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The Differential Geometry of Two-Phase Interfaces

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Coherent as well as incoherent interfaces associated with simple two-phase boundaries have been analyzed in terms of the concepts of differential geometry. Such tensor quantities as distortion, torsion and curvature have been developed and are all shown to give significant insight in describing the Burgers circuits and dislocation content of such boundaries.

Introduction

In a recent study (Marcinkowski, Sadananda & Cullen, 1975) it was shown how two-phase interfaces could be treated in terms of simple geometric arguments. Both fully coherent and incoherent interfaces were treated. It would now appear appropriate to apply the somewhat abstract but powerful techniques of differential geometry to the same problem. The goal was twofold. In the first place, it was desired to gain a stronger physical insight into the various tensor quantities provided by the differential geometric approach. Secondly, it was hoped that the techniques of differential geometry would add further to the understanding of two-phase interfaces.

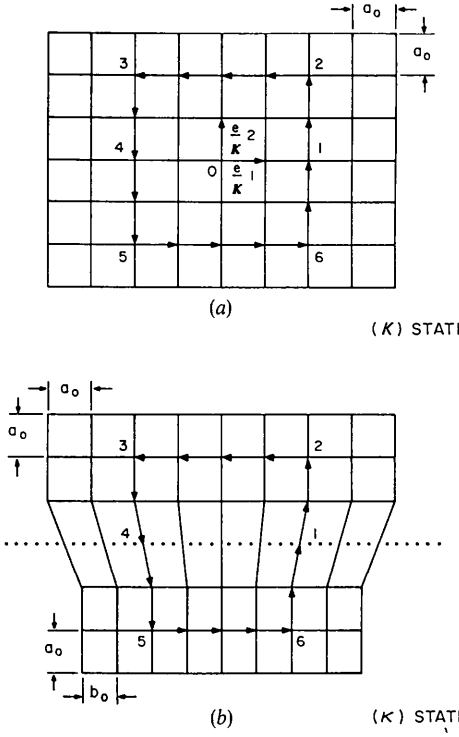

Fig. 1. Continuous two-phase interface. (*a*) Initial state. (*b*) Final state.

Distortion and metric tensors associated with a two-phase interface

Let us first consider the perfect crystal, shown in Fig. 1(*a*), of lattice constant a_0. This can also be thought of as the initial state and will be designated by uppercase Latin indices, *i.e.* K, L, *etc.* This state can now be deformed to produce the (κ) state shown in Fig. 1(*b*). This will be called the final state, designated by lowercase Greek letters, *i.e.* κ, λ, *etc.* It is clear from inspection of the figure that it represents a coherent boundary (shown dotted) separating two phases of lattice constant a_0 and b_0. We can now associate a distortion tensor $\mathbf{A}_K^\kappa$ with the deformation that produces the (κ) state from the (K) state which is defined as follows:

$$dx^\kappa = \mathbf{A}_K^\kappa dx^K \tag{1a}$$

and

$$dx^K = \mathbf{A}_\kappa^K dx^\kappa \tag{1b}$$

where dx^κ and dx^K are differential elements of length in the deformed and undeformed states respectively. The distortions can also be expressed as

$$\mathbf{e}_\kappa = \mathbf{A}_\kappa^K \mathbf{e}_K \tag{2a}$$

and

$$\mathbf{e}_K = \mathbf{A}_K^\kappa \mathbf{e}_\kappa \tag{2b}$$

where $\mathbf{e}_\kappa$ and $\mathbf{e}_K$ are local base vectors in the deformed and undeformed states respectively. For the specific case of Fig. 1 we may write for $\mathbf{A}_\kappa^K$

$$\mathbf{A}_\kappa^K = \begin{pmatrix} A_1^1 & A_1^2 & A_1^3 \\ A_2^1 & A_2^2 & A_2^3 \\ A_3^1 & A_3^2 & A_3^3 \end{pmatrix} = \begin{pmatrix} A_1^1 & 0 & 0 \\ A_2^1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{3}$$

where A_2^1 is some suitable function which accounts for the horizontal displacement of the vertical planes in Fig. 1(*a*) while

$$A_1^1 = f_2 + V f_1 \tag{4}$$

where f_1 and f_2 are defined as

$$f_1 = \frac{1}{\exp\left(a_K x^2\right) + 1} \tag{5a}$$

and

$$f_2 = \frac{1}{\exp(-a\overset{K}{x}{}^2)+1}. \tag{5b}$$

The function f_1 is shown in Fig. 2 where the coordinate $\overset{K}{x}{}^2$ is measured with respect to the local coordinate system located at the position of the potential two-phase boundary in Fig. 1(*a*). Thus, for $\overset{K}{x}{}^2 \to -\infty$, $f_2=0$ and $A_1^1=V$, while for $\overset{K}{x}{}^2 \to +\infty$, $f_1=0$ and $A_1^1=f_2=1$. Right at the potential boundary where $\overset{K}{x}{}^2=0$, $A_1^1=(1+V)/2$. Fig. 1(*b*) was drawn with $V=4/5$, *i.e.* $b_0=4/5\ a_0$. Thus the function given by (4) seems to be an appropriate one where the parameter a can be chosen so as to adjust the width of the distorted zone across the potential boundary. For finite values of $a>0$ the boundary is continuous except for $a=\infty$, in which case it becomes discontinuous. The distortion given by (3) can be visualized as arising from a phase change which results in a decrease in volume. Thus, (4) can be written out in full as

$$A_1^1 = \frac{1+V\exp(-a\overset{K}{x}{}^2)}{1+\exp(-a\overset{K}{x}{}^2)} \tag{6}$$

while the inverse quantity $\mathbf{A}_K^\kappa$ can be simply found from the following relation:

$$\mathbf{A}_K^\kappa \mathbf{A}_\lambda^K = \delta_\lambda^\kappa \tag{7}$$

where δ_λ^κ is the Kronecker delta defined as

$$\delta_\lambda^\kappa = \begin{cases} 1 \text{ for } \kappa=\lambda \\ 0 \text{ for } \kappa\neq\lambda. \end{cases} \tag{8}$$

For simplicity, we have chosen the volume change to occur along the $\overset{K}{x}{}^1$ direction only so that A_2^2 and A_3^3 in (3) are set equal to 1. We can thus now use (7) to write for $\mathbf{A}_K^\kappa$

$$\mathbf{A}_K^\kappa = \begin{pmatrix} A_1^1 & 0 & 0 \\ A_2^1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{9a}$$

where

$$A_1^1 = \frac{1+\exp(-a\overset{K}{x}{}^2)}{1+V\exp(-a\overset{K}{x}{}^2)} \tag{9b}$$

while A_2^1 is some suitable function which again accounts for the displacement of the vertical planes in Fig. 1(*b*).

It is now possible to tear (Kondo, 1962) the elastically strained (κ) state of Fig. 1(*b*) so as to obtain the (k) state configuration shown in Fig. 3(*a*). This may be referred to as an imperfectly torn crystal since only a portion of the elastic strain is relaxed. Full removal of the elastic strain is accomplished by the perfectly torn state (k^1) illustrated in Fig. 3(*b*). An equivalent perfect tearing similar to that of the (k^1) state is shown by the (k^2) state of Fig. 4(*a*). Note that in all of the torn states, new free surfaces are created, and may be considered as a fundamental feature of these particular states.

The (k) state of Fig. 3(*a*) may be derived from the (K) state by means of the distortion tensor

$$\mathbf{A}_k^K = \begin{pmatrix} A_1^1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{10}$$

which, except for the vanishing of the A_2^1 term, is

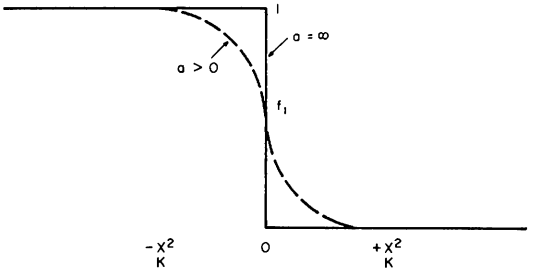

Fig. 2. Distribution function associated with the distortion of a two-phase interface.

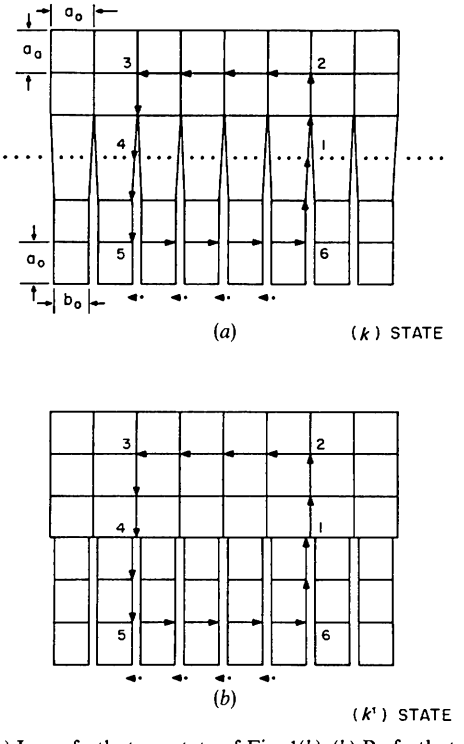

Fig. 3. (*a*) Imperfectly torn state of Fig. 1(*b*). (*b*) Perfectly torn state of Fig. 1(*b*).

identical to that given by (3). The perfectly torn (k^1) state of Fig. 3(b) can also be represented by (10) where A_1^1 is again given by (4), but with a set equal to ∞. However, under these conditions this function possesses no limiting value for $\underset{K}{x}^2=0$, and can thus not be defined. In order to overcome this difficulty, it is better to write the component A_1^1 of the distortion tensor $\mathbf{A}_{k1}^K$ as

$$A_1^1=\{H(+\underset{K}{x}^2)\}_2+\{VH(-\underset{K}{x}^2)\}_1 \tag{11}$$

where $H(-\underset{K}{x}^2)$ and $H(+\underset{K}{x}^2)$ are Heaviside functions defined by

$$H(-\underset{K}{x}^2)=\begin{cases}0 \text{ if } \underset{K}{x}^2>0\\ 1 \text{ if } \underset{K}{x}^2<0\end{cases} \tag{12a}$$

and

$$H(+\underset{K}{x}^2)=\begin{cases}0 \text{ if } \underset{K}{x}^2<0\\ 1 \text{ if } \underset{K}{x}^2>0\,.\end{cases} \tag{12b}$$

The curly bracket notation is used in (11) to emphasize the fact that each phase may be treated separately. (11) is simply another way of writing (4) for $a\to\infty$. The inverse $\bar{A}_1^1$ of (11) is readily found from (11) and (7) to be

$$\bar{A}_1^1=\{H(+\underset{K}{x}^2)\}_2+\left\{\frac{1}{V}H(-\underset{K}{x}^2)\right\}_1. \tag{13}$$

The distortions given by (11) and (13) can also be used to generate the perfectly torn (k^2) state of Fig. 4(a) and the dislocated (k^3) state of Fig. 4(b) from the initial (K) state. In particular

$$\mathbf{A}_K^{k2}=\mathbf{A}_K^{k3}\equiv\mathbf{A}_K^{k1} \tag{14a}$$

and

$$\mathbf{A}_{k2}^K=\mathbf{A}_{k3}^K\equiv\mathbf{A}_{k1}^K. \tag{14b}$$

It is important to note that the dislocated state (k^3) can be generated from the torn (k^2) state by the introduction of extra matter. Nevertheless, the (k^2) and (k^3) states can be generated from the same distortion tensor as given by (14). This particular point has important ramifications, as will be discussed later.

A metric tensor $\mathbf{g}_{\kappa\lambda}$ can also be associated with the (κ) state of Fig. 1(b) since

$$\mathbf{g}_{\kappa\lambda}=\mathbf{e}_\kappa\,.\,\mathbf{e}_\lambda \tag{15a}$$

which with the aid of (2a) becomes

$$\mathbf{g}_{\kappa\lambda}=\mathbf{A}_\kappa^K\mathbf{A}_\lambda^L\mathbf{e}_K\,.\,\mathbf{e}_L=\mathbf{A}_\kappa^K\mathbf{A}_\lambda^L\delta_{KL}=\mathbf{A}_\kappa^K\mathbf{A}_\lambda^K \tag{15b}$$

where the Kronecker delta in the above equation arises because the initial-state coordinates are Cartesian. From (15b) and (3), we can now write

$$\mathbf{g}_{\kappa\lambda}=\begin{pmatrix}g_{11}&g_{12}&0\\ g_{21}&g_{22}&0\\ 0&0&1\end{pmatrix}. \tag{16}$$

The metric tensor for the (K) state is obviously given by

$$\mathbf{g}_{KL}=\delta_{KL} \tag{17}$$

since the coordinates are Cartesian, while for the $\mathbf{g}_{kl}$ state, we can write from (10) and an expression of the form given by (15b):

$$\mathbf{g}_{kl}=\begin{pmatrix}g_{11}&0&0\\ 0&1&0\\ 0&0&1\end{pmatrix} \tag{18a}$$

where

$$g_{11}=\left[\frac{1+V\exp(-a\underset{K}{x}^2)}{1+\exp(-a\underset{K}{x}^2)}\right]^2. \tag{18b}$$

In the case of the (k^1), (k^2) and (k^3) states, the metric tensor is again of the same form as that given by (18a) but with

$$g_{11}=\{H^2(+\underset{K}{x}^2)\}_2+\{V^2H^2(-\underset{K}{x}^2)\}_1\,. \tag{19}$$

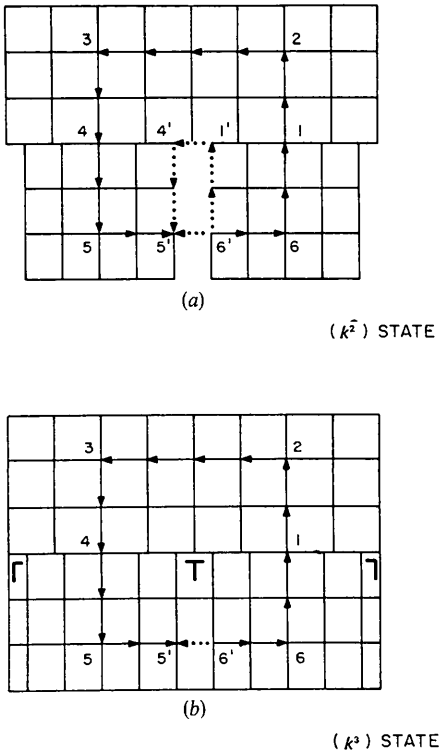

Fig. 4. (a) Alternative perfectly torn state to that shown in Fig. 3(b). (b) Dislocated (discontinuous) two-phase interface of Fig. 1(b).

Burgers circuit associated with a two-phase interface

It is now possible to define Burgers circuits with respect to each of the states shown in Figs. 1, 3 and 4.

In particular, the equivalent paths 1–2–3–4–5–6–1 are shown for each of these states. The closure failure or Burgers vector $\mathbf{b}^{\kappa}$ associated with a given path may be written in terms of the following line integral (Kröner, 1959)

$$\mathbf{b}^{\kappa} = -\oint \mathbf{A}^{\kappa}_{K} \mathrm{d}x^{K} . \tag{20a}$$

It is important to note that the above integration path must be taken with respect to the initial (K) state of the crystal. (20a) can be expanded with the aid of (9) to give

$$\underset{\kappa}{b}{}^{1} = -\int_{2}^{3} A^{1}_{1}\mathrm{d}\underset{K}{x}{}^{1} - \int_{3}^{5} A^{1}_{2}\mathrm{d}\underset{K}{x}{}^{2} - \int_{5}^{6} A^{1}_{1}\mathrm{d}\underset{K}{x}{}^{1} - \int_{6}^{2} A^{1}_{2}\mathrm{d}\underset{K}{x}{}^{2} = 0 . \tag{20b}$$

The same holds true for all other components of $\mathbf{b}^{\kappa}$. This is not a surprising result since the volume distortions in Fig. 1(b) are just compensated by the lateral displacements of the vertical planes, so that no closure failure obtains. In the case of the (k) state of Fig. 3(a), we can write

$$\mathbf{b}^{k} = -\oint \mathbf{A}^{k}_{K} \mathrm{d}x^{K} \tag{21a}$$

which with the aid of (10) gives

$$\underset{k}{b}{}^{1} = -\int_{2}^{3} A^{1}_{1}\mathrm{d}\underset{K}{x}{}^{1} - \int_{5}^{6} A^{1}_{1}\mathrm{d}\underset{K}{x}{}^{1} . \tag{21b}$$

This particular closure failure corresponds to the sum of all four gaps associated with the Burgers circuit of Fig. 3(a) generated by the tearing process, and which are denoted by dotted arrows. In the case of the remaining three states (k^1), (k^2) and (k^3) we may write

$$\mathbf{b}^{k^1} = -\oint \mathbf{A}^{k^1}_{K} \mathrm{d}x^{K} \tag{22a}$$

$$\mathbf{b}^{k^2} = -\oint \mathbf{A}^{k^2}_{K} \mathrm{d}x^{K} \tag{22b}$$

$$\mathbf{b}^{k^3} = -\oint \mathbf{A}^{k^3}_{K} \mathrm{d}x^{K} . \tag{22c}$$

Because of (14a), the above relations are all equivalent, and more specifically are of the form given by (21b). In view of (13), (22) gives

$$\underset{k^1}{b}{}^{1} = \underset{k^2}{b}{}^{1} = \underset{k^3}{b}{}^{1} = \{4\}_2 - \left\{\frac{4}{V}\right\}_1 = \frac{4}{V}(V-1) = -1 . \tag{23}$$

This numerical result corresponds either to the one extra half plane (6′–5′) shown dotted in Fig. 4(b) or to its omission, also shown by the dotted line 6′–5′ in Fig. 4(a). It is also significant to point out that the closure failure 5′–6′ in Fig. 4(a) is also equivalent to the sum of the surface closure failures 6′–1′–4′–5′ in this same figure. The vectors 6′–1′ and 4′–5′ may be viewed as cancelling with one another to give 4′–1′ or equivalently 6′–5′. In spite of the fact that the (k), (k^1) and (k^2) states possess closure failures, it is not strictly correct to speak of such states as dislocated states. Instead, such states are said to have associated with them an anholonomic object (Zorawski, 1967) which is a measure of the amount of free surface associated with them. The (k^3) state, on the other hand, contains extra matter and thus represents a true dislocated state. The meanings of these terms will become more clear in the following sections.

The line integrals of (21a) and (22) can now be converted into surface integrals by means of Stoke's theorem (Schouten, 1951) so as to obtain an alternative representation for the closure failure. In particular, in the case of (22b), we may write

$$\mathbf{b}^{k^2} = -\int_{s} \partial_{[K}\mathbf{A}^{k^2}_{L]}\mathrm{d}F^{KL} = -\tfrac{1}{2}\int_{s} [\partial_K \mathbf{A}^{k^2}_{L} - \partial_L \mathbf{A}^{k^2}_{K}]\mathrm{d}F^{KL} \tag{24a}$$

where ∂_K denotes the operator $\partial/\partial x^K$. (24a) can be written more specifically as

$$\underset{k^2}{b}{}^{1} = \int_{s} \partial_2 A^{1}_{1}\mathrm{d}\underset{K}{F}{}^{12} \tag{24b}$$

since $\mathrm{d}\underset{K}{F}{}^{12} = -\mathrm{d}\underset{K}{F}{}^{21} = \mathrm{d}\underset{K}{x}{}^{1}\mathrm{d}\underset{K}{x}{}^{2}$. We can further write (24b) as

$$\underset{k}{b}{}^{1}_{2} = \left\{\int_{-\infty}^{+\infty} \delta(\underset{K}{x}{}^{2})\mathrm{d}x^{2}\int \mathrm{d}x^{1}\right\}_2 + \left\{-\frac{1}{V}\int_{-\infty}^{+\infty} \delta(\underset{K}{x}{}^{2})\mathrm{d}x^{2}\int \mathrm{d}x^{1}\right\}_1 \tag{24c}$$

where (13) has been utilized along with the following relations (de Wit, 1973)

$$\partial_2 H(-\underset{K}{x}{}^{2}) = -\delta(\underset{K}{x}{}^{2}) \tag{25a}$$

and

$$\partial_2 H(+\underset{K}{x}{}^{2}) = \delta(\underset{K}{x}{}^{2}) \tag{25b}$$

where $\delta(\underset{K}{x}{}^{2})$ is the Dirac delta function defined such that it is equal to zero whenever $\underset{K}{x}{}^{2} \neq 0$. These functions also have the following property

$$\int_{-\infty}^{+\infty} \delta(\underset{K}{x}{}^{2})\mathrm{d}x^{2} = 1 \tag{26}$$

so that the evaluation of (24c) reduces to that of (23) obtained by the line integral method.

The closure failure $\mathbf{b}^{k^2}$ can be expressed in still a third way by writing (24a) as

$$\mathbf{b}^{k^2} = -\int_s \mathbf{A}^K_{l^2} \mathbf{A}^L_{m^2} \partial_{[K} \mathbf{A}^{k^2}_{L]} \mathrm{d}F^{l^2 m^2} \tag{27a}$$

or still more compactly as

$$\mathbf{b}^{k^2} = -\int_s \mathbf{\Omega}_{\dot{l}^2 \dot{m}^2}{}^{k^2} \mathrm{d}F^{l^2 m^2} \tag{27b}$$

where the quantity $\mathbf{\Omega}_{\dot{l}^2 \dot{m}^2}{}^{k^2}$ is termed the anholonomic object and is given by

$$\mathbf{\Omega}_{\dot{l}^2 \dot{m}^2}{}^{k^2} = \mathbf{A}^K_{l^2} \mathbf{A}^L_{m^2} \partial_{[K} \mathbf{A}^{k^2}_{L]} = \tfrac{1}{2} \mathbf{A}^K_{l^2} \mathbf{A}^L_{m^2} [\partial_K \mathbf{A}^{k^2}_L - \partial_L \mathbf{A}^{k^2}_K]. \tag{28}$$

It is apparent that whereas the integration in (24*a*) is carried out with respect to initial-state coordinates, that in (27*b*) is done with respect to final-state coordinates. Utilizing (11) and (13), we can now write for the specific component

$$\underset{k^2}{\Omega}_{\dot{1}\dot{2}}{}^1 = -\tfrac{1}{2} A^1_1 A^2_2 \partial_2 A^1_1 = \{-\tfrac{1}{2} \delta(\underset{k^2}{x}{}^2)\}_2 + \{\tfrac{1}{2} \delta(\underset{k^2}{x}{}^2)\}_1 \tag{29}$$

which when substituted into (27*b*) again gives the same result as that obtained from (23). Similar to (27), we can now write (22*c*) as

$$\mathbf{b}^{k^3} = \int_s \mathbf{S}_{\dot{l}^3 \dot{m}^3}{}^{k^3} \mathrm{d}F^{l^3 m^3} \tag{30}$$

where $\mathbf{S}_{\dot{l}^3 \dot{m}^3}{}^{k^3}$ is termed the torsion tensor and written as (Kröner, 1958)

$$\begin{aligned} \mathbf{S}_{\dot{l}^3 \dot{m}^3}{}^{k^3} &= -\mathbf{A}^K_{l^3} \mathbf{A}^L_{m^3} \partial_{[K} \mathbf{A}^{k^3}_{L]} \\ &= -\tfrac{1}{2} \mathbf{A}^K_{l^3} \mathbf{A}^L_{m^3} [\partial_K \mathbf{A}^{k^3}_L - \partial_L \mathbf{A}^{k^3}_K]. \end{aligned} \tag{31}$$

It was first shown by Kondo (1955) that a non-vanishing torsion tensor signifies the presence of dislocations. In particular, we can write

$$\underset{k^3}{S}_{\dot{1}\dot{2}}{}^1 = -\underset{k^2}{\Omega}_{\dot{1}\dot{2}}{}^1. \tag{32}$$

This result was again first demonstrated by Kondo (1955) and underscores the close relation between the torsion tensor and the anholonomic object. Utilization of (32), (31), (30) and (29) again gives $\underset{k^3}{b}{}^1 = \underset{k^2}{b}{}^1$, in agreement with (23) and Fig. 4.

A further importance of the torsion tensor lies in the fact that it is a measure of the dislocation density (Kröner, 1958). This can be seen by writing (22*c*) in differential form as

$$\mathrm{d}\mathbf{b}^{k^3} = \mathbf{S}_{\dot{l}^3 \dot{m}^3}{}^{k^3} \mathrm{d}F^{l^3 m^3} = \mathbf{S}_{\dot{l}^3 \dot{m}^3}{}^{k^3} \boldsymbol{\varepsilon}^{n^3 l^3 m^3} \mathrm{d}F_{n^3} = \boldsymbol{\alpha}^{n^3 k^3} \mathrm{d}F_{n^3} \tag{33}$$

where the quantity $\boldsymbol{\alpha}^{n^3 k^3}$ is defined as the dislocation density given by

$$\boldsymbol{\alpha}^{n^3 k^3} = \boldsymbol{\varepsilon}^{n^3 l^3 m^3} \mathbf{S}_{\dot{l}^3 \dot{m}^3}{}^{k^3} \tag{34}$$

while $\boldsymbol{\varepsilon}^{n^3 l^3 m^3}$ is the permutation tensor defined by

$$\boldsymbol{\varepsilon}^{n^3 l^3 m^3} = \mathbf{e}^{n^3 l^3 m^3} / \sqrt{g} \tag{35}$$

and where $\mathbf{e}^{n^3 l^3 m^3}$ are the permutation symbols, while g is the determinant of the metric tensor $\mathbf{g}_{k^3 l^3}$ (Fung, 1965). For the specific component α^{31} we obtain

$$\underset{k^3}{\alpha}{}^{31} = \{\delta(\underset{k^3}{x}{}^2)\}_2 + \left\{-\delta(\underset{k^3}{x}{}^2) \frac{1}{V}\right\}_1 \tag{36a}$$

which upon integration in the manner of (26) gives

$$\underset{k^3}{\alpha}{}^{31} = \frac{V-1}{V} = -\tfrac{1}{4}. \tag{36b}$$

The fraction in the above equation simply refers to the number of extra half planes per four planes of the original reference lattice, *i.e.* one. The first superscript in $\boldsymbol{\alpha}^{n^3 k^3}$ refers to the dislocation line direction, while the second pertains to the direction of its Burgers vector. Similarly to (33), we may also utilize (27*b*) to obtain

$$\boldsymbol{\alpha}^{n^2 k^2} = -\boldsymbol{\varepsilon}^{n^2 l^2 m^2} \mathbf{\Omega}_{\dot{l}^2 \dot{m}^2}{}^{k^2}. \tag{37}$$

Strictly speaking, the above relation gives the density of newly created free surfaces created by the perfect tearing process. It is apparent that

$$\underset{k^2}{\alpha}{}^{31} = \underset{k^3}{\alpha}{}^{31}. \tag{38}$$

The above relation once again underscores the close connection between the anholonomic object and the torsion tensor. It is in fact this close relation that has enabled Zorawski (1967) to formulate his theory of dislocations on the basis of the anholonomic object rather than torsion. Finally, it is a relatively straightforward matter to show that both $\mathbf{S}_{\dot{\lambda}\dot{\mu}}{}^{\kappa}$ and $\mathbf{\Omega}_{\dot{\lambda}\dot{\mu}}{}^{\kappa}$ associated with Fig. 1(*b*) are zero. This is to be expected since the Burgers circuit corresponding to this state has associated with it neither dislocations nor newly created free surfaces.

Some further fundamental tensor quantities associated with a two-phase interface

Let us consider next the parallel displacement of a vector $\mathbf{c}^\lambda$ through a distance $\mathrm{d}x^\mu$. According to Kröner (1959) and Schouten (1954), this gives rise to a change $\mathrm{d}\mathbf{c}^\kappa$ which can be expressed as

$$\mathrm{d}\mathbf{c}^\kappa = -\mathbf{\Gamma}^\kappa_{\mu\lambda} \mathbf{c}^\lambda \mathrm{d}x^\mu \tag{39}$$

where $\mathbf{\Gamma}^\kappa_{\mu\lambda}$ is termed the connection. In those cases where only elastic distortions are involved, such as the (κ) state, we may write (Schouten, 1954)

$$\mathbf{\Gamma}^\kappa_{\mu\lambda} = \left\{{}^{\kappa}_{\mu\lambda}\right\} \tag{40}$$

where $\left\{{}^{\kappa}_{\mu\lambda}\right\}$ is the Christoffel symbol of the second kind given by

$$\left\{{}^{\kappa}_{\mu\lambda}\right\} \overset{\text{def}}{=} \tfrac{1}{2} \mathbf{g}^{\kappa\sigma} (\partial_\mu \mathbf{g}_{\lambda\sigma} + \partial_\lambda \mathbf{g}_{\mu\sigma} - \partial_\sigma \mathbf{g}_{\mu\lambda}). \tag{41}$$

A relation of the type given by (40) describes a Riemannian space and may be denoted by V_n (Schouten, 1954). Furthermore, the connection $\mathbf{\Gamma}^\kappa_{\mu\lambda}$ is said to be

metric with respect to $\mathbf{g}_{\mu\lambda}$. Under these conditions the covariant derivative of $g_{\mu\lambda}$ vanishes, *i.e.*

$$\nabla_\mu \mathbf{g}_{\lambda\kappa} \overset{\text{def}}{=} \partial_\mu \mathbf{g}_{\lambda\kappa} - \mathbf{\Gamma}^\sigma_{\mu\lambda}\mathbf{g}_{\rho\kappa} - \mathbf{\Gamma}^\sigma_{\mu\kappa}\mathbf{g}_{\sigma\kappa} = 0. \tag{42}$$

If however the above condition is not satisfied, we may write

$$\mathbf{Q}_{\mu\lambda\kappa} = -\nabla_\mu \mathbf{g}_{\lambda\kappa}. \tag{43}$$

Under these conditions, $\mathbf{\Gamma}^\kappa_{\mu\lambda}$ is not metric with respect to $\mathbf{g}_{\mu\lambda}$ and we must rewrite (40) as (Schouten, 1954; Bilby, Gardner, Grinberg & Zorawski, 1966):

$$\mathbf{\Gamma}^\kappa_{\mu\lambda} = \left\{ {\kappa \atop \mu\lambda} \right\} + \tfrac{1}{2}(\mathbf{Q}_{\mu\lambda}{}^{\cdot\kappa} + \mathbf{Q}_{\lambda\cdot\mu}^{\ \ \kappa} - \mathbf{Q}^\kappa{}_{\cdot\mu\lambda}). \tag{44}$$

(44) would hold, for example, if the metric $\mathbf{g}_{\mu\lambda}$ were defined with respect to a different coordinate system, *i.e.* $\underset{K}{\mathbf{g}}_{\mu\lambda}$. Physically, this state of affairs would be equivalent to utilizing a measuring device or ruler of variable length. The manifold defined by (44) is termed an A_n. Clearly, for a V_n, as expressed by (40), lengths are conserved upon parallel transport.

For the dislocated (k^3) state which possesses the metric $\mathbf{g}_{ml}$, the connection may be written as (Schouten, 1954)

$$\mathbf{\Gamma}^{k^3}_{m^3 l^3} = \left\{ {k^3 \atop m^3 l^3} \right\} + \mathbf{S}_{m^3 l^3}{}^{\cdot k^3} - \mathbf{S}_{l^3}{}^{k^3}{}_{\cdot m^3} + \mathbf{S}^{k^3}{}_{\cdot m^3 l^3} \tag{45}$$

where the asymmetric part of $\mathbf{\Gamma}^{k^2}_{m^3 l^3}$ is simply

$$\mathbf{\Gamma}^{k^3}_{[m^3 l^3]} = \mathbf{S}_{m^3 l^3}{}^{\cdot k^3} \tag{46}$$

and where the torsion is that given by (32). In view of the following relations:

$$\mathbf{S}_{l^3}{}^{k^3}{}_{\cdot m^3} = \mathbf{g}_{m^3 o^3}\mathbf{g}^{k^3 n^3}\mathbf{S}_{l^3 n^3}{}^{\cdot o^3} \tag{47a}$$

and

$$\mathbf{S}^{k^3}{}_{\cdot m^3 l^3} = \mathbf{g}_{l^3 o^3}\mathbf{g}^{k^3 n^3}\mathbf{S}_{n^3 m^3}{}^{\cdot o^3} \tag{47b}$$

we can utilize (45) to write the following two components of $\mathbf{\Gamma}^{k^3}_{m^3 l^3}$

$$\underset{k^3}{\mathit{\Gamma}}{}^1_{12} = \left\{ {1 \atop 12} \right\}_{k^3} + 2\underset{k^3}{S}{}_{12}{}^1 = 0 \tag{48a}$$

while

$$\underset{k^3}{\mathit{\Gamma}}{}^1_{12} = \left\{ {1 \atop 21} \right\}_{k^3}. \tag{48b}$$

The first of these relations follows from

$$\left\{ {1 \atop 12} \right\}_{k^3} = \left\{ {1 \atop 21} \right\}_{k^3} = \tfrac{1}{2}\mathbf{g}^{11}(\partial_2 \underset{k^3}{g}_{11}) = -\underset{k^3}{S}{}_{12}{}^1 \tag{49}$$

where the metric tensors have already been given by (19). In terms of (39), the component $\underset{k^3}{\mathit{\Gamma}}{}^1_{21}$, given by (48*b*), measures the change in length $\mathrm{d}\mathbf{c}^1$ of a test vector $\mathbf{c}^1$ as it undergoes a parallel displacement over the distance $\mathrm{d}x^2$. This change is of course equal to zero because of (29) and (32), so that once again, the (k^3) state exhibits distant parallelism. The reason for this of course is that $\mathbf{\Gamma}^{k^3}_{m^3 l^3}$ is metric with respect to $\mathbf{g}_{m^3 l^3}$. If such were not the case, it would be necessary to rewrite (45) as (Schouten, 1954)

$$\mathbf{\Gamma}^{k^3}_{m^3 l^3} = \left\{ {k^3 \atop m^3 l^3} \right\} + \mathbf{S}_{m^3 l^3}{}^{\cdot k^3} - \mathbf{S}_{l^3}{}^{k^3}{}_{\cdot m^3} + \mathbf{S}^{k^3}{}_{\cdot m^3 l^3} + \tfrac{1}{2}(\mathbf{Q}_{m^3 l^3}{}^{\cdot k^3} + \mathbf{Q}_{l^3}{}^{k^3}{}_{\cdot m^3} - \mathbf{Q}^{k^3}{}_{\cdot m^3 l^3}). \tag{50}$$

Finally, for the perfectly torn (k^2) state, we can write, similar to (45),

$$\mathbf{\Gamma}^{k^2}_{m^2 l^2} = \left\{ {k^2 \atop m^2 l^2} \right\} - \mathbf{\Omega}_{m^2 l^2}{}^{\cdot k^2} + \mathbf{\Omega}_{l^2}{}^{k^2}{}_{\cdot m^2} - \mathbf{\Omega}^{k^2}{}_{\cdot m^2 l^2}. \tag{51}$$

In view of (32) it is apparent that the analysis of $\mathbf{\Gamma}^{k^2}_{m^2 l^2}$ is identical to that of $\mathbf{\Gamma}^{k^2}_{m^3 l^3}$. For example

$$\mathbf{\Gamma}^{k^2}_{[m^2 l^2]} = -\mathbf{\Omega}_{m^2 l^2}{}^{\cdot k^2} \tag{52}$$

while

$$\left\{ {1 \atop 12} \right\}_{k^2} = \left\{ {1 \atop 21} \right\}_{k^2} = -2\underset{k^2}{\Omega}{}_{12}{}^1. \tag{53}$$

If $\mathbf{\Gamma}^{k^2}_{m^2 l^2}$ is not metric with respect to $\mathbf{g}_{m^2 l^2}$, we must write the connection in a manner similar to that of (50).

Another item of interest is the Riemann–Christoffel curvature tensor defined as (Schouten, 1954)

$$\mathbf{R}_{\mu\lambda\nu}{}^{\cdot\kappa} = 2\partial_{[\mu}\mathbf{\Gamma}^\kappa_{\lambda]\nu} + 2\mathbf{\Gamma}^\kappa_{[\mu|\rho|}\mathbf{\Gamma}^\rho_{\lambda]\nu} \tag{54a}$$

or in expanded form as

$$\mathbf{R}_{\mu\lambda\nu}{}^{\cdot\kappa} = \partial_\mu \mathbf{\Gamma}^\kappa_{\lambda\nu} - \partial_\lambda \mathbf{\Gamma}^\kappa_{\mu\nu} + \mathbf{\Gamma}^\kappa_{\mu\rho}\mathbf{\Gamma}^\rho_{\lambda\nu} - \mathbf{\Gamma}^\kappa_{\lambda\rho}\mathbf{\Gamma}^\rho_{\mu\nu}. \tag{54b}$$

The importance of this quantity lies in the fact that it determines the integrability conditions of $\mathbf{\Gamma}^\kappa_{\lambda\nu}$ (Schrödinger, 1954), *i.e.* when this quantity vanishes, integrability with respect to $\mathbf{\Gamma}^\kappa_{\lambda\nu}$ obtains. It can be shown from equations of the type given by (40), (45) and (51), used in conjunction with (54), that the curvature tensor vanishes for all of the states considered in the present study. This is an important finding since it shows that these spaces all possess teleparallelism or absolute parallelism. Physically this means that a vector displaced by parallel transfer from one point to another is independent of path. This is obviously true for all of the Burgers circuits considered thus far.

The final item of interest concerns the nature of the strain tensors associated with the states thus far described. In particular, we may write

$$\mathbf{e}_{\kappa\lambda} = (\mathbf{g}_{\kappa\lambda} \underset{K}{\mathbf{g}}_{\kappa\lambda})/2 \tag{55a}$$

$$\mathbf{e}_{k^2 l^2} = (\mathbf{g}_{k^2 l^2} - \underset{K}{\mathbf{g}}_{k^2 l^2})/2 \tag{55b}$$

$$\mathbf{e}_{k^3 l^3} = (\mathbf{g}_{k^3 l^3} - \underset{K}{\mathbf{g}}_{k^3 l^3})/2. \tag{55c}$$

The last two equations are equal and involve pure plastic strains, whereas (55*a*) gives the sum of both the plastic and elastic strains. The elastic strain, however, may be separated out as follows

$$\underset{E}{\mathbf{e}}_{\kappa\lambda} = (\mathbf{g}_{\kappa\lambda} - \underset{k^2}{\mathbf{g}}_{\kappa\lambda})/2 \tag{56}$$

where $\underset{k^2}{\mathbf{g}}_{\kappa\lambda}$ is the metric associated with the (κ) state, just as $\underset{K}{\mathbf{g}}_{\kappa\lambda}$ was the metric associated with the (K) state.

Summary and conclusions

The techniques of differential geometry have been applied to both coherent and incoherent two-phase

interfaces. Various tensor quantities such as distortion, torsion and curvature have been developed in terms of the Burgers circuit and are shown to give what is perhaps the most complete description available until now of the Burgers vector and dislocation density associated with such two-phase interfaces.

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Efficient Structure-Factor Calculation for Large Molecules by the Fast Fourier Transform

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A method is presented for calculating structure factors by Fourier inversion of a model electron density map. The cost of this method and of the standard methods are analyzed as a function of number of atoms, resolution, and complexity of space group. The cost functions were scaled together by timing both methods on the same problem, with the same computer. The FFT method is $3\frac{1}{2}$ to 7 times less expensive than conventional methods for non-centrosymmetric space groups.

Structure factor calculation is one of the major expenses in refinement of macromolecular structures. The purpose of this paper is to show how the fast Fourier transform (FFT) method can be used to calculate structure factors, and to compare FFT structure-factor calculation with conventional methods in terms of convenience, speed, and economy. A specific comparison of the two methods for the space group $P6_122$ has been carried out as part of a project in this laboratory to refine the structure of thermolysin, a proteolytic enzyme from *Bacillus thermoproteolyticus* (Matthews, Weaver & Kester, 1974). It will be shown that the FFT structure-factor calculation is considerably less expensive than any of the direct-summation methods.

A. Calculation of structure factors by the FFT method

The fast Fourier transform algorithm can only compute finite discrete Fourier transforms. Therefore we must construct a model electron density map sampled on a grid and invert it to obtain our structure factors. The calculation of such a model map presents two problems which must be solved in order to use this method. First, a procedure must be devised to solve the sampling problem; otherwise the model electron density map must be constructed on a very fine grid, which greatly increases the computer storage requirements and the cost of the calculation. Second, a convenient functional representation must be found for the electron density distribution of a single atom. Sayre (1951) discussed these problems in some detail. In the following sections we describe ways of solving these problems, and also discuss programming strategy.

A.1. *The sampling problem*

The FFT algorithm can only be used to calculate the *finite discrete* Fourier transform of a function sampled at regular intervals on a grid. The act of sampling a continuous function implies potential loss