The differential geometry of internal surfaces

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A GENERALIZED formulation of internal boundaries in crystals has been made using the methods of differential geometry. In particular, a number of important tensor quantities such as distortion, torsion, lattice connection, curvature, Burgers vector, dislocation density and Burgers circuit have been derived with respect to an arbitrary internal boundary and related explicitly to the dislocation content of such boundaries.

Otrzymano uogólniony opis granic wewnętrznych w krasztalach, korzystając z metod geometrii różniczkowej. W szczególności, wyprowadzono szereg ważnych wielkości tensorowych, takich jak odkształcenie, skręcenie, połączenia sieciowe, krzywizna, wektor Burgersa, gęstość dyslokacji i obwód Burgersa, w odniesieniu do dowolnej granicy wewnętrznej; wielkości te związano w sposób jawny z zawartością dyslokacyjną takich granic.

Получено обобщенное описание внутренних границ в кристаллах, используя методы дифференциальной геометрии. В частности выведен ряд важных тензорных величин, таких как деформация, кручение, соединения в решетке, кривизна, вектор Бюргерса, плотность дислокаций и периметр Бюргерса по отношению к произвольной внутренней границе; эти величины связаны явным образом с дислокационным содержанием таких границ.

1. Introduction

IT HAS BEEN previously shown [1] that the continuum theory of dislocations could be applied to grain boundaries in order to obtain a deeper insight into the nature of the dislocations contained therein. The still more general methods of differential geometry were demonstrated [2] to provide an even more powerful means of dealing with the structure of grain boundaries. The goal of the present study is to extend the differential geometric analysis of grain boundaries to more general two-phase interfaces since it has recently been shown [3] that the coincidence site lattice theory of grain boundaries can be applied with remarkable generality to two-phase interfaces.

2. Distortion tensors associated with internal surfaces

Consider the single phase crystal shown in Fig. 1a which is divided into two parts by the dashed vertical line. The crystal can then be cut along the dashed line, after which grains #1 and #2 may be rotated by $+\theta/2$ and $-\theta/2$ to produce the torn state shown in Fig. 1b. Extra material may now be added to the torn state the generate the final state illustrated in Fig. 1c which is in fact a symmetric tilt type grain boundary. We will denote the initial state by upper case Latin letters, i.e. $K. L$, etc., the torn state by lower case Latin letters, i.e. k, l, etc., and the final state by lower case Greek letters, i.e. $\varkappa, \lambda$, etc.
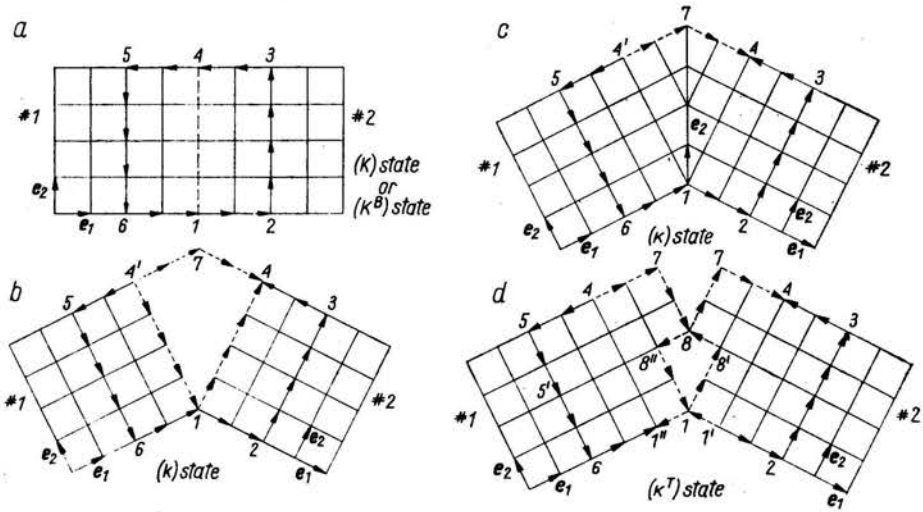
FIG. 1. Steps illustrating the formation of a symmetric tilt type grain boundary. a) Initial reference state; b) Torn state; c) Dislocated state; d) Torn dislocated state of c.

Note that the dislocated state $(\varkappa)$ contains severe elastic distortions at the grain boundary. These strains can, however, be completely removed by the tearing process shown in Fig. 1d. This will be referred to as the $(\varkappa^T)$ state. A set of local base vectors $\mathbf{e}_K$, $\mathbf{e}_k$, $\mathbf{e}_\varkappa$ and $\mathbf{e}_{\varkappa^T}$ can next be associated with each of the four states illustrated in Fig. 1 along with the components dx^K, dx^k, $dx^\varkappa$ and $dx^{\varkappa^T}$. These may be related to one another by equations of the type (4)

$$(2.1) \qquad dx^k = A_K^k dx^K,$$
$$dx^K = A_k^K dx^k$$

etc. where A_K^k and A_k^K are termed distortion tensors. Similarly, the base vectors are related to one another as follows:

$$(2.2) \qquad \mathbf{e}_k = A_k^K \mathbf{e}_K,$$
$$\mathbf{e}_K = A_K^k \mathbf{e}_k$$

etc. The (K) and (k) states of Fig. 1 may be connected to one another by the following distortion:

$$(2.3) \qquad A_K^k = \{A_K^k H(-x^1)\}_1 + \{A_K^k H(+x^1)\}_2;$$
$$ 1 \quad K \qquad\quad 2 \quad K$$

where $H(-x^1)$ and $H(+x^2)$ are Heaviside functions defined by
$ K K$

$$(2.4)_1 \qquad\qquad H(-x^1) = \begin{cases} 0 & \text{if} \quad x^1 > 0, \\ & \quad K \\ 1 & \text{if} \quad x^1 < 0, \\ & \quad K \end{cases}$$
$$ K$$

while

$$(2.4)_2 \qquad H(+x^1) = \begin{cases} 0 & \text{if} \quad x^1 < 0, \\ 1 & \text{if} \quad x^1 > 0. \end{cases}$$

The distortions A^k_K and A^k_K, on the other hand, are given by

$$(2.5)_1 \qquad A^k_K = \begin{pmatrix} A^1_1 & A^2_1 & A^3_1 \\ A^1_2 & A^2_2 & A^3_2 \\ A^1_3 & A^2_3 & A^3_3 \end{pmatrix} = \begin{pmatrix} \cos\theta/2 & -\sin\theta/2 & 0 \\ \sin\theta/2 & \cos\theta/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and

$$(2.5)_2 \qquad A^k_K = \begin{pmatrix} \cos\theta/2 & \sin\theta/2 & 0 \\ -\sin\theta/2 & \cos\theta/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The curly bracket notation has been utilized in Eq. (2.3) to emphasize the fact that the two grains may be treated separately.

We will now note that whereas the (K) state has associated with it one unique coordinate system, while states (k) and $(\varkappa^T)$ have two, the $(\varkappa)$ state in Fig. 1c has at least three. In this latter case, one set of coordinates is associated with each of the grains, and one with the grain boundary itself. There are other local coordinates in the vicinity of the grain boundary associated with the elastic distortions. It is apparent that the coordinates within the grain boundary are one-dimensional. They in turn may be associated with a grain boundary state (K^B). The grain boundary coordinate may be related to those within the grain interiors, i.e. $(\varkappa)$ state as follows:

$$(2.6) \qquad \mathbf{e}_{K^B} = A^{\varkappa}_{K^B} \mathbf{e}_{\varkappa},$$

where in the specific case of Fig. 1c, Eq. (2.6) gives

$$(2.7)_1 \qquad \underset{K^{B2}}{\mathbf{e}} = A^1_2 \underset{\varkappa^1}{\mathbf{e}} + A^2_2 \underset{\varkappa^2}{\mathbf{e}}$$

or

$$(2.7)_2 \qquad \underset{K^{B2}}{\mathbf{e}} = \frac{\sin\theta/2}{\cos\theta/2} \underset{\varkappa^1}{\mathbf{e}} + \frac{\cos\theta/2}{\cos\theta/2} \underset{\varkappa^2}{\mathbf{e}}.$$

The distortion $A^{\varkappa}_{K^B}$ can also be written as

$$(2.8) \qquad A^{\varkappa}_{K^B} = A^K_{K^B} A^{\varkappa}_K,$$

where

$$(2.9) \qquad A^K_{K^B} = \begin{pmatrix} \dfrac{1}{\cos\theta/2} & 0 & 0 \\ 0 & \dfrac{1}{\cos\theta/2} & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

while

$(2.10)_1$
$$A_K^\varkappa \equiv A_K^k$$
$$\quad 1 \qquad 1$$

and

$(2.10)_2$
$$A_K^\varkappa \equiv A_K^k.$$
$$\quad 2 \qquad 2$$

More generally, we can write, similar to Eq. (2.3),

(2.11)
$$A_{K^B}^\varkappa = \{A_{K^B}^\varkappa H(-x^1)\}_1 + \{A_{K^B}^\varkappa H(+x^1)\}_2.$$
$$\qquad\quad 1 \qquad K^B \qquad\quad 2 \qquad K^B$$

The above distortions are not strictly true at all points in the vicinity of the grain boundary because of elastic strains. However, as we shall see later this problem can be avoided.
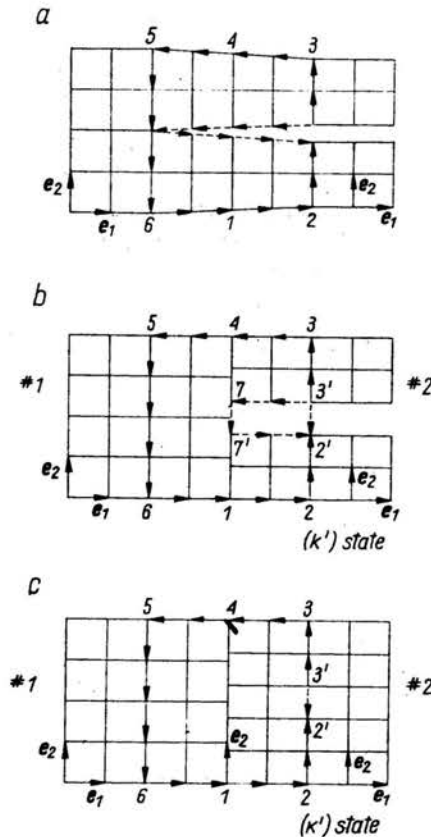

FIG. 2. a) Imperfectly torn; b) Perfectly torn; c) Dislocated states associated with a simple two-phase interface.

Let us now consider the simple two-phase interface shown in Fig. 2. As in the case of Fig. 1, we may denote three states by (K^1), (k^1) and $(\varkappa^1)$ where the superscript 1 has been used to differentiate these states from those in Fig. 1. In addition, state (K^1) is identical

to state (K), and is thus not shown. The (k^1) state can be generated from the (K^1) state by means of the following distortion:

$$(2.12) \qquad A_{k1}^{K1} = \{A_{k1}^{K1} H(-x^1)\}_1 + \{A_{k1}^{K1} H(+x^1)\}_2,$$
$$\qquad\qquad\qquad 1 \quad K^1 \qquad\quad 2 \quad K^1$$

where

$$(2.13)_1 \qquad\qquad\qquad A_{k1}^{K1} = \delta_{k1}^{K1},$$
$$\qquad\qquad\qquad\qquad 1$$

while

$$(2.13)_2 \qquad\qquad\qquad A_{k1}^{K1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & V & 0 \\ 0 & 0 & 1 \end{pmatrix},$$
$$\qquad\qquad\qquad\qquad 2$$

where the distortion given by Eq. (2.12) connects the following base vectors:

$$(2.14) \qquad\qquad\qquad \mathbf{e}_{k1} = A_{k1}^{K1} \mathbf{e}_{K1}.$$

The above equations show that only grain #2 undergoes a volume distortion in accordance with the construction in Fig. 2b. In particular, V was chosen as 4/5 in this figure. The (k^1) state may be referred to as a perfectly torn state, as compared to that in Fig. 2a, which may be termed an imperfectly torn state. In particular, the tearing occurs only along the horizontal coordinates, while in Fig. 2b it occurs along both the horizontal and vertical coordinates. It also follows that the discontinuous function given by Eq. (2.12) no longer holds for Fig. 2a. It is important to note that the tearing operations associated with the transformations $(K) \to (k)$ and $(K^1) \to (k^1)$ correspond to the following relations:

$$(2.15)_1 \qquad\qquad\qquad dx^k \overset{*}{=} \delta_K^k dx^K$$

and

$$(2.15)_2 \qquad\qquad\qquad dx^{k1} \overset{*}{=} \delta_{K1}^{k1} dx^{K1}.$$

In other words, all of the components are dragged along by the distortions (5). This is also equivalent to associating the following point transformations with the coordinate transformations

$$(2.16)_1 \qquad\qquad\qquad P_{.L}^K \overset{*}{=} A_k^K \delta_L^k$$

and

$$(2.16)_2 \qquad\qquad\qquad P_{.L1}^{K1} \overset{*}{=} A_{k1}^{K1} \delta_{L1}^{k1}.$$

If new material is added to grain #2 to fill up the space left by the distortion in Fig. 2b, we obtain the $(\varkappa^1)$ state configuration shown in Fig. 2c. We can describe this state with respect to a grain boundary state (K^{1B}) as follows:

$$(2.17) \qquad A_{K1B}^{\varkappa1} = \{A_{K1B}^{\varkappa1} H(-x^1)\}_1 + \{A_{K1B}^{\varkappa1} H(+x^1)\}_2,$$
$$\qquad\qquad\qquad 1 \quad K^{1B} \qquad\quad 2 \quad K^{1B}$$

where

$$(2.18)_1 \qquad\qquad\qquad A_{K1B}^{\varkappa1} = \delta_{K1B}^{\varkappa1},$$
$$\qquad\qquad\qquad\qquad 1$$

while

(2.18)₂
$$
\underset{2}{A}{}^{\varkappa 1}_{K^1 B} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \dfrac{1}{V} & 0 \\ 0 & 0 & 1 \end{pmatrix}.
$$

It is clear that Eqs. (2.18) satisfy an equation of the type given by Eq. (2.6), i.e.

(2.19)
$$
\underset{K^{1B}}{e} = A^{\varkappa 1}_{K^1 B}\, e_{\varkappa 1}.
$$

We are now in a position to turn our attention to the more general boundary shown in Fig. 3 which consists of both rotations as well as volume changes. For this case we may write

(2.20)
$$
A^{\varkappa 2}_{K 2 B} = \{\underset{1}{A}{}^{\varkappa 2}_{K^{2B}} H(-x^1)\}_1 + \{\underset{2}{A}{}^{\varkappa 2}_{K^{2B}} H(+x^1)\}_2,
$$

where

(2.21)₁
$$
\underset{1}{A}{}^{\varkappa 2}_{K 2 B} = \underset{1}{A}{}^{\varkappa}_{K^B},
$$

while

(2.21)₂
$$
\underset{2}{A}{}^{\varkappa 2}_{K 2 B} = \begin{pmatrix} \dfrac{1}{V}\dfrac{\cos\theta/2}{\cos\theta/2} & \dfrac{1}{V}\dfrac{\sin\theta/2}{\cos\theta/2} & 0 \\ -\dfrac{1}{V}\dfrac{\sin\theta/2}{\cos\theta/2} & \dfrac{1}{V}\dfrac{\cos\theta/2}{\cos\theta/2} & 0 \\ 0 & 0 & 1 \end{pmatrix}.
$$

As was the case of Eq. (2.11), the above relations are not strictly applicable in the vicinty of the grain boundary due to the presence of elastic strains; however, this presents no problem. In order to derive the (k^2) state of Fig. 3a, we may write

(2.22)
$$
A^{K 2}_{k 2} = \{\underset{1}{A}{}^{K 2}_{k 2} H(-x^1)\}_1 + \{\underset{2}{A}{}^{K 2}_{k 2} H(+x^1)\}_2
$$

where

(2.23)₁
$$
\underset{1}{A}{}^{K 2}_{k 2} \equiv A^{K}_{k}
$$

and

(2.23)₂
$$
\underset{2}{A}{}^{K 2}_{k 2} \equiv \begin{pmatrix} \dfrac{1}{V}\cos\theta/2 & -\dfrac{1}{V}\sin\theta/2 & 0 \\ \dfrac{1}{V}\sin\theta/2 & \dfrac{1}{V}\cos\theta/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}.
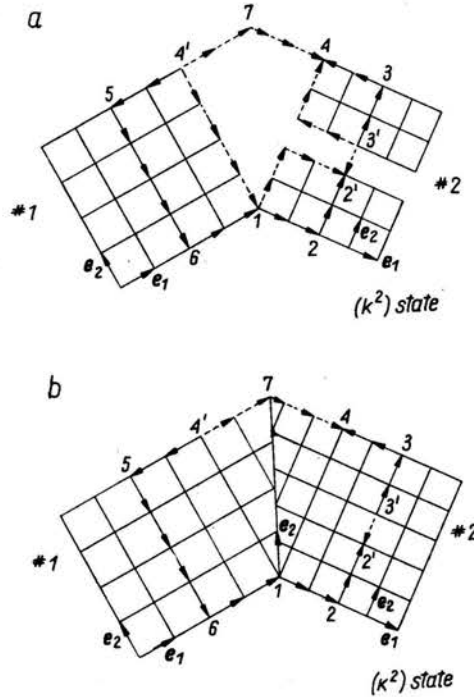$$

FIG. 3. a) Torn; b) Dislocated states associated with a more generalized boundary.

3. Burgers vector and dislocation density associated with internal surfaces

Consider the reference or Burgers circuit 1-2-3-4-5-6-1 associated with the (K^B) state of Fig. 1a. Note that the (K^B) state in this figure differs from the (K) state only by a scale factor given by Eq. (2.9). The corresponding circuit in the dislocated state $(\varkappa)$ is shown in Fig. 1c where the closure failures 4'-7 and 7-4 are denoted by dotted arrows. We may express these closure failures by the following line integral [4, 6]:

$$(3.1) \qquad b^\varkappa = -\oint A^\varkappa_{K\beta} dx^{K^B},$$

where the distortion tensor is given by Eq. (2.11). When Eq. (3.1) is applied to Fig. 2c we⸴ obtain

$$(3.2)_1 \qquad \underset{\varkappa}{b^1} = \underset{2^1\,1-2}{-A^1 \Delta x^1} \underset{2^2\,2-3}{-A^1 \Delta x^2} \underset{2^1\,3-4}{-A^1 \Delta x^1} \underset{1^1\,4-5}{-A^1 \Delta x^1} \underset{1^2\,5-6}{-A^1 \Delta x^2} \underset{1^1\,6-1}{-A^1 \Delta x^1},$$

where Δx^1 etc. are the distances from point 1 to 2 etc. in Fig. 1a. With the aid of Eq.
$1-2$
(2.11), Eq. (3.2) reduces to

$$(3.2)_2 \qquad \underset{\varkappa}{b^1} = \{\underset{2^2\,2-3}{-A^1 \Delta x^2}\}_2 + \{\underset{1^2\,5-6}{-A^1 \Delta x^2}\}_1$$

or

$$(3.2)_3 \qquad \underset{\varkappa}{b^1} = \{4\tan\theta/2\}_2 + \{4\tan\theta/2\}_1.$$

In terms of Fig. 1c, Eq. (3.2) becomes

$$(3.2)_4 \qquad\qquad b^1_{\varkappa} = \{\varDelta x^1\}_2 + \{\varDelta x^1\}_1.$$
$$\phantom{(3.2)_4 \qquad\qquad b^1_{\varkappa} =} 7-4 \qquad 4'-7$$

Let us now consider the $(\varkappa^T)$ state of Fig. 1d which is the torn counterpart of the $(\varkappa)$ state. Here again we can write

$$(3.3) \qquad\qquad b^{\varkappa^T} = -\oint A^{\varkappa^T}_{K^{B}} dx^{K^B}$$

and since $A^{\varkappa^T}_{K^{B}} \equiv A^{\varkappa}_{K^{B}}$, Eq. (3.3) gives a closure failure identical to that of Eq. (3.2), as is evident from Fig. 1d. We also obtain additional free surfaces resulting from the tearing operation which are given by

$$(3.4) \qquad\qquad b^{\varkappa^T} = \oint A^{\varkappa^T}_{K^{B}} dx^{K^B}$$

which, except for the absence of the negative sign, is identical to Eq. (3.3). We thus have in terms of Fig. 1d

$$(3.5) \qquad\qquad b^1_{\varkappa^T} = \{\ \varDelta x^1 + \varDelta x^1\ \}_2 + \{\ \varDelta x^1 + \varDelta x^1\ \}_1$$
$$\phantom{(3.5) \qquad\qquad b^1_{\varkappa^T} =} 8'-8 \quad 1'-1 \qquad 8-8'' \quad 1-1''$$

as well as

$$(3.6)_1 \qquad\qquad b^2_{\varkappa^T} = \{A^2\,\varDelta x^2\}_2 + \{A^2\,\varDelta x^2\}_1$$
$$\phantom{(3.6)_1 \qquad\qquad b^2_{\varkappa^T} =} 2^2\,2-3 \qquad 1^2\,5-6$$

or

$$(3.6)_2 \qquad\qquad b^2_{\varkappa^T} = \{\ \varDelta x^2 + \varDelta x^2\ \}_2 + \{\varDelta x^2 + \varDelta x^2\ \}_1.$$
$$\phantom{(3.6)_2 \qquad\qquad b^2_{\varkappa^T} =} 8-7 \quad 1-8' \qquad 7-8 \quad 8''-1$$

For the torn (k) state of Fig. 1b we may write

$$(3.7) \qquad\qquad b^k = \oint A^k_k dx^K.$$

In view of Eq. (2.15)$_1$, Eq. (2.3) can be rewritten as

$$(3.8) \qquad\qquad A^k_k = \{\delta^k_k H(-x^1)\}_1 + \{\delta^k_k H(+x^1)\}_2$$
$$ 1 \qquad K \qquad 2 \qquad K$$

which, when substituted into Eq. (3.7) yields

$$(3.9)_1 \qquad\qquad b^2_k = \{\varDelta x^2\}_2 + \{\varDelta x^2\}_1.$$
$$ 2-3 \qquad 5-6$$

or

$$(3.9)_2 \qquad\qquad b^2_k = \{4\}_2 + \{-4\}_1,$$

while in terms of Fig. 1b

$$(3.9)_3 \qquad\qquad b^2 = \{\varDelta x^2\}_2 + \{\varDelta x^2\}_1.$$
$$ 1-4 \qquad 4'-1$$

This result is thus identical to that given by Eqs. (3.6). At this point we can attribute the closure failure given by Eqs. (3.1) and (3.3) to extra planes within the crystal, i.e. dislocations, while those given by Eqs. (3.4) and (3.7) are due to the creation of free surfaces. This will become more clear as we procede further with this analysis. Another intriguing

aspect of this problem manifests itself in that b^2_k given by Eq. $(3.9)_3$ is equivalent to $b^1_\varkappa$ given by Eq. $(3.2)_4$. This is indicated in Fig. 1b by the fact that the vector sums 4'-1-4 and 4'-7-4 are equivalent. This implies that we can write

$(3.10)_1$
$$b^k = \oint A^k_{KB} dx^{KB},$$

where

$(3.10)_2$
$$A^k_{KB} = -A^\varkappa_{KB}.$$

Continuing on to the $(\varkappa^1)$ state of Fig. 2c, we may write

$(3.11)_1$
$$b^{\varkappa^1} = -\oint A^{\varkappa^1}_{K_1B} dx^{K_1B},$$

which with the help of Eq. (2.17) gives

$(3.11)_2$
$$b^2_{\varkappa^1} = \{-A^2 \Delta x^2\}_{2^2 2-3} + \{-A^2 \Delta x^2\}_{1^2 5-6}$$

or

$(3.11)_3$
$$b^2_{\varkappa^1} = \left\{-\frac{1}{V}(4)\right\}_2 + \{4\}_1$$

or in terms of Fig. 2c

$(3.11)_4$
$$b^2_{\varkappa^1} = \{-1\}_2 \equiv \left\{\Delta x^2\right\}_{\substack{2 \\ 3'-2'}}.$$

A little care must now be exercised in obtaining b^{k^1}. In particular, if we write, similar to Eq. (3.7)

(3.12)
$$b^{k^1} - \oint A^{k^1}_{K_1} dx^{K_1}$$

and then employ Eq. $(2.15)_2$, we obtain

(3.13)
$$b^2_{k^1} = \{4\}_2 + \{-4\}_1.$$

However, the surface closure failure occurs at the boundary between the two phases so that we must write instead of Eq. (3.12)

(3.14)
$$b^{K_1B} = \varphi A^{K_1B}_{k_1} dx^{k_1},$$

where

(3.15)
$$A^{K_1B}_{k_1} \equiv A^{k_1B}_{\varkappa^1},$$

which can be obtained from Eq. (2.17). Equation (3.14) can therefore be expanded as

(3.16)
$$b^2_{K^{1B}} = \{V(4)\}_2 + \{-4\}_1 = \left\{-\frac{4}{5}\right\}_{1B} = \left\{\Delta x^2\right\}_{\substack{1B \\ 7-7'}}.$$

There are other components $b^1_{k^1}$ associated with Fig. 2b given by the dotted lines 3'-7 and 7'-2'; however, they may be considered as cancelling with one another. Also, since the vector sum 3'-7-7'-2' is equivalent to 3'-2' in Fig. 2b, we may write, similar to Eqs. (3.10)$_2$,

$(3.17)_1$
$$b^{k1} = \oint A^{k1}_{K1B} dx^{K1B},$$

where

$(3.17)_2$
$$A^{k1}_{K1B} = -A^{k1}_{K1B}.$$

We next turn our attention to the $(\varkappa^2)$ state of Fig. 3b where we can write

(3.18)
$$b^{\varkappa 2} = -\oint A^{\varkappa 2}_{K2B} dx^{K2B}.$$

From Eq. (2.20) we can use Eq. (3.18) to find

$(3.19)_1$
$$b^1_{\varkappa^2} = \{4\tan\theta/2\}_1 + \left\{\left(\frac{5}{4}\right)4\tan\theta/2\right\}_2,$$

which in terms of Fig. 3b gives

$(3.19)_2$
$$b^1_{\varkappa^2} = \{ \underset{4'-7}{\Delta x^1} \}_1 + \{ \underset{7-4}{\Delta x^1} \}_2,$$

while the second component is found to be

(3.20)
$$b^2_{\varkappa^2} = \{4\}_1 + \left\{-4\left(\frac{5}{4}\right)\right\}_2 = -\{1\}_2 \equiv \{ \underset{3'-2'}{\Delta x^2} \}_2.$$

It is a relatively straightforward matter to obtain the surface closure failures associated with the (k^2) state of Fig. 3a utilizing the methods described earlier with respect to states (k) and (k^1).

With the aid of Stoke's theorem, the line integral given by Eq. (3.1) may be converted into a surface integral [5, 7] as follows:

$(3.21)_1$
$$b^{\varkappa} = -\oint A^{\varkappa}_{KB} dx^{KB} = -\int_s \partial_{[MB} A^{\varkappa}_{KB]} dF^{MBKB}$$

or in expanded form as

$(3.21)_2$
$$b^{\varkappa} = -\oint A^{\varkappa}_{KB} dx^{KB} = -\frac{1}{2}\int_s [\partial_{MB} A^{\varkappa}_{KB} - \partial_{KB} A^{\varkappa}_{MB}] dF^{MBKB}.$$

Thus the surface integral provides an alternate method of obtaining $b^{\varkappa}$. In particular, when applied to the grain boundary shown in Fig. 1c, Eq. (3.21) gives

$(3.22)_1$
$$b^1_{\varkappa} = -\frac{1}{2}\int_s [\partial_1 A^1_2 dF^{12} - \partial_1 A^1_2 dF^{21}]$$

which, with the aid of Eq. (2.11), becomes

$(3.22)_2$
$$b^1 = \left\{ -\frac{1}{2} \int_s [\partial_1 \underset{K^B}{H}(-x^1)\tan\theta/2\, dF^{12} - \partial_1 \underset{K^B}{H}(-x^1)\tan\theta/2\, dF^{21}] \right\}_1$$
$$+ \left\{ -\frac{1}{2} \int_s [-\partial_1 \underset{K^B}{H}(+x^1)\tan\theta/2\, dF^{12} + \partial_1 \underset{K^B}{H}(+x^1)\tan\theta/2\, dF^{21}] \right\}_2.$$

Since $dF^{12} = -dF^{21}$, and from the following relations (2.8)

$(3.23)_1$
$$\partial_1 \underset{K^B}{H}(-x^1) = -\underset{K^B}{\delta}(x^1)$$

and

$(3.23)_2$
$$\partial_1 \underset{K^B}{H}(+x^1) = +\underset{K^B}{\delta}(x^1),$$

where $\underset{K^B}{\delta}(x^1)$ is the Dirac delta function defined such that $\delta(x^1) = 0$ for $x^1 \neq 0$, we can write Eq. $(3.22)_2$ as

(3.24)
$$b^1 = \left\{ \int_s \underset{K^B}{\delta}(x^1)\tan\theta/2\, dx^1 dx^2 \right\}_1 + \left\{ \int_s \underset{K^B}{\delta}(x^1)\tan\theta/2\, dx^1 dx^2 \right\}_2.$$

Note that in the $(K^B) \to (\varkappa)$ transformation, the component dx^2 is dragged, so that in accordance with Eqs. (2.15) we can write $\underset{K^B}{dx^2} = \underset{\varkappa}{dx^2}$. Also, since the delta function satisfies the following relation:

(3.25)
$$\int_{-\infty}^{+\infty} \delta(x^1)dx^1 = 1,$$

and since $\int dx^2 = 4$, Eq. (3.24) reduces to

(3.26)
$$b^1 = \{4\tan\theta/2\}_1 + \{4\tan\theta/2\}_2$$

which is identical to Eq. $(3.2)_3$ obtained by the line integral method.

Rather than discuss the Burgers circuit in terms of integrals with respect to a reference (K^B) state, as has been done thus far, it now becomes instructive to consider the corresponding Burgers circuit with respect to the final state $(\varkappa)$. This can be done by writing Eq. $(3.21)_2$ as

$(3.27)_1$
$$b^\varkappa = -\int_s \frac{1}{2} A_\lambda^{LB} A_\mu^{MB} [\partial_{LB} A_{MB}^\varkappa - \partial_{MB} A_{LB}^\varkappa] dF^{\lambda\mu}$$

or alternately as

$(3.27)_2$
$$b^\varkappa = -\int_s S_{\lambda\mu}^{\cdots\varkappa} dF^{\lambda\mu},$$

where the quantity $S_{\lambda\mu}^{\cdots\varkappa}$ is termed the torsion tensor and is given by [5, 7]:

(3.28)
$$S_{\lambda\mu}^{\cdots\varkappa} = \frac{1}{2} A_\lambda^{LB} A_\mu^{MB} [\partial_{LB} A_{MB}^K - \partial_{MB} A_{LB}^\varkappa].$$

In terms of Fig. 1c the above equation becomes

(3.29)$_1$
$$S_{12}^{\cdot\cdot1} = \frac{1}{2}[A_1^1 A_2^2 - A_1^2 A_2^1]\partial_1 A_2^1.$$
$\varkappa$

We must now be careful in defining the inverses $A_\lambda^{L^B}$. Specifically, they represent the dragging of the components dx^1 and dx^2 to dx^1 and dx^2 respectively, so that $A_\lambda^{L^B} = \delta_\lambda^{L^B}$.
$\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad \varkappa \quad\quad \varkappa \quad K^B \quad\quad K^B$
This makes the bracketed term in Eq. (3.29) equal to unity, so that in view of Eq. (2.11) it finally becomes

(3.29)$_2$
$$S_{12}^{\cdot\cdot1} = \left\{-\frac{1}{2}\tan\theta/2\,\delta(x^1)\right\}_1 + \left\{-\frac{1}{2}\tan\theta/2\,\delta(x^1)\right\}_2.$$
$\varkappa \quad\quad\quad\quad\quad\quad\quad\quad \varkappa \quad\quad\quad\quad\quad\quad\quad\quad \varkappa$

When the above expression is substituted into Eq. (3.27)$_2$, we again obtain the same result as that given by Eq. (3.26). Also inportant to note is the fact that the presence of a non-vanishing $S_{\varkappa\cdot}^{\cdot\cdot\mu}$ is synonymous with the presence of dislocations, as was first pointed out by KONDO [9].

Turning our attention again to the $(\varkappa^1)$ state of Fig. 2c, we can utilize Eq. (3.21)$_2$ to obtain

(3.30)$_1$
$$b^2 = -\frac{1}{2}\int_s [\partial_1 A_2^2 dF^{12} - \partial_1 A_2^2 dF^{21}]$$
$\varkappa^1$

which, with the help of Eq. (2.17), yields

(3.30)$_2$
$$b^2 = \left\{\int_s \delta(x^1)dx^1 dx_2\right\}_1 + \left\{-\frac{1}{V}\int_s \delta(x^1)dx^1 dx^2\right\}_2$$
$\varkappa^1 \quad\quad\quad K^{1B} \quad\quad\quad\quad\quad\quad\quad\quad\quad K^{1B}$

or

(3.30)$_3$
$$b^2 = \{4\}_1 + \left\{-\frac{1}{V}(4)\right\}_2.$$
$\varkappa^1$

This is the same result given by Eq. (3.11)$_3$. The torsion tensor associated with the $(\varkappa^1)$ state can be found to be

(3.31)$_1$
$$S_{12}^{\cdot\cdot2} = \frac{1}{2}[A_1^1 A_2^2 - A_1^2 A_2^1]\partial_1 A_2^2$$
$\varkappa^1$

which, together with Eq. (2.17), gives

(3.31)$_2$
$$S_{12}^{\cdot\cdot2} = \left\{-\frac{1}{2}\delta(x^1)\right\}_1 + \left\{\frac{1}{2}\delta(x^1)\right\}_2.$$
$\varkappa^1 \quad\quad\quad\quad\quad\quad \varkappa^1 \quad\quad\quad\quad\quad\quad \varkappa^1$

When the above relation is substituted into the following equation:

(3.32)
$$b^{\varkappa^1} = -\int S_{\lambda^1\mu^1}^{\cdot\cdot\varkappa^1}dF^{\lambda^1\mu^1},$$

we obtain the same result given by Eq. (3.30)$_3$. A surface integral of the type given by Eq. (3.32) can also be written for the (x^2) state of Fig. 3b. In this case there are two components of the torsion tensor given by

$$(3.33)_1 \qquad \underset{x^2}{S_{12}^{\cdot\cdot 1}} = \left\{ -\frac{1}{2} \tan \theta/2 \delta(x^1) \right\}_{\underset{x^2}{1}} + \left\{ -\frac{1}{2} \tan \theta/2 \delta(x^1) \right\}_{\underset{x^2}{2}}$$

and

$$(3.33)_2 \qquad \underset{x^2}{S_{12}^{\cdot\cdot 2}} = \left\{ -\frac{1}{2} \delta(x^1) \right\}_{\underset{x^2}{1}} + \left\{ \frac{1}{2} \delta(x^1) \right\}_{\underset{x^2}{2}}.$$

The surface integrals discussed thus far have all been associated with closure failures due to dislocations. The same reasoning can be applied to the torn states to obtain closure failures due to the creation of free surfaces. In particular, analogous to Eqs. (3.21), we may write

$$(3.34) \qquad b^k = \oint A_K^k dx^K = \frac{1}{2} \int_s [\partial_M A_K^k - \partial_K A_M^k] dF^{MK}.$$

For the (k) state of Fig. 1b, the above relation gives

$$(3.35)_1 \qquad \underset{k}{b^2} = \int_s \partial_1 A_2^2 dF^{12}$$

which in turn, using Eq. (2.15)$_1$, yields

$$(3.35)_2 \qquad \underset{k}{b^2} = \left\{ -\int_s \underset{k}{\delta(x^1)} dx^1 dx^2 \right\}_1 + \left\{ \int_s \underset{k}{\delta(x^1)} dx^1 dx^2 \right\}_2$$

and is identical to the line integral result of Eqs. (3.9)$_2$. Equation (3.34) can also be written in terms of (k) state coordinates as

$$(3.36) \qquad b^k = \int_s \Omega_{im}^{\cdot\cdot k} dF^{lm}$$

where $\Omega_{im}^{\cdot\cdot k}$ is termed the anholonomic object and defined as [5, 10]

$$(3.37) \qquad \Omega_{im}^{\cdot\cdot k} = \frac{1}{2} A_l^L A_m^M [\partial_L A_M^k - \partial_M A_L^k].$$

Equations (3.36) and (3.37) are thus of the same forms as Eqs. (3.27)$_2$ and (3.28) respectively, but have physically different meanings. In the case of the (k) state, Eq. (3.37) yields

$$(3.38) \qquad \underset{k}{\Omega_{12}^{\cdot\cdot 2}} = \left\{ -\frac{1}{2} \underset{k}{\delta(x^1)} \right\}_1 + \left\{ \frac{1}{2} \underset{k}{\delta(x^1)} \right\}_2$$

which, when substituted into Eq. (3.36), again gives the same result as that of Eq. (3.9)$_2$. In the case of the (k^1) state of Fig. 2b, the anholonomic object becomes

$$(3.39) \qquad \underset{K^{1B}}{\Omega_{12}^{\cdot\cdot 2}} = \left\{ -\frac{1}{2} \underset{K^{1B}}{\delta(x^1)} \right\}_1 + \left\{ \frac{1}{2} V \underset{K^{1B}}{\delta(x^1)} \right\}_2,$$

where use has been made of Eq. (3.15). Strictly speaking, there is also a component $\Omega_{12}^{\cdot\cdot1}$ associated with the horizontal torn surfaces in Fig. 2b and can in principle be found, but will not be considered further. In a similar manner, an anholonomic object associated with the torn surfaces of the (k^2) state can also be found.

Having determined the torsion tensor, we are now in a position to find the dislocation density tensor utilizing the following relation [11]:

$$(3.40) \qquad \alpha^{\nu\varkappa} = -\varepsilon^{\nu\mu\lambda} S_{\mu\lambda}^{\cdot\cdot\varkappa},$$

where $\varepsilon^{\nu\mu\lambda}$ is the permutation tensor defined as

$$(3.41) \qquad \varepsilon^{\nu\mu\lambda} = e^{\nu\mu\lambda}/\sqrt{g}$$

and where $e^{\nu\mu\lambda}$ is the permutation symbol, while g is the determinant of the metric tensor. The index ν refers to the normal to the 1-2 plane, while $\varkappa$ corresponds to the Burgers vector component. Thus, for the $(\varkappa)$ state Eq. (3.40) gives

$$(3.42)_1 \qquad \underset{\varkappa}{\alpha^{31}} = -2S_{12}^{\cdot\cdot1}$$

which, in view of Eq. $(3.29)_2$ gives, after integrating as per Eq. (3.25)

$$(3.42)_2 \qquad \underset{\varkappa}{\alpha^{31}} = \{\tan\theta/2\}_1 + \{\tan\theta/2\}_2$$

which, in terms of Fig. 1c is simply

$$(3.42)_3 \qquad \underset{\varkappa}{\alpha^{31}} = \left\{ \frac{\overset{\Delta x^1}{4'-7}}{\underset{1-4'}{\Delta x^2}} \right\}_1 + \left\{ \frac{\overset{\Delta x^1}{7-4}}{\underset{1-4}{\Delta x^2}} \right\}_2 .$$

In the case of the $(\varkappa^1)$ state.

$$(3.43)_L \qquad \underset{\varkappa^1}{\alpha^{32}} = 2S_{21}^{\cdot\cdot2}/\sqrt{g}$$

or in view of Eq. $(3.42)_2$

$$(3.43)_2 \qquad \underset{\varkappa^1}{\alpha^{32}} = \{1\}_1 + \left\{ -\frac{1}{V} \right\}_2 = \frac{V-1}{V} .$$

In terms of Fig. 2c

$$(3.43)_3 \qquad \underset{\varkappa^1}{\alpha^{32}} = -1/4$$

which simply represents the number of extra half planes for every four planes of the deformed crystal. Finally, for the $(\varkappa^2)$ state we can use Eqs. (3.33) to obtain

$$(3.44)_1 \qquad \underset{\varkappa^2}{\alpha^{31}} = \{\tan\theta/2\}_1 + \left\{ \frac{1}{V} \tan\theta/2 \right\}_2$$

while

$$(3.44)_2 \qquad \underset{\varkappa^2}{\alpha^{32}} = \{1\}_1 + \left\{ \frac{1}{V} \right\}_2 .$$

The numerical value of the second term in Eq. $(3.44)_1$ is $2.5/4$ which designates the number of extra half planes in grain #2 along the x^1 direction divided by the number of planes in the original reference crystal along the x^2 direction.

A density can also be associated with the newly created surfaces formed by the tearing process. Similar to Eq. (3.40), we can write [10]

$$(3.45) \qquad \alpha^{nk} = \varepsilon^{nml} \Omega_{mi}^{\cdot\cdot k}.$$

Utilizing Eq. (3.38), the above becomes

$$(3.46)_1 \qquad \underset{k}{\alpha^{32}} = \{-1\}_1 + \{1\}_2.$$

In terms of Fig. 1b, the above equation is simply

$$(3.46)_2 \qquad \underset{k}{\alpha^{32}} = \left\{ \frac{\dfrac{\Delta x^2}{4'-1}}{\dfrac{\Delta x^2}{1-4}} \right\}_1 + \left\{ \frac{\dfrac{\Delta x^2}{1-4}}{\dfrac{\Delta x^2}{1-4}} \right\}_2 .$$

In a similar manner we can write for the $(\varkappa^1)$ state, using Eq. (3.39),

$$(3.47) \qquad \underset{k^1}{\alpha^{32}} = \{-1\}_1 + \{V/V\}_2.$$

Thus we have the interesting result that in a torn crystal which contains no dislocations, α^{nk} is always unity and is a simple consequence of the fact that no extra half planes are involved in such torn states. Such however, is not the case for the $(\varkappa^T)$ state shown in Fig. 1d. Here we can write

$$(3.48) \qquad b^{\varkappa^T} = -\int_s [S_{\lambda\tau\mu\tau}^{\cdot\cdot\cdot\cdot\varkappa^T} - \Omega_{\lambda\tau\mu\tau}^{\cdot\cdot\cdot\cdot\varkappa^T}] dF^{\lambda\tau\mu\tau},$$

where

$$(3.49) \qquad S_{\lambda\tau\mu\tau}^{\cdot\cdot\cdot\cdot\varkappa^T} = \Omega_{\lambda\tau\mu\tau}^{\cdot\cdot\cdot\cdot\varkappa^T}.$$

This means that the closure failure due to the creation of free surfaces just balances those due to dislocations. This applies only to the components $\underset{\varkappa^T}{S_{12}^{\cdot\cdot 1}}$ and $\underset{\varkappa^T}{\Omega_{12}^{\cdot\cdot 1}}$ as is obvious from inspection of Fig. 1d. It also follows from Eqs. (3.40) and (3.45) that

$$(3.50) \qquad \underset{R}{\alpha^{\nu^T \varkappa^T}} = -\underset{\Omega}{\alpha^{\nu^T \varkappa^T}}.$$

Thus we see that under certain conditions we are able to use the anholonomic object in place of the torsion. This is the basis upon which ŻÓRAWSKI [10] is able to develop a theory of defects which depends exclusively on the quantity $\Omega_{\lambda\mu}^{\cdot\cdot\varkappa}$ rather than $S_{\lambda\mu}^{\cdot\cdot\varkappa}$. In general, however, it must be remembered that they are fundamentally different quantities

4. Lattice connection and curvature associated with internal surfaces

It is of interest now to look into some further aspects of the tensor quantities treated in the previous section. In particular, when a vector c^λ is displaced parallel to a distance dx^μ, it undergoes a change $dc^\varkappa$ given by [5]

$$(4.1) \qquad dc^\varkappa = -\Gamma_{\mu\lambda}^\varkappa c^\lambda dx^\mu,$$

where $\Gamma^{\varkappa}_{\mu\lambda}$ is termed the lattice connection. In general, $\Gamma^{\varkappa}_{\mu\lambda}$ can be written as

(4.2)
$$\Gamma^{\varkappa}_{\mu\lambda} = \{{\varkappa \atop \mu\lambda}\} + (S^{\cdot\cdot\varkappa}_{\mu\lambda} - \Omega^{\cdot\cdot}_{\mu\nu}) - (S^{\cdot\varkappa}_{\lambda\cdot\mu} - \Omega^{\cdot\varkappa}_{\lambda\cdot\mu}) + (S^{\varkappa}_{\cdot\mu\lambda} - \Omega^{\varkappa}_{\cdot\mu\lambda}),$$

where $\{{\varkappa \atop \mu\lambda}\}$ are Christoffel symbols of the second kind given by

(4.3)
$$\{{\varkappa \atop \mu\lambda}\} = \frac{1}{2} g^{\varkappa\sigma}(\partial_\mu g_{\lambda\sigma} + \partial_\lambda g_\mu - \partial_\sigma g_{\mu\lambda}).$$

Now $g_{\varkappa\lambda}$ can, at the most, be only a function of x^1 so that only terms of the type $g^{\varkappa\sigma}\partial_1 g_{\varkappa\sigma}$ need be considered in Eq. (4.3), The non-vanishing components of $\{\varkappa \atop \mu\lambda\}$ thus become $\{1 \atop 11\}$ and $\{2 \atop 12\}$. In the latter case we may write

(4.4)
$$\{{2 \atop 12}\} = \{-\delta(x^1)\}_1 + \{+\delta(x^1)\}_2 = 0.$$

Thus the above component vanishes both within the grains as well as in the grain boundary itself. The component $\{1 \atop 11\}$, however, need not vanish within the grains because of the elastic distortion near the grain boundary as discussed previously. In any event the quantity $\{\varkappa \atop \mu\lambda\}$ is symmetric with respect to the two lower indices as is apparent from Eq. (4.3). Also, since the torsion tensor is antisymmetric with respect to the lower indices [5], it follows that

(4.5)
$$\Gamma^{\varkappa}_{[\mu\lambda]} = S^{\cdot\cdot\varkappa}_{\mu\lambda}.$$

This can easily be proved by utilizing the relations

(4.6)$_1$
$$S^{\cdot\varkappa}_{\lambda\cdot\mu} = g_{\mu\sigma} g^{\varkappa\rho} S^{\cdot\cdot\sigma}_{\lambda\rho}$$

and

(4.6)$_2$
$$S^{\varkappa}_{\cdot\mu\lambda} = g_{\lambda\sigma} g^{\varkappa\rho} S^{\cdot\cdot\sigma}_{\rho\mu}$$

in Eq. (4.2), and taking $\Omega^{\cdot\cdot\varkappa}_{\mu\lambda} = 0$, which is certainly the case for the $(\varkappa)$ state of Fig. 1c. Now, along certain regions near the grain boundary, in particular along the Burgers circuit of Fig. 1c, Eq. (4.3) holds since $\{\varkappa \atop \mu\lambda\} = 0$. We can therefore write Eq. (4.1) as

(4.7)
$$dc^{\varkappa} = -S^{\cdot\cdot\varkappa}_{\mu\lambda} c^{\lambda} dx^{\mu}.$$

The above equation has a simple physical meaning in terms of Fig. 1c. Specifically, we may rewrite it as

(4.8)
$$dc^1 = -S^{\cdot\cdot1}_{12} c^3 dx^1.$$

Thus, utilizing Eq. (3.29)$_2$, when a test vector c^2 of magnitude $\Delta x^2_{1-4'}$ is moved along x^1 and encounters the grain boundary, it changes by $\Delta x^1_{4'-7}$ in grain #1 and Δx^1_{7-4} in grain #2, i.e. by just the closure failure associated with the dislocations. We thus have yet another

and still more fundamental means of interpreting the torsion tensor. In the case of the (x^1) state, Eq. (4.7) gives

(4.9)
$$\underset{x^1}{dc^2} = -S_{\cdot 12}^{\cdot\cdot 2}c^2 dx^1.$$

Physically this means that if a vector $c^2 = \Delta x^2$ is transported along x^1 from grain #1
$$6-5$$
to grain #2, it undergoes a change

(4.10)
$$\underset{x^1}{dc^2} = \{4\}_1 + \{-5\}_2 = -1,$$

where Eq. (3.31)$_1$ has been utilized. Thus dc^2 is just the closure failure Δx^2 in Fig. 2c.
$$\underset{x^1}{} \qquad\qquad 3'-3$$
An expression similar to Eq. (4.7) can also be written for dc^{x^2} and the results are straightforward.

If now the space under consideration contains only $\Omega_{mi}^{\cdot\cdot k}$, then Eqs. (4.1) and (4.2) give

(4.11)
$$dc^k = \Omega_{mi}^{\cdot\cdot k}c^l dx^m.$$

In terms of the torn state of Fig. 1b the above equation together with Eq. (3.38) 60 yields

(4.12)$_1$
$$\underset{k}{dc^2} = \underset{k}{\Omega_{\cdot 12}^{\cdot\cdot 2}}c^2 dx^1$$

so that if we take $c^2 = \Delta x^2$ in Fig. 1b, Eq. (4.12)$_1$ gives
$$6-5$$

(4.12)$_2$
$$\underset{k}{dc^2} = \{-4\}_1 + \{+4\}_2,$$

which means that this test vector is reduced from 4 to 0 in grain #1 and then increased from 0 to 4 in grain #2. In the case of the (k^1) state we have

(4.13)$_1$
$$\underset{k^1}{dc^2} = \underset{k^1}{\Omega_{\cdot 12}^{\cdot\cdot 2}}c^2 dx^1$$

which, with the help of Eq. (3.39) yields

(4.13)$_2$
$$\underset{k^1}{dc^2} = \{-4\}_1 + \{\sqrt{4}\}_2 = \{-4/5\}_1.$$

This is the same result given by Eq. (3.16) and simply represents the change in length of the test vector $c^2 = 4$ as it moves across the grain boundary along x^1.

Finally, we have for the (x^T) state of Fig. 1d, from Eqs. (4.1) and (4.2)

(4.14)
$$dc^{x^T} = -(S_{\mu\cdot\tau_\lambda}^{\cdot\tau}i^{x^T} - \Omega_{\mu\cdot\tau_\lambda}^{\cdot\tau}i^{x^T})c^{\lambda^T}dx^{\mu^T}.$$

Since the component $(S_{\cdot 12}^{\cdot\cdot 1} - \Omega_{\cdot 12}^{\cdot\cdot 1}) = 0$, a test vector $c^2 = \Delta x^2$ in Fig. 1d will remain
$$5'-5$$
unchanged, i.e. $c^2 = \Delta x^2$, right up to the surface of the crystal. It will then shrink to zero
$$8-7$$
upon further transport along x^1 due to the presence of $\Omega_{\cdot 12}^{\cdot\cdot 2}$.

2*

In concluding this section it is important to note that Eq. $(3.27)_2$ for the closure failure associated with a given Burgers circuit is not the most general expression. In particular, we may write [5, 7, 9, 11]

$$(4.15) \qquad b^\varkappa = - \int\limits_s \left[S^{\cdot\cdot\varkappa}_{\nu\mu} + \frac{1}{2} R^{\cdot\cdot\cdot\varkappa}_{\nu\mu\lambda} c^\lambda \right] dF^{\nu\mu},$$

where $R^{\cdot\cdot\cdot\varkappa}_{\nu\mu\lambda}$ is the Riemann-Christoffel curvature tensor given by [5]

$$(4.16) \qquad R^{\cdot\cdot\cdot\varkappa}_{\nu\mu\lambda} = \partial_\nu \Gamma^\varkappa_{\nu\lambda} - \partial_\mu \Gamma^\varkappa_{\nu\lambda} + \Gamma^\varkappa_{\nu\rho} \Gamma^\rho_{\mu\lambda} - \Gamma^\varkappa_{\mu\rho} \Gamma^\rho_{\nu\lambda}.$$

It has already been shown that this tensor vanishes for the grain boundaries [2] and two-phase interfaces [12], so the earlier expression for the closure failure given by Eq. $(3.27)_2$, is sufficient. This is also in agreement with the constructions in Fig. 1, 2 and 3.

5. Summary and conclusions

A differential geometric formulation has been carried out with respect to generalized two-phase interfaces. In particular, such characteristic tensor quantities as distortion, torsion, anholonomic object, lattice connection, curvature, Burgers vector, dislocation density and Burgers circuit have all been defined with respect to such internal surfaces. It is shown that such procedures give a concise and complete description of any type of internal boundary.

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