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Twinning in barium titanate crystals*.

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Single crystals of barium titanate have been grown in these laboratories by a technique based on the method due to Remeika (1954). The investigation of the domain structure and electrical properties of barium titanate crystals has received considerable attention (e.g. Merz, 1952, 1954), but few details have been published of the interesting crystallographic features displayed by crystals grown from solution in potassium fluoride.

The so-called 'butterfly twin' crystals obtained consist of two triangular plates joined along the hypotenuse at an acute angle. A narrow, well developed face is present along the junction of the plates (Fig. 1(*a*)). Occasionally crystals are found which have the plates joined at an obtuse angle. Crystals of the latter type possess a sharp edge along the junction (Fig. 1(*b*)). It may be noted in Fig. 1(*a*) that in the acute-angled crystals tapering of the thickness of the plates occurs near to the junction. This is presumably due to restricted access of solution to the narrow space between the two crystal plates.

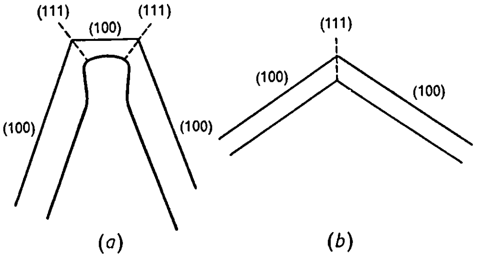

Fig. 1. Sections through the junction of $BaTiO_3$ twinned crystals. (*a*) Acute-angled 'butterfly twin'; (*b*) obtuse-angled crystal.

Measurement of the angle between the wings for a large number of crystals showed it to be approximately constant. The small variations observed may be ascribed to differences in the axial ratio of the structure cell, together with variations in the ratio of *a* to *c* domains (Forsbergh, 1949) at the junction.

The mean value obtained is consistent with a (114) twinning plane. Consideration of the atomic arrangement for the (114) plane, however, did not suggest a definite reason for such twinning. Furthermore, the small face at the junction of the acute-angled crystals would have the indices 221 for a (114) twinning plane. Such a face should rapidly disappear during growth owing to differential growth rates between (221) and (100).

Table 1. *Calculated and observed angles between the 'wings' of barium titanate twin crystals*

	Type of crystal	Calculated angle	Observed angle
Acute-angled twins	Entirely *a* domain ($c/a = 1{\cdot}01$)	39° 18′	—
	Entirely *c* domain ($c/a = 1{\cdot}01$)	38° 34′	—
	Equal *a* and *c* domains present (equivalent to $c/a = 1$)	38° 58′	—
	Mean observed value	—	38° 49′
Obtuse-angled twins	Equal *a* and *c* domains present (equivalent to $c/a = 1$)	109° 29′	—
	Mean observed value	—	109° 31′

A close study of many crystals has shown that, in fact, two twinning planes are present in each 'butterfly twin', both of which are (111) planes. The observed narrow face at the junction is thus a (100) face, and is consequently retained throughout the development of the crystal. The obtuse-angled crystals possess only a single (111) twinning plane and thus have a sharp junction.

The dendritic type of growth, which is readily obtained from potassium fluoride solution, also shows (111) twinning. In this case sheets of crystals are formed in which either tabular crystals or pyramids project on both sides and in all possible orientations from the common (111) plane.

Twinning in barium titanate thus conforms to established twinning laws for cubic crystals. The 'butterfly twin' habit is evidently a result of the prevalence of twinning, although the reasons for the precise form of this twin are not yet clear.

References

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On the structure of the crystal form *A′* of *n*-pentadecanoic acid.

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The structure described by von Sydow (1954) has been refined using difference syntheses. A temperature factor $\exp\,[-B\sin^2\theta/\lambda^2]$, with $B = 3{\cdot}0$ Å^2, has been applied. The coordinates of the hydrogen atoms were derived as in von Sydow (1954), and these values agree very well with the maxima obtained in the (F_o-F_c) synthesis where only the oxygen and carbon atoms were included in the calculation of F_c. The coordinates of the heavier atoms are collected in Table 1, and observed and calculated structure factors in Table 2. $R_1 = 0{\cdot}14$ when non-observed reflexions are omitted.

No change of signs is obtained for the observed reflexions, so the electron-density projection shown in the earlier paper is almost the same as that obtained with the values in Table 2 of this paper.

The two rows of carbon atoms are not quite straight, as was supposed earlier. Therefore, the subcell theory could not be used in the structure-factor calculations. The suggestion that the chains are helically twisted has been strengthened by these new results.

Reference

Sydow, E. von (1954). *Acta Cryst.* 7, 529.

Table 1. *Coordinates of the atoms*

Atom	y/b	z/c
O_1	0·244	0·0041
O_2	0·621	0·0434
C_1	0·401	0·0350
C_2	0·306	0·0540
C_3	0·459	0·0926
C_4	0·341	0·1160
C_5	0·516	0·1532
C_6	0·373	0·1798
C_7	0·575	0·2131
C_8	0·410	0·2433
C_9	0·630	0·2735
C_{10}	0·454	0·3062
C_{11}	0·681	0·3337
C_{12}	0·497	0·3681
C_{13}	0·725	0·3941
C_{14}	0·547	0·4308
C_{15}	0·767	0·4546

Table 2. *Observed and calculated structure factors*

hkl	$\|F_o\|$	F_c
000	272	—
001	32	+33
002	7	+ 8
003	23	+25
004	< 5	+ 1
005	16	+18
006	< 6	− 6
007	6	+10
008	8	−12
009	< 7	+ 3
0,0,10	9	−12
0,0,11	< 8	+ 1
0,0,12	13	−13
0,0,13	< 8	− 2
0,0,14	14	−14
0,0,15	< 9	− 5
0,0,16	10	+ 5
0,0,17	<10	− 3
010	110	−100
011	18	−18
012	30	−27
013	13	− 7
014	10	−10
015	< 8	− 1
016	< 8	+ 3
017	< 8	+ 3
018	< 9	+ 6
019	< 9	+ 4
0,1,10	<10	+10
0,1,11	<10	+ 3
0,1,12	<10	0
0,1,13	<11	+ 3
0,1,14	<11	− 2
0,1,15	48	+49
0,1,16	23	+23
0,1,17	19	−19
0,1,18	<12	+ 1
$01\bar{1}$	40	−27
$01\bar{2}$	70	+54
$01\bar{3}$	< 7	− 9
$01\bar{4}$	22	+16
$01\bar{5}$	< 7	− 8
$01\bar{6}$	13	+14
$01\bar{7}$	< 8	− 3
$01\bar{8}$	15	+16
$01\bar{9}$	< 8	+ 5
$0,1,\overline{10}$	16	+16
$0,1,\overline{11}$	9	+ 9
$0,1,\overline{12}$	19	+16
$0,1,\overline{13}$	10	+16
$0,1,\overline{14}$	18	+14
$0,1,\overline{15}$	12	+17
$0.1,\overline{16}$	25	−25
$0,1,\overline{17}$	62	+58
$0,1,\overline{18}$	<11	+12
0,2,13	<13	+ 8
0,2,14	21	+22
0,2,15	30	−34
0,2,16	15	−18
0,2,17	<14	− 1
$02\bar{1}$	<10	− 5
$02\bar{2}$	17	−21
$02\bar{3}$	<10	−14
$0,2,\overline{16}$	<12	+ 6
$0,2,\overline{17}$	18	−25
$0,2,\overline{18}$	39	−42
$0,2,\overline{19}$	17	+15
$0,2,\overline{20}$	<13	−10

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On the structure of the crystal form *B′* of *n*-pentadecanoic acid, and On the structure of the crystal form *B* of stearic acid: correction.

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In the above papers (von Sydow, 1954, 1955) the results given by Vand, Morley & Lomer (1951) concerning the structure of the crystalline *C*-form of lauric acid have been erroneously interpreted. In this form the chain planes of two molecules coupled together with hydrogen bonds are not perpendicular but parallel.

In the *B*-form of stearic acid (von Sydow, 1955), which has the same space group as the *C*-form, the chain planes of two such molecules are also parallel. In the *B′*-form of *n*-pentadecanoic acid (von Sydow, 1954), however, the planes are perpendicular, as was stated in the original paper.

References

Sydow, E. von (1954). *Acta Cryst.* 7, 823.
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Vand, V., Morley, W. M. & Lomer, T. R. (1951). *Acta Cryst.* 4, 324.