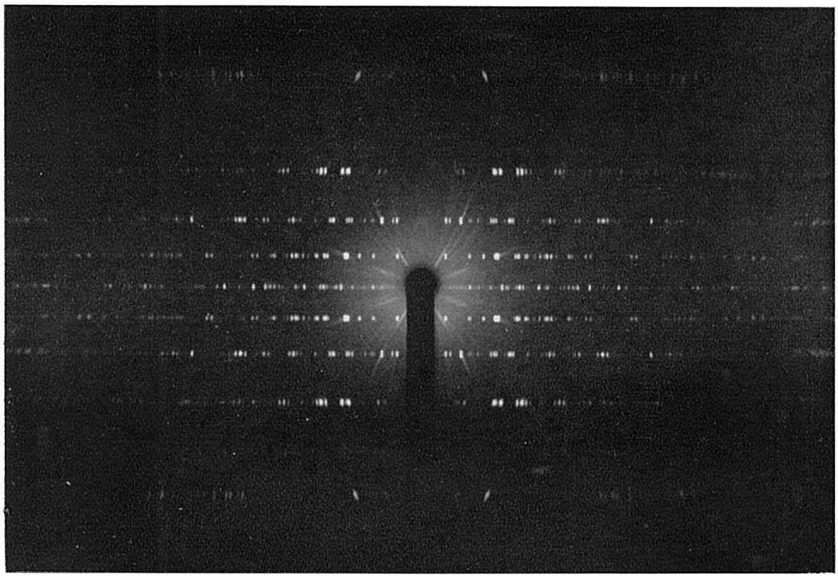

Fig. 1. Rotation photograph about c-axis.

photograph split mostly into two, except for the reflexions on the slanting straight line a^*. (Fig. 2) There are, therefore, two sets of reciprocal lattice lines which cross the slanting straight line a^*. They cross, too, each other on that slanting straight line a^*. Close observation with hand lens discloses that the reflexions on the line B, (Fig. 2) which is about 91° apart from the slanting straight line a^*, split crossways into two, that is, there are two slanting straight lines, b_1^* and b_2^*, (Fig. 2) which closely adjoin. The zero layer Weissenberg photograph was transformed into ordinary reciprocal net plane. The only way to decipher such a reciprocal net plane is that which deduce two direct lattices, A_1 B_1 C_1 D_1 and A_2 B_2 C_2 D_2, (Fig. 3) which are related by a reflexion across a direct lattice line [010]. The fact suggests the twinning on (100). The specimen used in the present investigation does not give any information which suggests the twinning

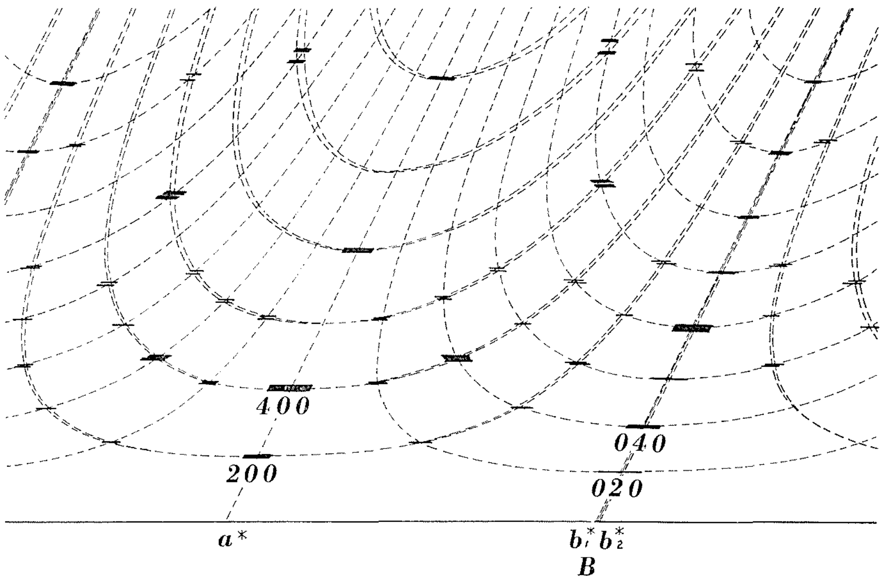

Fig. 2. The zero layer Weissenberg diagram.

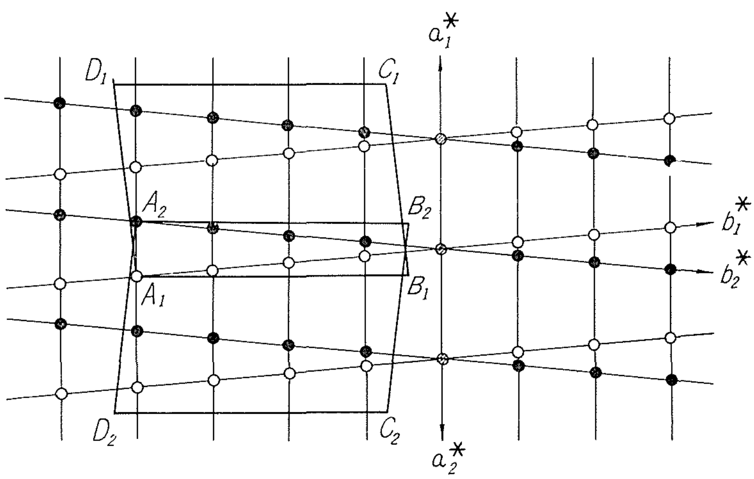

Fig. 3. *hk0* reciprocal net plane. The angle between b_1* and b_2* is exaggerated.

on (010). If such a twinning be present, the reciprocal lattice lines crossing the slanting straight lines, b_1* and b_2*, should consist of two sets of ones. This is, however, not the case.

The reflexions on the 1st and 2nd layer equi-inclination Weissenberg photographs (Fig. 4 and Fig. 5) split into two, three or four. Higher order reflexions are more conspicuous than lower order reflexions in splitting into four. The reflexions on the line A (Fig. 5) split crossways into two. The line A is, therefore,

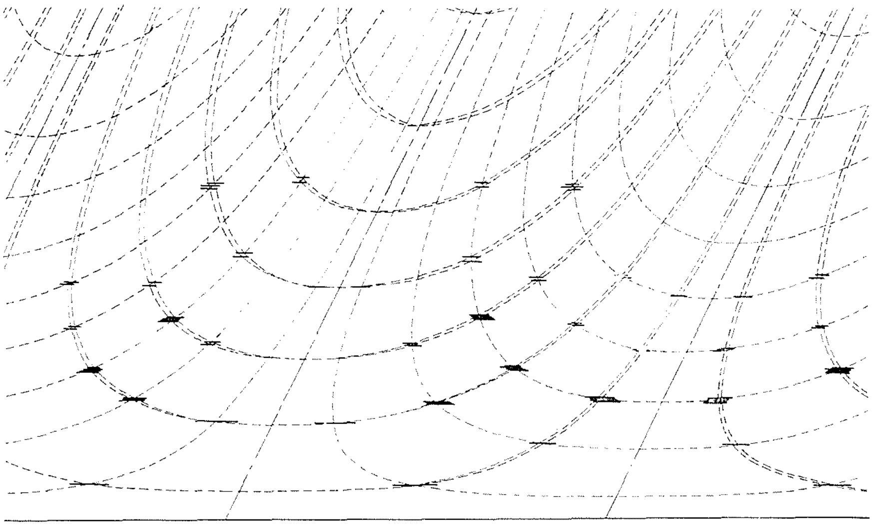

Fig. 4. The 1st layer equi-inclination Weissenberg diagram.

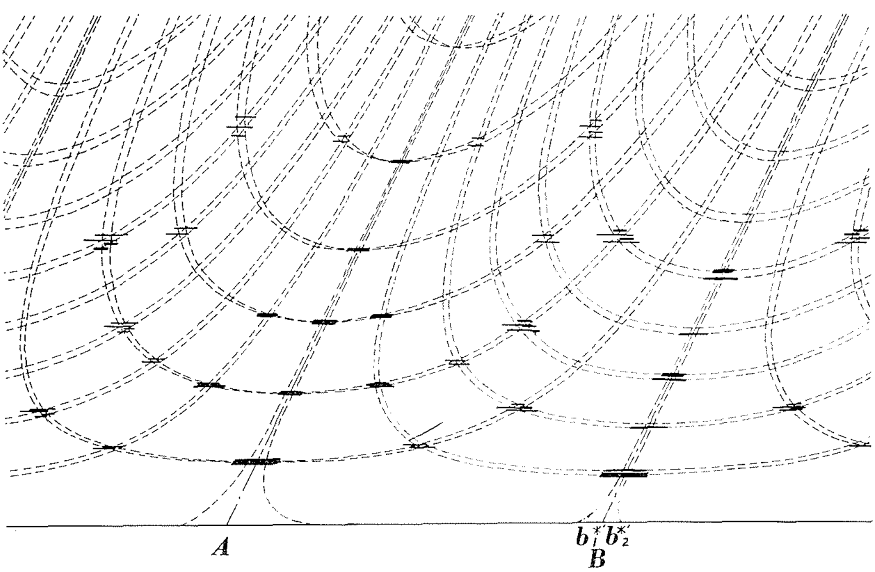

Fig. 5. The 2nd layer equi-inclination Weissenberg diagram.

on longer a reciprocal lattice line. There are two sets of reciprocal lattice lines which cross the line A. They cross each other on that line A. On the other hand, the reflexions on the line B, (Fig. 5) which is about 91° apart from the line A, split longitudinally and crossways into four. There are, therefore, two lines, $b_1^{*\prime}$ and $b_2^{*\prime}$. (Fig. 5) The reciprocal lattice lines crossing the lines, $b_1^{*\prime}$ and $b_2^{*\prime}$, are doubled respectively. Of the reflexions which form an assemblage, two being short and two long, the two short reflexions always appear outwardly and the two long reflexions inwardly on the right side to the line A, while the situation is reverse on the left side. (Fig. 6) The 2nd layer Weissenberg photograph was transformed into ordinary reciprocal net plane. (Fig. 7) The only way to decipher such a reciprocal net plane is that which deduce four direct lattices, A_1 B_1 C_1 D_1, A_2 B_2 C_2 D_2 and A_1' B_1' C_1' D_1', A_2' B_2' C_2' D_2'; the formers are related to the latters by the rotation of 180° respectively, the relationship between A_1 B_1 C_1 D_1 and A_2 B_2 C_2 D_2 is the same as described above.

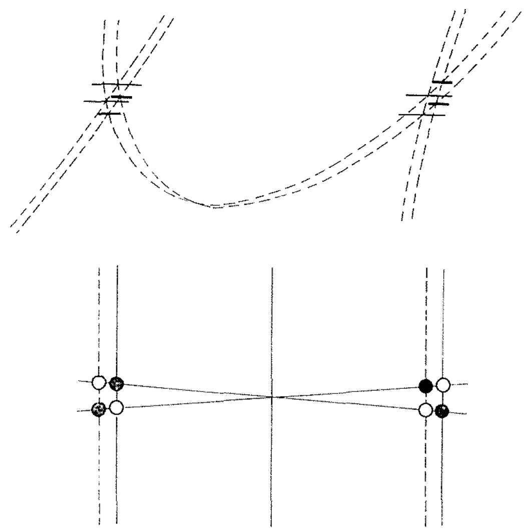

Fig. 6. Relationship between two corresponding reflexion assemblages on the right and left side of line A.

The results obtained from the zero layer Weissenberg and the 1st and 2nd layer equi-inclination Weissenberg photographs indicate that there are two kinds of twinning, one is the twinning by [001], the other is that on (100).

The lattice dimension c was calculated from the rotation photograph, and a^* and b^* were from the zero layer Weissenberg photograph giving indices to the reflexions on the slanting straight lines as shown in Fig. 2. The axial angle γ was

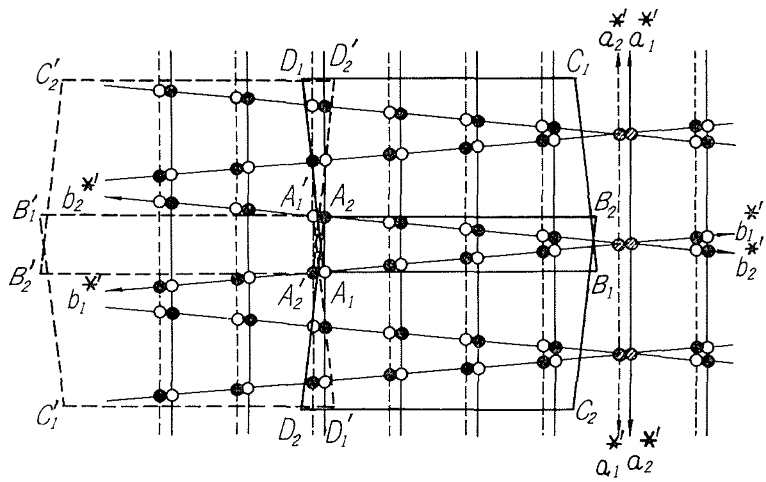

Fig. 7. The 2nd layer reciprocal net plane. The angle between $b_1^{*\prime}$ and $b_2^{*\prime}$ is exaggerated.

calculated from the z component between the slanting straight lines, a^* and b_1^*, on the zero layer Weissenberg photograph, and the axial angles α and β were by the method of level offsets. The cell-dimensions and interaxial angles obtained are as follows:

$$a=11.73\pm0.01\ \text{Å} \qquad \alpha=90°51'\pm0.1°$$
$$b=16.42\pm0.01\ \text{Å} \qquad \beta=90°08'\pm0.1°$$
$$c=\ 7.65\pm0.01\ \text{Å} \qquad \gamma=91°08'\pm0.1°.$$

Consequently, axial ratio: $a:b:c=0.714:1:0.466$. Space group is $F\bar{1}$, since reflexions appear when $h+k=2n$ and $k+l=2n$, and the present mineral is, as known from the morphology, centrosymmetrical. The unit cell contains $4[K_2Ca_2Mg(SO_4)_4\cdot2H_2O]$.

Consideration

The space group of polyhalite has long been unknown, although in 1938 PEACOCK suggested that it might be triclinic face-centered. By the present investigation it has been disclosed to be $F\bar{1}$, so far as the crystal axes are selected after PEACOCK. The mineral has been described by PEACOCK to be twinned on (010) and (100), but according to the present investigation the twinning of the mineral occurs in two ways, one is the twinning by [001], the other is that on (100). The mineral may seem as if it were twinned on (010) and (100) outwardly, owing to the two kinds of twinning said above and also to the fact that the axial angles are nearly 90°. The twinnings might extend to a submicroscopic scale.

The axial ratio obtained from the lattice constants is $a:b:c=0.714:1:0.466$ as described above, which is in good agreement with the ratio $a:b:c=0.7176:1:0.4657$ given by PEACOCK.

Reference

PEACOCK, M. A. (1938) The relation of leightonite to polyhalite, Am. Min., 23, 38.