Planar faults, designated $F_1$, $F_2$, and $F_3$, with intermixed dislocations in metastably retained hexagonal-BaTiO$_3$ ceramics, were found and analyzed by transmission electron microscopy. Only faults with one, two, and four extra $c$-layers parallel to the basal plane have been identified. Fault vectors $R_{F_1} = R_{F_3} = 1/6[0221]$, $R_{F_2} = R_{F_3} = 1/3[0111]$, $R_{F_3} = 1/3[0112]$, and $R_{F_3} = R_{F_2} = R_{F_1} = 1/6[0221]$ were determined adopting the $2\pi n\cdot R = 0$ (or $2\pi n$) criteria in combination with high-resolution imaging. Further, the embedded dislocations were half-partials with Burgers vectors $b = 1/3[1010]$ determined by the $g\cdot b = 0$ effective invisibility criteria in conjunction with the eligible fault vectors. A rotation by 60° about the $c$-axis was found between fault segments with $R_{F_2} = 1/6[0221]$ and $R_{F_3} = 1/6[0221]$ located on either side of a partial. Basal dislocations with $b_0 = 1/3[1210]$ have dissociated into two prism-plane Shockley half-partials with $b_{0s} = 1/3[1100]$ by glide in the fault plane (0002) according to $1/3[1210] \rightarrow 1/3[1100] + 1/3[0110]$. The fault segment $F'_3$ encompassed by two half-partials is an extrinsic complex stacking fault.

1. Introduction

High-temperature hexagonal (h-) BaTiO$_3$ (P6$_3$/mmc, No. 194) have been retained metastably at room temperature with acceptor doping, for example, Mg$^{2+}$ or Fe$^{3+}$, substituting for the Ti$^{4+}$ site, or by hot pressing in low oxygen partial pressures. The 6H-polype (i.e., h-BaTiO$_3$) is not ferroelectric; another hexagonal phase ($P_2_1$ (No. 17)) only becomes ferroelectric at $\sim 77$ K ($\sim 196$ C). Although doped with acceptor oxide Ga$_2$O$_3$, h-BaTiO$_3$ has been explored for microwave dielectrics; unlike the tetragonal phase, its practical applications are still limited. Fault vectors ($R_q$) in the h-BaTiO$_3$ ceramics prepared by hot pressing in a graphite die assembly were analyzed and how these faults were generated in low oxygen partial pressures has been proposed. It was suggested that the stacking faults described as interleaved c-BaTiO$_3$, lamellae embedded in h-BaTiO$_3$ matrix are growth faults due to local oxygen excess accommodated by extra corner-sharing $c$-layer(s). The faults consisted of extra $c$-layers relative to the $(\text{che}_{2})(\text{che}_{2})(\text{che}_{2})$ (or equivalently (CBC)(ABA)) stacking sequence of 6H-polytype. They contained no dislocations. Here, we report on an analysis concentrating on planar faults, intermixed with dislocations, which have been divided into several segments. With dislocations running across the faults, the fault fringe contrast was distinctive on either side of a dislocation. A fringe contrast of alternate visible-invisible bands in strong-beam images had appeared among the fault segments.

Eibl et al. have reported the presence of both perfect and partial dislocations in h-BaTiO$_3$ ceramics sintered at 1440°C in air, followed by annealing at 1400°C in an N$_2$-H$_2$ atmosphere. Similar to hexagonal close-packed metals (A$^3$ hcp), and D$_0$$_{19}$ intermetallics, the unit lattice translation vectors in h-BaTiO$_3$ are $1/3[1120]$, $\{1010\}$, and $[0001]$. Perfect dislocations with $b = 1/3[1120]$ and a pair of Shockley partials with $b'$ and $b'' = 1/3[1100]$, all lying in the basal plane, were identified. Dissociation of the former into a pair of Shockley half-partials, often found in hexagonal systems, has also occurred in h-BaTiO$_3$ by the classical reaction

$$b \rightarrow b' + b''$$

$$1/3[1210] \rightarrow 1/3[1100] + 1/3[0110]$$

Some of the perfect dislocations not lying in the basal plane had climbed. The Shockley half-partials were found to lie within widely extended planar stacking faults (EPSF). The fault vector of the portion of the stacking fault bordered by partial dislocations $D_3$ and $D_4$ in Eibl et al.'s work was $R_F = 1/3[1101]$ while that of the other portion was $R_F = 1/3[1101]$, such that the fault vectors have opposite components in the basal plane: [1100] and [1100]. It was concluded that the two fault vectors differed only in the components parallel to the basal plane, i.e., the prismatic components $1/3[1010]$ of the general form: $R_F = (n/6) [0001] + l/3[1010]$, by vectors other than the lattice vectors. In addition, the two segments of stacking fault, separated by one of the Shockley half-partials, lie in two distinct basal planes (i.e., $0001$ where $l = 1 - 6$) separated by $1/2c$ where $c = [0001]$.

In this study, the planar faults in hot-pressed h-BaTiO$_3$ found to be embedded with partial dislocations were determined for their type, fault vectors, and the intermixed dislocations for Burgers vectors by the transmission electron microscopy (TEM). All dislocations were half-partials with $b = 1/3[1010]$, consistent with those reported before by Eibl et al. Relationships between Burgers vectors and fault characteristics are discussed.

2. Experimental Procedure

A commercial hydrothermal BaTiO$_3$ powder (K-Plus (Boyertown, PA) was used in this study. The powder was stoichiometric and contained major impurities of residual carbon.

Manuscript No. 21138. Received November 9, 2005; approved March 29, 2006. 
We thank the National Science Council of Taiwan for funding support through contracts NSC 91-2216-E-110-018, 92-2216-E-110-003, 93-2216-E-110-015, and 94-2216-E-110-004.

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2Work was done while at NSYSU.
3Member, American Ceramic Society.
(<1000 ppm), soluble chloride (<250 ppm), and strontium (<500 ppm), according to the manufacturer. Samples were hot pressed at 1300°C for 2 h by a uniaxial pressure of ~25.8 MPa in a graphite die assembly using a Fuji Dempa (Osaka, Japan) multipurpose furnace equipped with a graphite resistance-heating element whose temperature was monitored by a W-Re thermocouple and a two-color pyrometer. Hot-pressed samples, while being kept in the graphite die, were furnace cooled to room temperature.

As-hot-pressed disks of 15 mm diameter were lightly polished to remove graphite and boron nitride (BN) coating from the graphite spacers that were inserted between the graphite punch and BaTiO$_3$ samples before hot pressing. Thin foils for TEM were prepared by the conventional technique of cutting with a diamond-embedded saw, grinding, and polishing to an ~30 μm thickness, and 1 μm of surface roughness before dimple grinding to an ~10 μm thickness in the center region. The thin sections were then Ar $^+$ ion-beam thinned (DuoMill™, Gatan, Pleasanton, CA) to electron transparency. Observations were made in a JEM™ AEM3010 (Tokyo, Japan), with a double-tilting stage of ±45° for the x-tilt and ±30° for the y-tilt, operating at 300 kV.

III. Results

Stacking faults were observed in almost all h-BaTiO$_3$ grains. Grains were spherulitic in shape although not grown abnormally.\(^1\)\(^,\)\(^2\)

(1) General Observations—Fringe Patterns

Selecter area diffraction patterns were indexed\(^3\) corresponding to the standard triangles of the stereographic projection. Seven sets of faults are discernible from one of the h-BaTiO$_3$ grains imaged in strong beam bright field (BF) (Fig. 1). Spot streaking suggests that the foil contains planar defectsinclining to the beam direction at deviation parameter $s_g \neq 0$ (Figs. 1(a) and (b)).\(^5\)\(^,\)\(^10\) Only six of them, designated as $F_1$–$F_6$, have been fully characterized. Faults $F_5$ and $F_6$ were visible (Fig. 1(a)) when imaged with $g = 1014$. Faults $F_5$ and $F_6$ are partly superimposed in projection, producing a complex fringe pattern that remains symmetrical in BF. They are entirely similar to faults $F_5$ and $F_6$ in a previous report.\(^5\)

Four dislocations, $d_1$–$d_4$, were detected in the field of view (Fig. 1(a)). Two of them, $d_1$ and $d_2$, with the respective Burgers vectors $b_{d_1}$ and $b_{d_2}$, lie within fault $F_1$, thus dividing $F_1$ into three segments, $F_1$–$F_1$–$F_1$, which show alternate fringe contrast. Using $g = 1014$, the inner segment $F_1$ was visible (indicated by (O)) while the rest of the fault, on both sides of $F_1$, was invisible (indicated by (X)), i.e., fault contrast was reversed across both dislocations $d_1$ and $d_2$. Nevertheless, the fringe patterns revealed by a strong-beam BF image were symmetrical and complementary (for $s_g = 0$) about a foil center.\(^11\) Extreme fringe contrast was both dark in BF image, and the dark–dark (D–D) fringe pattern of $F_1$ is indicated in Fig. 1(a). The fringes were however asymmetrical in CDF image where the extreme fringe contrast became dark–bright (D–B). The contrast characteristics are similar to those reported\(^5\) before, which allows us to conclude as of the $\alpha$-type fault\(^11\) with fault vectors (R), thus directly related to the lattice displacement vectors of hexagonal crystals.

Fault $F_1$ is bordered by dislocation $d_2$, as indicated in Fig. 1(c). Dislocation $d_4$ with Burgers vector $b_{d_4}$ sits in the foil alongside with fault $F_3$. Causing no change in the fringe pattern, it is not in contact with the fault. Nevertheless, its presence indicates that h-BaTiO$_3$ was plastically deformed during hot pressing by the movement of dislocations $b_{d_4} = 1/3[1010]$. Faults $F_1$–$F_4$ are invisible (X) while $F_5$ and $F_6$ remain visible (O) both from $g = 1014$ and 1104. All these faults are invisible from $g = 2110$ and visible from $g = 2114$, accordingly (Figs. 1(a)–(d)). They are of a wedge shape as the foil thickness continuously decreases toward the left of the image.

(2) Determination of Fault Vectors for Faults $F_1$–$F_6$ and $F_d$

The eligible fault vectors for $F_1$–$F_6$ were determined by the three-step procedure\(^5\) described previously: (1) application of the invisibility criteria under diffraction contrast and under

![Fig. 1](https://example.com/fig1.jpg)  
*Fig. 1. Contrast analysis for faults $F_1$–$F_6$ using (a) $g = 1014$, (b) $g = 1104$, (c) $g = 2110$, and (d) $g = 2114$ (bright-field image, transmission electron microscopy).*
high-resolution imaging; (2) count of the extra c-layers; and (3) identification of displacement along prismatic directions, were followed to determine the eligible fault vectors for \( F_1 \)–\( F_6 \).

(A) Faults \( F_1 \)–\( F_4 \). Faults \( F_1 \)–\( F_4 \) are visible under \( g = 2114 \). (Fig. 1(d)), 1013, and 1103 while \( F_5 \) and \( F_6 \) are visible under \( g = 1014 \) and 1104 in \( Z = [0441] \) (Figs. 1(a) and (b)). The results for fault vectors \( R_{F_1} \), \( R_{F_2} \), \( R_{F_3} \), and \( R_{F_4} \) are shown in Table I; the faults exhibit five, six, and eight layers. All the faults determined here are of the \( R_{F_{im}} \) type, none of the \( R_{F_i} \) \( R_{F(1)} \) type, for example \( F_8 \) in Wu and Lu,\(^3\) has been observed.

The fault vectors for \( R_{F_1} \) are \( 1/6[0221] \), \( 1/6[2021] \), and \( 1/6[2201] \), consistent with observed diffraction contrast and a five-layer fault (with the stacking sequence of \( \text{cchccch} \), containing one extra c-layer) determined from the HR image. The characteristic zig–zag feature of the \( \text{cchccch} \) stacking sequence (with the c-layer indicated by open circles and the h-layer by full circles) in unfaulted \( \text{h-BaTiO}_3 \) was identified from \( Z = [1210] \). Both the zig–zag occurred at the h-layer (i.e., the B-layer in \( \text{CBCABA} \)) and is indicated by full circles in Fig. 2(a). Fault \( F_1 \) may be described by a total of nine layers (i.e., \( \text{R5+L4} \)) consisting of five right-inclined zig layers (designated \( \text{R5} \)) and four zig layers (designated \( \text{L4} \)) by counting twice the turning point at the h-layers (indicated by full circles). Tilting the foil by 30° clockwise to the consecutive \( [0110] \), fault \( F_1 \) containing five layers in total, although embedded in the unfaulted \( \text{cchccch} \) stacking sequence of \( \text{h-BaTiO}_3 \), could still be differentiated by the three c-layers appearing between two h-layers, as indicated by open circles (for c-layers) and full circles (for h-layers) in Fig. 2(b). This is shown in Fig. 2(b) from the framed region of Fig. 2(b) at a higher magnification: the lattice spacings of \( d_{[2110]} = 0.286 \text{ nm} \) and \( d_{[0006]} = 0.233 \text{ nm} \) are also indicated. Unlike the projection on \( (1210) \), whether the h-layer or the c-layer has shifted along \( [2110] \) cannot be discerned from \( Z = [0110] \), although the fault-containing five layers may still be differentiated.

On the other hand, \( R_{F_2} \) and \( R_{F_3} \) are six-layer faults with \( \text{cchet(chc)} \), whereas \( R_{F_4} \) is eight-layered with \( \text{cchet(chc)} \). The eligible fault vectors for \( F_1 \)–\( F_4 \) are summarized in the “number of layers” column in Table I.

(B) Faults \( F'_1 \), \( F_5 \), and \( F_6 \). Faults \( F'_1 \), \( F_5 \), and \( F_6 \) exhibit a \( \text{cchet(chc)} \) stacking sequence, identical to that of \( F_1 \). Eligible fault vectors could only be confirmed by investigating HR images for \( Z = [1210] \) where five-layer faults containing one extra c-layer may be distinguished. For faults \( F'_1 \), \( F_5 \), and \( F_6 \) only three of the six \( \{0110\} \) prismatic directions \( R_{F_1} = R_{F_5} = R_{F_6} = 1/6[0221], 1/6[2021], \) and \( 1/6[2201] \) are valid, referring to the “number of layers” column in Table I. The eligible fault vectors (Table I), projected on \( [0001] \), are illustrated schematically in Fig. 3.

There is a 60°-rotation correspondence between fault vectors \( R_{F_1} = 1/6[0221] \) and \( R_{F_1} = 1/6[0221] \) (Table I), and faults \( F_1 \) and \( F'_1 \) exhibit contrast reversal across dislocations \( d_1 \) and \( d_2 \) (demonstrated in Figs. 1(a) and (b)). The fact that a clockwise 60° rotation of \( F_1 \) (and likewise for faults \( F_2 \)–\( F_6 \)) about \( [0001] \)}
produces non-eligible shear vectors suggests that they are not the \( \pi \)-rotation type.\(^4\)\(^5\)

(c) Fault \( F_0 \) and Partial Dislocation \( d_c \). The fault shown in Fig. 4(a) found in other areas of the foil is interrupted by one of two partials \( d_c \) with Burgers vector \( b_{dc} = 1/3[1100] \) to two segments \( F_0 \) with fault vectors \( 1/6[0221], 1/6[2201] \), and \( 1/6[2201] \), and \( F_o' \) with fault vectors \( 1/6[0221], 1/6[2201] \), and \( 1/6[2201] \) when they differ by a 60° rotation about \([0001]\) (Table I). The true line direction \( u = [2110] \) of partial dislocation \( d_c \) determined by trace analysis suggests that it is a 30°-mixed type. Fault slab, as indicated, can be differentiated unambiguously in Figs. 4(b) and (c). Both segments being five-layer faults of the stacking sequence (chc)(chc) containing one extra c-layer are evidenced from HR images on either side of partial \( d_c \), shown in Fig. 4(d) for \( F_0 \) and Fig. 4(e) for \( F_o' \). The nine-layer stacking sequence of right-inclined fault \( F_0 \) containing (R5+L4)-layers (indicated in Fig. 4(d)) remains unaltered on moving across partial dislocation \( d_c \) to left-inclined fault \( F_o' \) of (L5+R4)-layers (Fig. 4(e)). Moving across the partial dislocation, similar to faults \( F_2, F_5 \), the fault vectors have simply rotated by 60°. Similar to \( F_1 \), the stacking sequence is retained across the partial, i.e. \( d_1 \) and \( d_2 \) in \( F_1 \) and \( d_1 \) and \( d_2 \) in \( F_o' \) (Table II).

(3) Determination of Burgers Vectors, Line Directions for Dislocations Associated with Faults

All dislocations having Burgers vectors \( b = 1/3[1100] \) are prism-plane partials. The term “prism-plane dislocations” suggested by Heuer\(^1\)\(^4\) is adopted here instead of prismatic dislocations to avoid confusion with prismatic loops. Burgers vectors are as follows: \( b_{d_1} = 1/3[1100] \), \( b_{d_2} = 1/3[0110] \), and \( b_{dc} = b_{d_4} = 1/3[1010] \), as given in Table II. True directions have been determined by trace analysis. Only dislocation \( d_2 \) is of the screw type; others are of mixed type of 60° for \( d_1 \) and \( d_4 \), and 30° for \( d_2 \). The prism-plane partials are glissile in the (0002) basal plane in which they are lying.

IV. Discussion

We have compared the present results of fault vectors with those reported previously, placing emphasis particularly on why dislocations \( d_1 \) and \( d_2 \) produce a fault fringe contrast reversal.

(1) Eligible Fault Vectors

Fault vectors determined in this study belong to one of the two general types,\(^3\)\(^5\) \( R_{F_p} \) and \( R_{F_m} \), of the stacking faults in \( b-BaTiO_3 \). They correspond to \( R_{F_p} = n/6[0001] + 1/3[1010] \), \( n = 1, 2, 4, \) and 5 of the extrinsic nature. Each fault shows three possible fault vectors (Table I) as determined accordingly.

Interrupting the \( b-BaTiO_3 \) stacking sequence by inserting extra c-layer(s), contributing to the basal component \((n/6) e\) fault vectors \( R_{Fa} \)\(^3\)\(^5\) has been clearly evidenced from HR images, for example \( 1/6[6221] \) in Fig. 2(a) for fault \( F_1 \). Displacements of the (chc)(chc) zig–zag feature\(^5\)\(^6\)\(^7\) along \((1010)\), for example \( 1/6[6221] \) in Fig. 2(a), have also enabled to determine the prismatic component \( p_{(11)} = 1/3[1010] \). The unfaulted stacking sequence modified by extra c-layers inserted along \([0001]\) taken\(^5\) to justify that only three prismatic components of the shear vectors along \((1010)\) are valid fault vectors is equally applicable to faults analyzed here.

When examining the stacking sequence along \([0001]\), possible shear vectors may again be grouped into two major classes depending on where in the unfaulted stacking sequence the first extra c-layer is inserted. The insertion of the extra c-layer occurring immediately after (CBC) generates left-inclined faults, e.g., \( F_1 \) in Fig. 4(e) (as shown in Fig. 5(a)). Right-inclined faults, e.g., \( F_1 \) in Fig. 2(a) and \( F_4 \) in Fig. 4(d), result from insertion after (ABA) (Fig. 5(b)).\(^3\)

All faults identified in the hot-pressed \( b-BaTiO_3 \) ceramics, i.e. \( F_{Fa} F_{Fa} \) in Wu and Lu,\(^5\) and \( F_1 F_3 \) in the present work are included in the stacking sequences for the five-, six-, seven-, eight-, and nine-layer faults shown schematically for the two groups of faults. So far, not all predicted faults (shown in Figs. 5(a) and (b)) have been encountered.

(2) Dislocation Glide or Climb in Basal Planes

The difference of \( 1/3[1100] \) between fault vectors \( R_{Fa} = 1/6[0221] \) and \( R_{F_a} = 1/6[0221] \) is equal to the Burgers vector of partial dislocation \( d_2 \), and that between \( R_{F_a} \) and \( R_{Fa} \) is again equal to \( b_{d_1} = 1/3[0110] \) of partial dislocation \( d_2 \). As both faults contained one extra c-layer (as evidenced by a similar five-layered fault \( F_o \) shown in Fig. 4(d)), dislocations \( d_1 \) and \( d_2 \) have

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Table I. Fault Vectors for \( F_1, F_1', F_2, F_3, F_5, F_6, F_{Fa}, \) and \( F_{Fa}' \) Determined by the \( 2\pi \cdot R = 0 \) or \( 2\pi \) Invisibility Criteria (\( R_e \) of 12 Variations), High-Resolution Imaging (HR), and Number of Layers of (Three Eligible Vectors)

<table>
<thead>
<tr>
<th>Type</th>
<th>Fault</th>
<th>HR (layers)</th>
<th>( R_e )</th>
<th>Number of layers</th>
</tr>
</thead>
<tbody>
<tr>
<td>( F_{Fa} )</td>
<td>( F_a, F_a )</td>
<td>5</td>
<td>( 1/6[0221], 1/6[2201], 1/6[2201] )</td>
<td>6 layers</td>
</tr>
<tr>
<td>( F_a, F_a )</td>
<td>( F_2, F_3 )</td>
<td>6</td>
<td>( 1/3[0111], 1/3[1011], 1/3[1011] )</td>
<td>8 layers</td>
</tr>
<tr>
<td>( R_{F_{Fa}} )</td>
<td>( F_4 )</td>
<td>8</td>
<td>( 1/6[0225], 1/6[2205], 1/6[2205] )</td>
<td>9 layers</td>
</tr>
<tr>
<td>( F_1 )</td>
<td>5</td>
<td>( 1/6[0221], 1/6[2201], 1/6[2201] )</td>
<td>5 layers</td>
<td></td>
</tr>
<tr>
<td>( F_5 )</td>
<td>( 1/3[0111], 1/3[1011], 1/3[1011] )</td>
<td>6 layers</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( F_6 )</td>
<td>( 1/3[0112], 1/3[1012], 1/3[1102] )</td>
<td>8 years</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( F_{Fa}' )</td>
<td>( 1/6[0225], 1/6[2205], 1/6[2205] )</td>
<td>9 layers</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Fig. 3. Fault vectors projected on (0001) showing the prismatic components, noting that \( F_3, F_5, F_6, F_1 \) although sharing the same prismatic component \((0110)\), were 120° between each other.
moved in the (0002) fault plane by glide, leaving the c-component of the fault vectors unchanged.

The unit lattice translation vectors are possible Burgers vectors for perfect dislocations. We have in h-BaTiO₃ the basal dislocation, \( \mathbf{b}_B = 1/3(1120) \), the prism-plane dislocation, \( \mathbf{b}_{Pr} = (1010) \), and the pyramidal dislocation, \( \mathbf{b}_{Py} = 1/3(2021) \). Similar to hcp A₃ metals, \( 1/3(1120) \) are the close-packed directions in h-BaTiO₃. Basal slip along the close-packed directions, \( 1/3(1120) \) (0001), is the easiest slip system. However, unlike the configurations reported by Eibl et al., only dissociated \( \mathbf{b}_{Pr} \), have been identified in hot-pressed samples, i.e., \( d_1, d_2 \) coplanar with fault \( F_1 \), and \( d_3, d_4 \) coplanar with \( F_2 \) and \( F_3 \), respectively. Perfect basal dislocations with \( \mathbf{b}_B = 1/3(1120) \) that would indicate possible shear in this direction have not yet been identified in hot-pressed h-BaTiO₃.

However, Shockley half-partials, \( d_1 \) and \( d_2 \) originated from the dissociation of basal dislocations \( \mathbf{b}_B = 1/3(1120) \) by the reaction \( \mathbf{b}_B \rightarrow \mathbf{b}_{d1} + \mathbf{b}_{d2} \):

\[
1/3[1210] \rightarrow 1/3[1100] + 1/3[0110]
\]

As basal dislocations had subsequently dissociated into two prism-plane half-partials (by Eq. (2)), they were observed in the present samples. Shear still occurs principally along \( (1120) \) in h-BaTiO₃, only that such basal dislocations induced plastically had dissociated. Therefore, plastic deformation took place predominantly through the easiest slip system \( 1/3(1120) \) (0002) in h-BaTiO₃ when a powder of \( \sim 120 \) nm was hot pressed at 1300 °C.

The dissociation of basal dislocations into partials \( d_1 \) and \( d_2 \) with \( \mathbf{b}_{d1} \) and \( \mathbf{b}_{d2} \) takes place by glide in (0002), the B-layer in (CBC) stacking sequence, as the \( c \) component of faults \( F_1 \) and \( F_1 \) is the same. The fault segment encompassed by partials \( d_1 \)

\[\text{Table II. True Directions, Type of Dislocations and the Relevant Slip Plane}\]

<table>
<thead>
<tr>
<th>Dislocation</th>
<th>True direction ( \mathbf{u} )</th>
<th>Burgers vector ( \mathbf{b} )</th>
<th>Slip plane</th>
<th>Dislocation type</th>
</tr>
</thead>
<tbody>
<tr>
<td>( d_1 )</td>
<td>[0110]</td>
<td>1/3[1100]</td>
<td>(0002)</td>
<td>Mixed (60°)</td>
</tr>
<tr>
<td>( d_2 )</td>
<td>[1210]</td>
<td>1/3[0110]</td>
<td>(0002)</td>
<td>Mixed (30°)</td>
</tr>
<tr>
<td>( d_3 )</td>
<td>1010</td>
<td>1/3[1010]</td>
<td>(0002)</td>
<td>Screw</td>
</tr>
<tr>
<td>( d_4 )</td>
<td>1100</td>
<td>1/3[1010]</td>
<td>(0002)</td>
<td>Mixed (60°)</td>
</tr>
<tr>
<td>( d_5 )</td>
<td>2110</td>
<td>1/3[1010]</td>
<td>(0002)</td>
<td>Mixed (30°)</td>
</tr>
</tbody>
</table>

\[\text{Fig. 4. Fault } F_a \text{ interrupted by partial dislocation } d_a, \text{ (a) bright-field image showing two segments } F_a \text{ and } F'_a; \text{ (b) and (c) are high-resolution images taken from either side of partial } d_a; \text{ (d) and (e) are higher magnifications of the local regions of (b) and (c).}\]
and \( d_2 \) is therefore a complex extrinsic stacking fault (CESF). The complex fault enveloped by partials \( d_1 \) and \( d_2 \) is fault segment \( F_1' \) that contains one extra \( c \)-layer with fault vector \( \mathbf{R}_{F_1'} = 1/6[022] \) (Fig. 2(a)). The fault vectors of \( F_1 \) and \( F_1' \) belong to two crystallographically distinctive groups of \( 1/6[022] \), whose projections on \((0002)\) together with \( \mathbf{b}_{d_1} \) and \( \mathbf{b}_{d_2} \), are shown schematically in Fig. 6.

Compared with the stacking fault energy \( \gamma_{SF} \approx 108 \text{ mJ/m}^2 \) of \( t\)-BaTiO\(_3\),\(^{15}\) the larger separation \( (d) \) between a pair of half-partial, \( d_1 \) and \( d_2 \), of \( \sim 500 \text{ nm} \) (Fig. 1(a)) indicates a significantly lower \( \gamma_{SF} \) in \( h\)-BaTiO\(_3\). However, this value cannot be estimated at present as no shear modulus for \( h\)-BaTiO\(_3\) is available in the literature. Partial separated by \( d=120 \text{ nm} \) found by Eibl et al.,\(^8\) being much narrower, may not lie in the same plane but in planes differing by \( (1/2)c \) indicate a climb dissociation of \( \mathbf{b}_0 \) into half-partial (nevertheless, similarly, by Eq. (2)). Fault segments on both sides of the partials \( D_4 \) and/or \( D_5 \) in Eibl et al. would have distinctive fault vectors with a characteristic stacking sequence containing different extra \( c \)-layers. This necessitates climb of partial dislocations upon dissociation in prism planes at the interface of the two stacking faults. One of a pair of half-partial migrated by a mixed glide in \((0002)\) and climb in \((1010)\) has indeed been determined.\(^{16}\)

The glide of \( d_1 \) with \( \mathbf{b}_{d_1} = 1/3[1100] \) on \((0002)\), the fault plane of \( F_1 \), has effectively rotated \( \mathbf{R}_{F_1} = 1/6[022] \) by \( 60^\circ \) clockwise to \( \mathbf{R}_{F_1} = 1/6[022] \). A complex stacking fault is created extrinsically in fault segment \( F_1' \) with \( \mathbf{R}_{F_1} \). Partial dislocation \( d_2 \) with \( \mathbf{b}_{d_2} = 1/3[0110] \) then restores \( \mathbf{R}_{F_1} \) back to \( \mathbf{R}_{F_1} \) in a similar fashion. Thus, bordering between faults \( F_1 \) and \( F_1' \) is an interface characterized by half-partial \( \mathbf{b}_{d_1} = 1/3[1100] \) (Fig. 6). Analogously, the interface across \( F_1 \) and \( F_1 \) is generated by \( \mathbf{b}_{d_2} = 1/3[0110] \). Consequently, the configuration of \( F_1 \) is restored after the trailing half-partial, \( \mathbf{b}_{d_2} \). Fault segments \( F_1-F_1' \) separated by dislocations \( d_1 \) and \( d_2 \) did not have identical shear vectors (Table I) due to the displacement of \( \mathbf{B} \) to \( \mathbf{A} \) (for \( F_1 \)) versus \( \mathbf{B} \) to \( \mathbf{C} \) (for \( F_1' \)) in \((0002)\) (Fig. 5).\(^5\) Nevertheless, the total number of nine layers in \( F_1 \) and \( F_1' \) remains unchanged across half-partial \( d_1 \) and \( d_2 \), i.e., \((R5+L4)\) to \((L5+R4)\), from a right-inclined fault \( F_1 \) in Fig. 2(a) to a left-inclined one (similar to that of \( F_1' \) in Fig. 4(e)). Dissociation of perfect basal dislocation \( \mathbf{b}_0 \) by a pure glide in \((0002)\) has resulted in an extended separation between half-partial, such that the observed for \( F_1-F_1' \) at \( d=500 \text{ nm} \) (Fig. 1(a)). Indeed, a separation of \( d=230 \text{ nm} \) for \( d_2 \) and its pair partial (which should have been located left of \( d_2 \) (Fig. 4(e)) if not milled off) was estimated from a lower magnification strong-beam image. When dissociation occurs by climb, such as that found by Eibl et al.,\(^8\) or a
mixed mechanism.\textsuperscript{16} half-partialss would have separated the initial fault into two fault segments consisting of different extra c-layers, i.e. differing in the c component of fault vectors \( \mathbf{F}_i \). Planar faults in \( h\)-BaTiO\(_3\) intersected by glide-dissociated half-partialss and divided into two or more segments of dissimilar fault vectors (Table I) but of similar stacking sequence (\( \mathbf{c} \mathbf{c} \mathbf{c} \mathbf{c} \mathbf{c} \mathbf{c} \)) found with \( F_i \) and \( F_i' \) (Figs. 4(d)–(e)). Whether climb dissociation\textsuperscript{8} of \( \mathbf{b}_d \) generated by plastic deformation occurs at all may be investigated by determining the fault vector for each of the fault segments. Climb of partials must occur whenever faults with different extra c-layers are encountered in dislocation dissociation. Fault vectors of such segments suggest that the intersecting dislocations have climbed by (\( \pi / 6 \))[0001] reported by Eibl et al.\textsuperscript{8} and Wu et al.\textsuperscript{16} If there are dislocations intersecting between a five-layer fault, e.g. \( F_1 \) and a six-layer fault, e.g. \( F_2 \), climb of \( \mathbf{b} = 1/3[1100] \) by \( 1/6[0001] \) must occur upon crossing from \( \mathbf{R}_{F_1} = 1/6[0221] \) to \( \mathbf{R}_{F_2} = 1/3[1011] \), although such dislocations were not observed here. Other combinations with different extra c-layers in stacking faults are therefore possible. This has consequently produced discrepant separations between half-partialss, such as \( d = 500 \) nm determined in the present study and \( \sim 120 \) nm reported by Eibl et al.\textsuperscript{8} and \( \sim 47–195 \) nm by Wu et al.\textsuperscript{16}

V. Conclusions

Eligible fault vectors determined for faults in metastably retained \( h\)-BaTiO\(_3\) with dislocations embedded were similar to those without the intersecting dislocations. Only three of the six prismatic components of \( (1010) \) were eligible for type II faults \( F_1-F_0 \) and \( F_0 \) (with \( \mathbf{F}_i \)) fault vectors) analyzed here. During hot pressing, the Shockley half-partialss with \( \mathbf{b}_p = 1/3[0110] \) were dissociated from basal dislocations with \( \mathbf{b}_d = 1/3[1120] \) by glide in (0002) and/or climb in prism planes of \( h\)-BaTiO\(_3\). The interface dislocation with \( \mathbf{b}_p = 1/3[0110] \) has affected a 60° rotation of fault segment \( F_1 \) with \( \mathbf{R}_{F_1} \) to \( F_1' \) with \( \mathbf{R}_{F_1'} \) about [0001], and then from \( F_1' \) back to \( F_1 \) by another rotation of 60° successively. Fault segments \( F_1-F_1' \) and \( F_1'-F_1 \) are bordered by a pair of half-partialss, \( d_1 \) and \( d_2 \), one leading and the other trailing. The fault segment \( F_1' \) enveloped by half-partialss is a CESF.

References
