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Differential geometry of phase transformations

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The foundations have been laid with respect to a generalized theory of phase transformations in solids. In particular, the methods of differential geometry have been employed and such important tensor quantities as distortion, metric, torsion, and anholonomic object have been developed with respect to such transformations. It is further shown that both Riemannian as well as non-Riemannian (dislocation) geometries are needed to describe these transformations properly.

1. Introduction

When a finite volume of a crystal undergoes a transformation into a new phase, each phase becomes separated from the other by a closed surface or interface. A theory of such interfaces has already been formulated by a number of investigators for a special class of transformations in which no diffusion of atoms is involved, i.e., the so-called martensitic transformations [1, 2]. However, no generalized theory has been proposed which would embody all classes of transformations. Furthermore, since the two-phase interface is an entity most properly described in terms of its dislocation content, such a theory should in essence be a dislocation theory. In addition, in order that the treatment be all encompassing, the most generalized type of geometric analysis should be employed. It has already been shown with respect to grain boundaries and two-phase interfaces that the techniques of differential geometry satisfy these conditions. This approach will therefore now be used for the problem of phase transformations.

2. Distortion tensors

Let us consider the perfect reference crystal shown in Fig. 1a which will be denoted by an upper case Roman letter, i.e., K, L etc. If it now undergoes a phase transformation such as a simple shear, the lattice distortion shown in Fig. 1b is obtained. The distorted lattice will be denoted by lower case Greek letters, i.e., κ, λ etc. We may write the distortion tensor which gives $(\mathrm{K}) \to (\kappa)$ as follows:

$$B_\kappa^{\mathrm{K}} = \begin{pmatrix} B_1^1 & B_1^2 & B_1^3 \\ B_2^1 & B_2^2 & B_2^3 \\ B_3^1 & B_3^2 & B_3^3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \tan\theta & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (1)$$

where the distortion tensor connects the base vectors in the two states according to

$$e_\kappa = B_\kappa^{\mathrm{K}} e_{\mathrm{K}} \quad (2)$$

In the case of Fig. 1b, $\tan\theta$ was taken as $\frac{1}{2}$. The metric tensor associated with the (κ) state can next be written as

$$b_{\kappa\lambda} = B_\kappa^{\mathrm{K}} B_\lambda^{\mathrm{K}} = \begin{pmatrix} 1 & \tan\theta & 0 \\ \tan\theta & (\tan^2\theta + 1) & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (3)$$

On the other hand, the metric tensor associated with the (K) state, a_{KL} is simply the Kronecker delta δ_{KL}. The metric tensors can in turn be used to measure distances in the two states as follows [3]:

$$(\mathrm{d}S)_{\mathrm{K}}^2 = a_{\mathrm{KL}} \mathrm{d}x^{\mathrm{K}} \mathrm{d}x^{\mathrm{L}} \quad (4a)$$

and

$$(\mathrm{d}S)_\kappa^2 = b_{\kappa\lambda} \mathrm{d}x^\kappa \mathrm{d}x^\lambda \quad (4b)$$

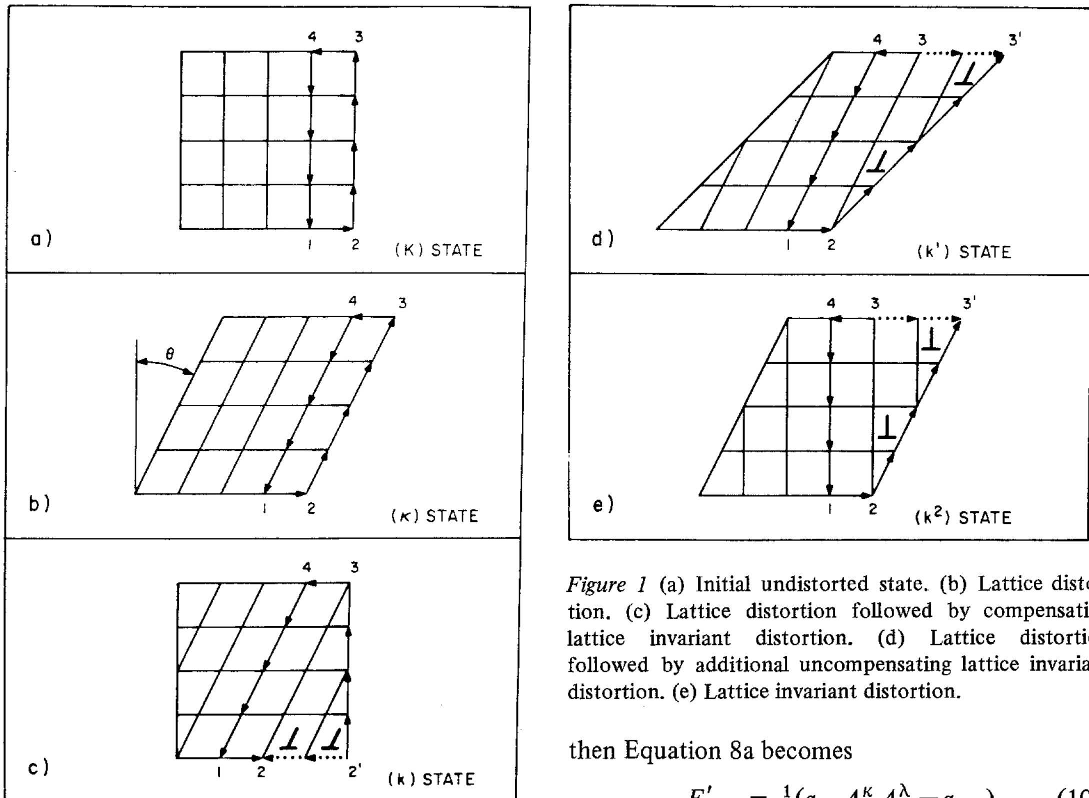

Figure 1 (a) Initial undistorted state. (b) Lattice distortion. (c) Lattice distortion followed by compensating lattice invariant distortion. (d) Lattice distortion followed by additional uncompensating lattice invariant distortion. (e) Lattice invariant distortion.

while

$$(dS)^2_\kappa - (dS)^2_K = (b_{\kappa\lambda} A^\kappa_K A^\lambda_L - a_{KL})\, dx^K dx^L \qquad (5a)$$

or

$$(dS)^2_\kappa - (dS)^2_K = (b_{\kappa\lambda} - a_{KL} A^K_\kappa A^L_\lambda)\, dx^\kappa dx^\lambda \qquad (5b)$$

The distortions A^κ_K connect the components of the two states as follows:

$$dx^\kappa = A^\kappa_K dx^K \qquad (6)$$

where

$$A^\kappa_K \equiv B^K_\kappa \qquad (7)$$

With the aid of Equations 5, we can define the following strain tensors:

$$E_{KL} = \tfrac{1}{2}(b_{\kappa\lambda} A^\kappa_K A^\lambda_L - a_{KL}) \qquad (8a)$$

or

$$E_{\kappa\lambda} = \tfrac{1}{2}(b_{\kappa\lambda} - a_{KL} A^K_\kappa A^L_\lambda) \qquad (8b)$$

The strain E_{KL} is obviously defined in terms of the (K) state coordinates, while $E_{\kappa\lambda}$ is in terms of the (κ) state coordinates. If the coordinates are dragged, i.e., $dx^K = dx^\kappa$ then

$$E_{\kappa\lambda} = E_{KL} = \overset{L}{e}_{\kappa\lambda} = \tfrac{1}{2}(b_{\kappa\lambda} - a_{\kappa\lambda}) \qquad (9)$$

If, on the other hand, the metric in state (κ) is kept the same as that in state (K), i.e., $a_{\kappa\lambda} = a_{KL}$, then Equation 8a becomes

$$E'_{KL} = \tfrac{1}{2}(a_{\kappa\lambda} A^\kappa_K A^\lambda_L - a_{KL}) \qquad (10a)$$

while if the metric in the (K) state is kept the same as that in the (κ) state, Equation 8b becomes

$$E'_{\kappa\lambda} = \tfrac{1}{2}(b_{\kappa\lambda} - b_{KL} A^K_\kappa A^L_\lambda) \qquad (10b)$$

In order to see how these strains all compare with one another, we can write, with the aid of Equation 7

$$E_{KL} = \begin{pmatrix} 0 & \tan\theta & 0 \\ \tan\theta & 2\tan^2\theta & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad (11a)$$

$$E_{\kappa\lambda} = \begin{pmatrix} 0 & \tan\theta & 0 \\ \tan\theta & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad (11b)$$

$$e_{\kappa\lambda} = \begin{pmatrix} 0 & \tfrac{1}{2}\tan\theta & 0 \\ \tfrac{1}{2}\tan\theta & \tfrac{1}{2}\tan^2\theta & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad (11c)$$

It is also a simple matter to show that

$$E'_{KL} = E'_{\kappa\lambda} = \overset{L}{e}_{\kappa\lambda} \qquad (11d)$$

Thus, we see that dragging of the metric gives the same strain as dragging of the coordinates. The following section will show that the former representation is more suitable for plastic deformation, while the latter formulation more vividly reflects the lattice deformation. The index L has been used in the last equation to indicate that the strain is due to the lattice distortion or transformation associated with (K) → (κ).

The (κ) state may next be plastically deformed to generate the (k) state shown in Fig. 1c. This is accomplished by means of the following distortion:

$$B^{\kappa}_{\mathrm{k}} = \begin{pmatrix} 1 & 0 & 0 \\ -\tan\theta & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{12}$$

This is simply a shear opposite to that given by Equation 1, so that the overall distortion in going from (K) → (k) is

$$B^{\mathrm{K}}_{\mathrm{k}} = B^{\mathrm{K}}_{\kappa} B^{\kappa}_{\mathrm{k}} = \delta^{\mathrm{K}}_{\mathrm{k}} \tag{13}$$

Thus, the metric tensor associated with the (k) state is

$$c_{\mathrm{kl}} = B^{\mathrm{K}}_{\mathrm{k}} B^{\mathrm{K}}_{\mathrm{l}} = \delta_{\mathrm{kl}} \tag{14}$$

We can thus write the lattice invariant or plastic strain in going from (κ) → (k) as

$$\overset{\mathrm{P}}{e}_{\mathrm{kl}} = \tfrac{1}{2}(c_{\mathrm{kl}} - b_{\mathrm{kl}}) = \begin{pmatrix} 0 & -\frac{1}{2}\tan\theta & 0 \\ -\frac{1}{2}\tan\theta & -\frac{1}{2}\tan^2\theta & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{15}$$

The total strain in going from (K) → (k) is obviously

$$\overset{\mathrm{T}}{e}_{\mathrm{kl}} = \overset{\mathrm{L}}{e}_{\mathrm{kl}} + \overset{\mathrm{P}}{e}_{\mathrm{kl}} = \tfrac{1}{2}(-a_{\mathrm{kl}} + c_{\mathrm{kl}}) = 0 \tag{16}$$

in accordance with the construction of Fig. 1c. The transformation strain is thus just compensated by the plastic strain.

If now a plastic distortion given by

$$B^{\kappa}_{\mathrm{k}^1} \equiv B^{\mathrm{K}}_{\kappa} \tag{17}$$

is superimposed on the (κ) state, we obtain the configuration shown in Fig. 1d, i.e., the shape and plastic distortions add together rather than compensate one another, as was the case for the (k) state shown in Fig. 1c. For the overall distortion, we can write

$$B^{\mathrm{K}}_{\mathrm{k}^1} = B^{\mathrm{K}}_{\kappa} B^{\kappa}_{\mathrm{k}^1} = \begin{pmatrix} 1 & 0 & 0 \\ 2\tan\theta & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{18}$$

from which we find

$$d_{\mathrm{k}^1\mathrm{l}^1} = B^{\mathrm{K}}_{\mathrm{k}^1} B^{\mathrm{K}}_{\mathrm{l}^1} = \begin{pmatrix} 1 & 2\tan\theta & 0 \\ 2\tan\theta & (4\tan^2\theta + 1) & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{19}$$

while the total strain in going from (K) → (k^1) is

$$\overset{\mathrm{T}}{e}_{\mathrm{k}^1\mathrm{l}^1} = \tfrac{1}{2}(d_{\mathrm{k}^1\mathrm{l}^1} - a_{\mathrm{k}^1\mathrm{l}^1}) = \begin{pmatrix} 0 & \tan\theta & 0 \\ \tan\theta & 2\tan^2\theta & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{20}$$

The (k^2) state shown in Fig. 1e can be derived from the (K) state by means of the following distortion:

$$B^{\mathrm{K}}_{\mathrm{k}^2} \equiv B^{\mathrm{K}}_{\kappa} \tag{21a}$$

from which it follows that

$$f_{\mathrm{k}^2\mathrm{l}^2} \equiv b_{\kappa\lambda} \tag{21b}$$

while

$$\overset{\mathrm{P}}{e}_{\mathrm{k}^2\mathrm{l}^2} \equiv \overset{\mathrm{L}}{e}_{\kappa\lambda} \tag{21c}$$

The distortions considered thus far involved no volume changes, i.e.,

$$\mathrm{Det}\,(A^{\mathrm{K}}_{\kappa}) = 1 \tag{22}$$

where Det signifies determinant. Let us now consider what is perhaps the simplest of all volume distortions given by

$$B^{\mathrm{K}}_{\kappa^1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & V & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{23}$$

The resulting (κ^1) state is shown in Fig. 2a where V has been chosen as 4/5. The metric tensor for this state becomes

$$g_{\kappa^1\lambda^1} = B^{\mathrm{K}}_{\kappa^1} B^{\mathrm{K}}_{\lambda^1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & V^2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{24}$$

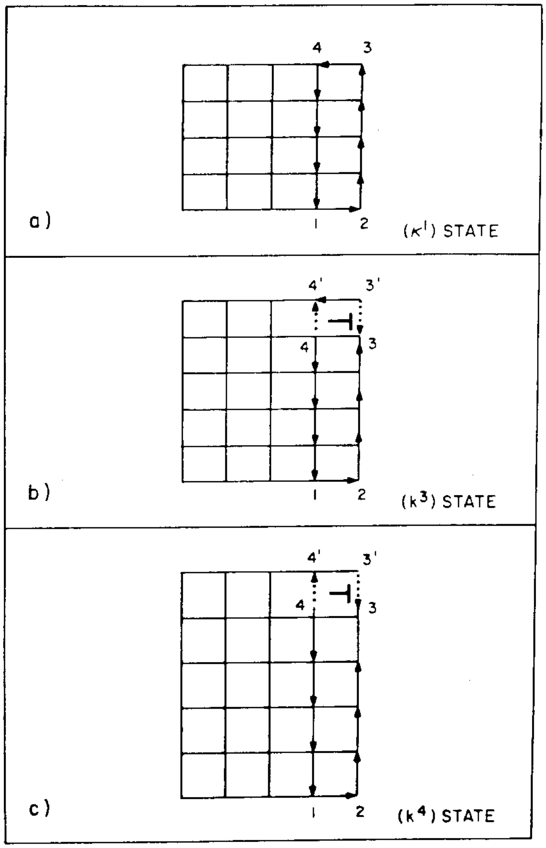

Figure 2 (a) Lattice distortion. (b) Lattice distortion followed by compensating lattice invariant distortion. (c) Lattice invariant distortion.

whereas the strain tensor is

$$\overset{L}{e}_{\kappa^1\lambda^1} = \tfrac{1}{2}(g_{\kappa^1\lambda^1} - a_{\kappa^1\lambda^1}) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \tfrac{1}{2}(V^2-1) & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (25)$$

In order to produce the plastically distorted (k^3) state shown in Fig. 2b from the (κ^1) state, we must write

$$B^{\kappa^1}_{k^3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/V & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (26)$$

so that the overall distortion becomes

$$B^{K}_{k^3} = B^{K}_{\kappa^1} B^{\kappa^1}_{k^3} = \delta^{K}_{k^3} \quad (27)$$

This means that the metric tensor for the (k^3) state is

$$h_{k^3 l^3} = \delta_{k^3 l^3} \quad (28)$$

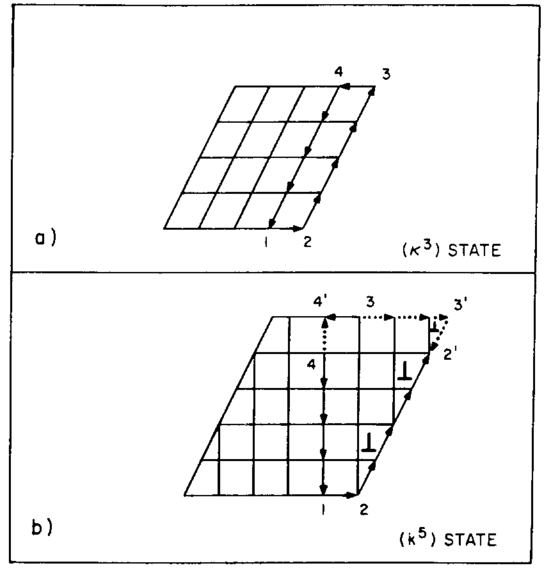

Figure 3 (a) Generalized lattice distortion. (b) Lattice distortion accompanied by lattice invariant distortion.

The plastic strain in going from (κ^1) → (k^3) is thus

$$\overset{P}{e}_{k^3 l^3} = \tfrac{1}{2}(h_{k^3 l^3} - g_{k^3 l^3}) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \tfrac{1}{2}(1-V^2) & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (29)$$

so that the overall strain in going from (K) → (k^3) is

$$\overset{T}{e}_{k^3 l^3} = \overset{L}{e}_{k^3 l^3} + \overset{P}{e}_{k^3 l^3} = 0 \quad (30)$$

If the distortion given by Equation 26 were applied to the (K) state crystal, i.e.

$$B^{K}_{k^4} \equiv B^{\kappa^1}_{k^3} \quad (31)$$

the (k^4) state shown in Fig. 2c would be obtained. The analogies between the shear distortions in Fig. 1 and the volume distortions in Fig. 2 are thus complete.

For the sake of generality, Fig. 3 shows a set of more generalized distortions. If, for example, we write

$$B^{K}_{\kappa^2} = \begin{pmatrix} V & 0 & 0 \\ 0 & V & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (32)$$

while

$$B^{\kappa^2}_{\kappa^3} \equiv B^{K}_{\kappa}$$

then state (κ^3) can be obtained from state (K) via the following distortion:

$$B^{\mathrm{K}}_{\kappa^3} = B^{\mathrm{K}}_{\kappa^2} B^{\kappa^2}_{\kappa^3} = \begin{pmatrix} V & 0 & 0 \\ V\tan\theta & V & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (33)$$

On the other hand, the (k^5) state depicted in Fig. 3b can be obtained from the (κ^3) state according to

$$B^{\kappa^3}_{\mathrm{k}^5} = \begin{pmatrix} 1/V & 0 & 0 \\ 0 & 1/V & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (34)$$

We can thus write

$$B^{\mathrm{K}}_{\mathrm{k}^5} = B^{\mathrm{K}}_{\kappa^3} B^{\kappa^3}_{\mathrm{k}^5} \equiv B^{\mathrm{K}}_{\kappa} \quad (35)$$

It follows that, whereas the (κ^3) state possesses only a lattice distortion, state (k^5) contains both a lattice and a plastic distortion.

3. Torsion tensor

Let us now consider the reference circuit 1–2–3–4–1 associated with the (K) state in Fig. 1a. The corresponding circuit in the (κ) state is shown in Fig. 1b. Now the closure failure or Burgers vector associated with any Burgers circuit can be written as [4]

$$b^{\kappa} = -\oint A^{\kappa}_{\mathrm{K}} \mathrm{d}x^{\mathrm{K}} \quad (36)$$

The above equation can be expanded to give

$$\underset{\kappa}{b^1} = -A^1_2 \underset{4-1}{\Delta x^2} - A^1_2 \underset{2-3}{\Delta x^2} = 4\tan\theta - 4\tan\theta = 0 \quad (37)$$

where $\underset{4-1}{\Delta x^2}$ etc. are the distances 4–1 etc. in Fig. 1a.

Considering next the (K) → (k^2) state transformation, we may write

$$b^{\mathrm{k}^2} = -\oint A^{\mathrm{k}^2}_{\mathrm{K}} \mathrm{d}x^{\mathrm{K}} \quad (38)$$

where $A^{\mathrm{k}^2}_{\mathrm{K}}$ must be written as

$$A^{\mathrm{k}^2}_{\mathrm{K}} = \underset{1}{A^{\mathrm{k}^2}_{\mathrm{K}}} H(-x^1) + \delta^{\mathrm{k}^2}_{\mathrm{K}} H(+x^1) \quad (39)$$

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

$$H(-x^1) = \begin{cases} 0 & \text{if } x^1 > 0 \\ 1 & \text{if } x^1 < 0 \end{cases} \quad (40a)$$

while

$$H(+x^1) = \begin{cases} 0 & \text{if } x^1 < 0 \\ 1 & \text{if } x^1 > 0 \end{cases} \quad (40b)$$

whereas

$$\underset{1}{A^{\mathrm{k}^2}_{\mathrm{K}}} \equiv B^{\mathrm{K}}_{\mathrm{k}^2} \quad (41)$$

as given by Equation 21a. The distance x^1 is measured from the rightmost face of Fig. 1a. Equation 38 can now be expanded to yield

$$\underset{\mathrm{k}^2}{b^1} = -A^1_2 \underset{4-1}{\Delta x^2} - A^1_2 \underset{2-3}{\Delta x^2} = 4\tan\theta - 0 \quad (42a)$$

The second term in the above equation is zero, since A^1_2 along the path 2–3 is zero. In terms of Fig. 1e, Equation 42a becomes

$$\underset{\mathrm{k}^2}{b^1} = 2 = \underset{3-3'}{\Delta x^2} \quad (42b)$$

The dislocations are indicated by their standard symbols. It is obvious that

$$b^{\mathrm{K}} = -\oint A^{\mathrm{K}}_{\mathrm{k}^2} \mathrm{d}x^{\mathrm{k}^2} = 0 \quad (43)$$

since there are no dislocations in the (K) state.

The line integral of Equation 38 may next be converted into a surface integral by means of Stokes' theorem to give [5]

$$b^{\mathrm{k}^2} = -\oint A^{\mathrm{k}^2}_{\mathrm{K}} \mathrm{d}x^{\mathrm{K}} = -\int_s \partial_{[\mathrm{L}} A^{\mathrm{k}^2}_{\mathrm{K}]} \mathrm{d}F^{\mathrm{LK}} \quad (44a)$$

Expanding, this yields

$$\underset{\mathrm{k}^2}{b^1} = -\int_s \partial_1 A^1_2 \mathrm{d}F^{12} = \int_s \tan\theta\, \delta(x^1) \mathrm{d}x^1 \mathrm{d}x^2 \quad (44b)$$

where $\delta(x^1)$ is the Dirac delta function which satisfies the following relation

$$\int_{-\infty}^{+\infty} \delta(x^1) \mathrm{d}x^1 = 1 \quad (45)$$

and arises from the fact that

$$\partial_1 H(-x^1) = -\delta(x^1) \quad (46)$$

Equation 44b can thus be rewritten as

$$\underset{\mathrm{k}^2}{b^1} = \tan\theta \int \mathrm{d}x^2 = 4\tan\theta \quad (47)$$

which is the same result as that given by Equation 42a.

The surface integral of Equation 44a can also be written with respect to final state coordinates as follows:

$$b^{\mathrm{k}^2} = -\int S_{1^2}{}^{\cdot}{}_{\mathrm{m}^2}{}^{\cdot}{}^{\mathrm{k}^2}\, \mathrm{d}F^{1^2 \mathrm{m}^2} \qquad (48)$$

where the quantity $S_{1^2}{}^{\cdot}{}_{\mathrm{m}^2}{}^{\cdot}{}^{\mathrm{k}^2}$ is termed the torsion tensor and is given by

$$S_{1^2}{}^{\cdot}{}_{\mathrm{m}^2}{}^{\cdot}{}^{\mathrm{k}^2} = A^{\mathrm{L}}_{1^2} A^{\mathrm{K}}_{\mathrm{m}^2}\ \partial_{[\mathrm{L}} A^{\mathrm{k}^2}_{\mathrm{K}]} \qquad (49)$$

The particular component of interest to us is

$$S_{1}{}^{\cdot}{}_{2}{}^{\cdot}{}^{1} = \tfrac{1}{2}\bar{A}^1_1 \bar{A}^2_2 \partial_1 A^1_2 = -\tfrac{1}{2}\tan\theta\, \delta(x^1) \qquad (50)$$

where the barred quantities $\bar{A}^1_1$ etc. signify inverses. Substitution of Equation 50 into 48 yields the same result as Equation 47.

Turning now to Fig. 1c, we may write

$$b^{\mathrm{k}} = -\oint A^{\mathrm{k}}_{\kappa} \mathrm{d}x^{\kappa} \qquad (51)$$

where

$$A^{\mathrm{k}}_{\kappa} = \underset{1}{A^{\mathrm{k}}_{\kappa}} H(-x^1) + \delta^{\mathrm{k}}_{\kappa} H(+x^1) \qquad (52)$$

and

$$\underset{1}{A^{\mathrm{k}}_{\kappa}} \equiv B^{\kappa}_{\mathrm{k}}.$$

Equation 51 can now be expanded to give

$$\underset{\mathrm{k}}{b^1} = -\underset{1}{A^1_2}\underset{4-1}{\Delta x^2} - A^1_2 \underset{2-3}{\Delta x^2} = -4\tan\theta - 0 \qquad (53\mathrm{a})$$

In terms of Fig. 1c, Equation 53a becomes

$$\underset{\mathrm{k}}{b^1} = -2 = \underset{2'-2}{\Delta x^2} \qquad (53\mathrm{b})$$

In the case of Fig. 1d

$$b^{\mathrm{k}^1} = -\oint A^{\mathrm{k}^1}_{\kappa}\, \mathrm{d}x^{\kappa} \qquad (54)$$

The above relation gives the same result as that given by Equation 42b.

With respect to Fig. 2, we may write

$$b^{\mathrm{k}^3} = -\oint A^{\mathrm{k}^1}_{\kappa^1} \mathrm{d}x^{\kappa^1} \qquad (55)$$

where

$$A^{\mathrm{k}^3}_{\kappa^1} = \underset{1}{A^{\mathrm{k}^3}_{\kappa^1}} H(-x^1) + \delta^{\mathrm{k}^3}_{\kappa^1} H(+x^1) \qquad (56)$$

and where

$$\underset{1}{A^{\mathrm{k}^3}_{\kappa^1}} \equiv B^{\kappa^1}_{\mathrm{k}^3} \qquad (57)$$

Substituting into Equation 55, we obtain

$$\underset{\kappa^1}{b^2} = -\underset{1}{A^2_2}\underset{4-1}{\Delta x^2} - A^2_2 \underset{2-3}{\Delta x^2} = \left(\frac{1}{V}\right)4 - 4 \qquad (58\mathrm{a})$$

which in terms of Fig. 2b becomes

$$\underset{\kappa^1}{b^2} = 1 = \underset{4-4'}{\Delta x^2} \qquad (58\mathrm{b})$$

Fig. 2b also shows the closure failure 3′–3 which is, in fact, a surface closure failure [6] and can be obtained by rewriting Equation 55 as

$$b^{\mathrm{k}^3} = \oint A^{\mathrm{k}^3}_{\kappa^1} \mathrm{d}x^{\kappa^1} \qquad (59)$$

The analogue of this condition for the (k^2) state is shown for the (k^6) state in Fig. 4a. Unlike Fig. 1e, the dislocations in Fig. 4a have surface steps associated with them given by 5–5′ and 2′–2. These may be obtained by rewriting Equation 38 as

$$b^{\mathrm{k}^6}_{\mathrm{K}} = \oint A^{\mathrm{k}^6}_{\mathrm{K}}\, \mathrm{d}x^{\mathrm{K}} \qquad (60)$$

where

$$A^{\mathrm{k}^6}_{\mathrm{K}} \equiv A^{\mathrm{k}^2}_{\mathrm{K}} \qquad (61)$$

while the corresponding closure failure associated with the dislocation is 3–3′ given by

$$b^{\mathrm{k}^6} = -\oint A^{\mathrm{k}^6}_{\mathrm{K}}\, \mathrm{d}x^{\mathrm{K}} \qquad (62)$$

If now the distortion tensor given by Equation 39 were to be rewritten as

$$A^{\mathrm{k}^7}_{\mathrm{K}} = \underset{1}{A^{\mathrm{k}^7}_{\mathrm{K}}} H(-x^1) \qquad (63)$$

where

$$\underset{1}{A^{\mathrm{k}^7}_{\mathrm{K}}} \equiv \underset{1}{A^{\mathrm{k}^2}_{\mathrm{K}}} \qquad (64)$$

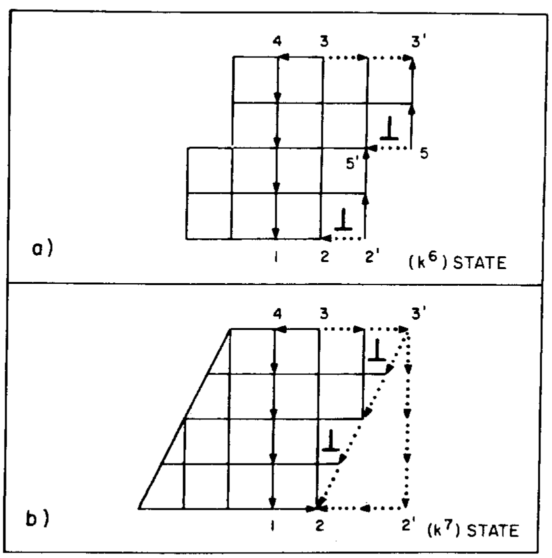

Figure 4 Torn configurations corresponding to the dislocated state in Fig. 1e.

the configuration shown in Fig. 4b would be obtained. A surface closure failure 3′–2 is now seen to be present, which in turn can be resolved into the two components 2′–2 and 3–3′. Both can be obtained from the following relation

$$b^{k^7} = \oint A^{k^7}_{K}\, dx^{K} \tag{65}$$

The (k^7) may be visualized as being created from the (κ^1) state by first tearing away the rightmost portion of this body. Equation 55 could be rewritten as [5, 7]

$$b^{k^3} = -\oint (S_{l^3 m^3}^{\cdot\ \cdot\ k^3} - \Omega_{l^3 m^3}^{\cdot\ \cdot\ k^3})\, dF^{l^3 m^3} \tag{66}$$

where

$$S_{l^3 m^3}^{\cdot\ \cdot\ k^3} = A^{\lambda^1}_{l^3} A^{\kappa^1}_{m^3}\, \partial_{[\lambda^1} A^{k^3}_{\kappa^1]} \tag{67a}$$

and

$$\Omega_{l^3 m^3}^{\cdot\ \cdot\ k^3} = A^{\lambda^1}_{l^3} A^{\kappa^1}_{m^3}\, \partial_{[\lambda^1} A^{k^3}_{\kappa^1]} \tag{67b}$$

It follows that

$$S_{l^3 m^3}^{\cdot\ \cdot\ k^3} = \Omega_{l^3 m^3}^{\cdot\ \cdot\ k^3} \tag{68a}$$

and, in particular,

$$S_{12}^{\cdot\cdot 2} = \tfrac{1}{2}\bar{A}^1_1 \bar{A}^2_2 \partial_1 A^2_2 = \tfrac{1}{2}[-\delta(x^1) + \delta(x^1)] \tag{68b}$$

When substituted into Equation 66, the above relations yield the same results as Equations 55 and 59. Here we see, though, that the torsion tensor $S_{l^3 m^3}^{\cdot\ \cdot\ k^3}$ measures the actual dislocation content, i.e., the closure failure 4–4′, while the quantity $\Omega_{l^3 m^3}^{\cdot\ \cdot\ k^3}$, termed the anholonomic object, measures the corresponding free surface associated with these dislocations. Obviously, $\Omega_{l^2 m^2}^{\cdot\ \cdot\ k^2}$ may be zero, as in the case of Fig. 1e, while $S_{l^2 m^2}^{\cdot\ \cdot\ k^2}$ remains finite. Conversely, $S_{l^7 m^7}^{\cdot\ \cdot\ k^7}$ may be zero, while $\Omega_{l^7 m^7}^{\cdot\ \cdot\ k^7}$ remains finite, as is true for the component $\Omega_{12}^{\cdot\cdot 2}$ which yields the closure failure 3′–2′ in Fig. 4b. States which possess an anholonomic object are said to be anholonomic or perfectly torn states since they possess no elastic distortions [5, 7].

Considering now the more generalized distortion shown in Fig. 3b, we can first write

$$A^{k^5}_{\kappa^3} = \underset{1}{A}{}^{k^5}_{\kappa^3} H(-x^1) + \delta^{k^3}_{\kappa^1} H(+x^1) \tag{69}$$

where

$$\underset{1}{A}{}^{k^5}_{\kappa^3} = B^{k^3}_{\kappa^5} \tag{70}$$

which can be used to find

$$S_{12}^{\cdot\cdot 1} = -\tfrac{1}{2} \tan\theta\, \delta(x^1) \tag{71a}$$

and

$$S_{12}^{\cdot\cdot 2} = \Omega_{12}^{\cdot\cdot 2} = \tfrac{1}{2}[-\delta(x^1) + \delta(x^1)] \tag{71b}$$

When substituted into the following equation

$$b^{k^5} = - (S_{l^5 m^5}^{\cdot\ \cdot\ k^5} - \Omega_{l^5 m^5}^{\cdot\ \cdot\ k^5})\, dF^{l^5 m^5} \tag{72}$$

we obtain the three closure failures shown dotted in Fig 3b.

4. Two-phase considerations

Let us now refer to the initial perfect reference state crystal (K^1) shown in Fig. 5a. Next, allow a certain region within the dotted area to undergo a lattice distortion given by Equation 1, followed by the plastic deformation given by Equation 12. The (K^1) state crystal is thus transformed to the (k^8) state crystal depicted in Fig. 5b. The transformed region is obviously identical to that illus-

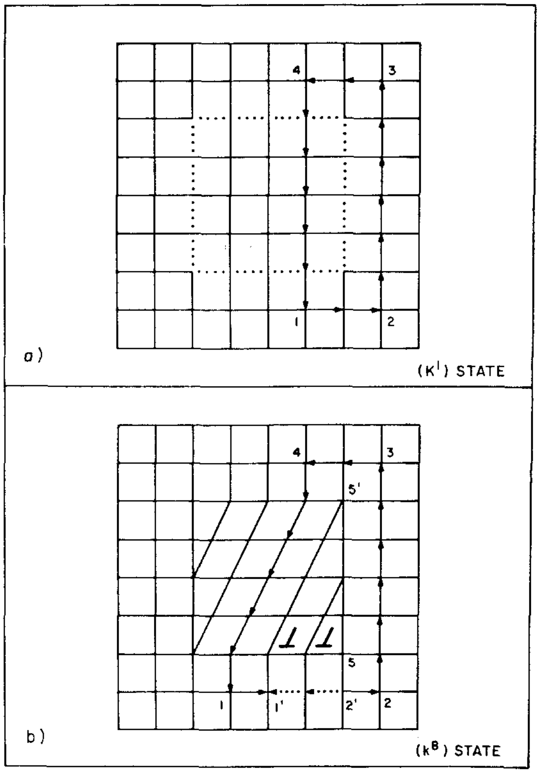

Figure 5 (a) Initial reference crystal in which (b) phase transformation takes place involving both lattice distortion followed by compensating plastic deformation.

trated in Fig. 1c. It is apparent that if the (K^1) crystal were to involve only the shape change, giving rise to the (κ) state crystal illustrated in Fig. 1b, then severe elastic distortions would be obtained. The configuration shown in Fig. 5b is thus of low energy. Furthermore, Burgers circuits taken in the (K^1) and (k^8) states lead to closure failures identical to those given in Figs. la and c respectively.

If now the dotted area shown in Fig. 5a undergoes lattice distortion given by Equation 23, the (k^9) state configuration shown in Fig. 6a is obtained. This is a perfectly torn configuration and consists of our newly-created free surfaces, but no dislocations. The perfect tearing eliminates the elastic strains that would otherwise be generated. In order to obtain the surface closure failure 5′–5 in Fig. 5a we must write

$$\underset{k^9}{\Omega}{}_{12}^{\cdot\cdot 2} = \{\tfrac{1}{2}\delta(x^1)\}_1 + \{-\tfrac{1}{2}\delta(x^1)\}_2 \qquad (73)$$

where the curly bracket notation is used to represent each phase separately, i.e., 1 for the transformed region and 2 for the untransformed area. When extra matter is added to the (k^9) state so as to fill up the hole, and thus eliminate the energy associated with the free surfaces, the (k^{10}) state configuration illustrated in Fig. 6a is produced. The new phase is obviously the same as that shown in Fig 2b and may be viewed as generated by the distortion given by Equation 26. In this case, there is a dislocation present given by the closure failure 1′–4′, but no free surfaces. This particular closure failure can be obtained from the following component of the torsion tensor:

$$\underset{k^{10}}{S}{}_{12}^{\cdot\cdot 2} = \{-\tfrac{1}{2}\delta(x^1)\}_1 + \{\tfrac{1}{2}\delta(x^1)\}_2 \qquad (74)$$

It is apparent that

$$\underset{k^{10}}{S}{}_{12}^{\cdot\cdot 2} \equiv -\underset{k^9}{\Omega}{}_{12}^{\cdot\cdot 2} \qquad (75)$$

Rather than have the compensating plastic distortion occur in the newly-formed phase, it may take place in the surrounding matrix. For example, Fig. 7a shows the transformation already discussed in Fig 1b with a corresponding compensating plastic distortion in the surrounding matrix. Under these conditions, the distortion must be written as

$$A_K^{k^{10}} = \{\underset{1}{A}{}_K^{k^{10}} H(-x^1)\}_1 + \{\underset{2}{A}{}_K^{k^{10}} H(+x^1)\}_2 \qquad (76)$$

where

$$A_K^{k^{10}} \equiv A_K^{\kappa} \qquad (77a)$$

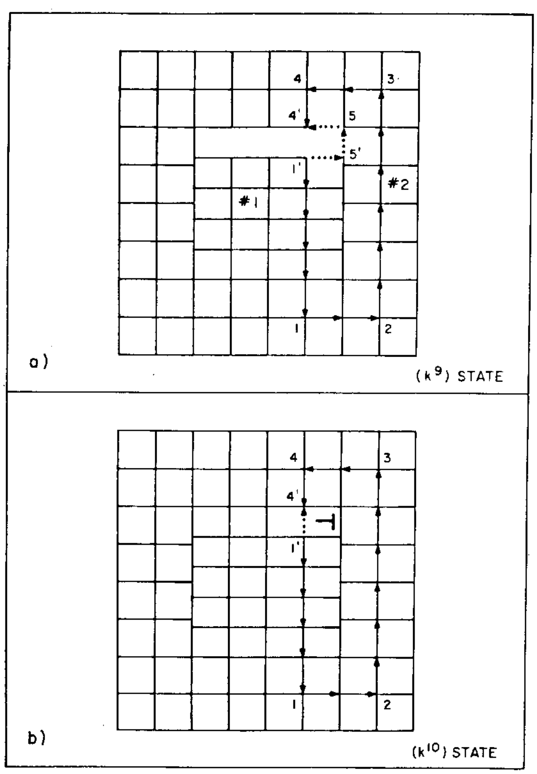

Figure 6 (a) Phase change which involves lattice distortion, followed by (b) compensating plastic deformation.

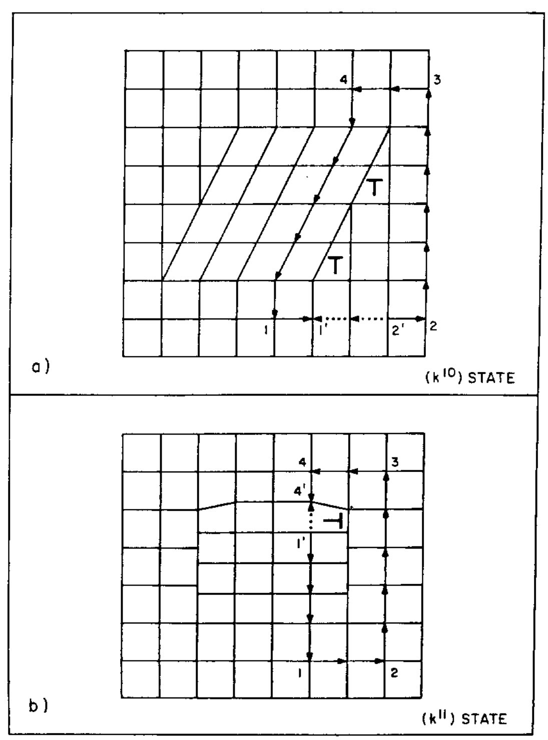

Figure 7 Lattice distortion followed by compensating plastic distortion in surrounding matrix.

while

$$\underset{2}{A}_{K}^{k^{10}} \equiv A_{K}^{k} \qquad (77b)$$

The lattice distortion associated with the transformation in Fig. 6a can also be accommodated by a plastic distortion which involves the removal of a horizontal plane on each side of the new phase. This results in the formation of the (k^{11}) state illustrated in Fig. 7b. Except for a relatively small residual elastic strain, the closure failure is essentially the same as that given for the (k^{10}) state of Fig. 6b.

All of the discussion up to now can be recast in a new light by reference to Fig. 8. In particular, the circle in Fig. 8a corresponds to the undeformed (K) state which, upon deformation to state (κ), takes the form of an ellipse. Similarly, the ellipse in Fig. 8b corresponds to the distorted state (k^3) which is generated from the (κ^1) state in Fig. 2. The compensating plastic distortion may be viewed as that which returns the ellipse back into the circle. More generally, the ellipse may be generated from the circle either by a lattice or a plastic distortion. Conversely, the circle may be generated from the ellipse either by a lattice or a plastic distortion. If the distortion involves the lattice, the coordinates are dragged, whereas if it is plastic, the metric tensor is dragged.

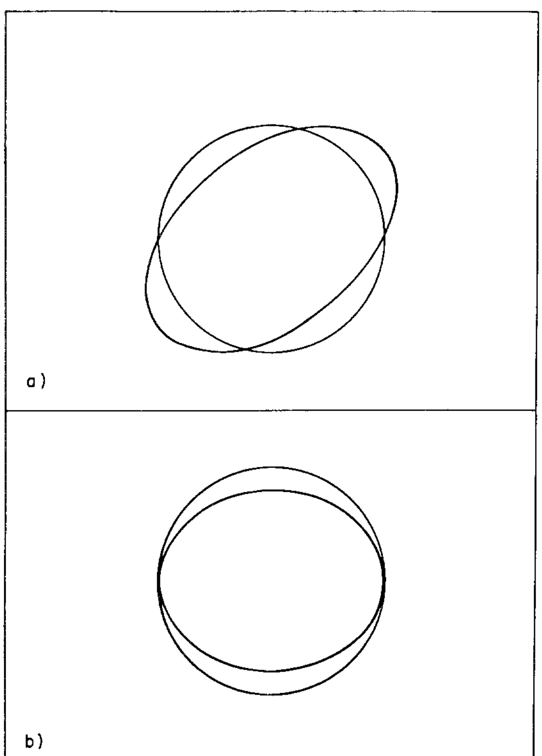

Figure 8 Alternative method of depicting lattice and plastic distortions shown in (a) Figs. 1a, b, c and (b) Figs. 2a, b.

We are now in a position to write a generalized distortion tensor associated with a phase transformation. In particular,

$$A_{K}^{k} = \{\underset{1}{A}_{K}^{k} H(-x^{K})\}_1 + \{\underset{2}{A}_{K}^{k} H(+x^{K})\}_2 \qquad (78)$$

where x^K is measured from the two-phase interface taken as the origin, while $\underset{1}{A}_{K}^{k}$ and $\underset{2}{A}_{K}^{k}$ correspond to the distortions giving rise to the new phase and the surrounding matrix respectively. In view of these considerations. it is apparent that the theory of the martensite transformation [1] is, in fact, a theory in which $\underset{2}{A}_{K}^{k}$ in the above equation is δ_{K}^{k} while $\underset{1}{A}_{K}^{k}$ involves only non-diffusional distortions. This latter restriction means that volume changes involving dragging of the metric tensor, such as occurs in the $(\kappa^1) \rightarrow (k^3)$ transformation, are not allowed. Furthermore, the present formulation is basically a dislocation theory, in contrast to previous treatments [1, 2].

The dislocation density associated with a two-phase interface may be written as [8]

$$\alpha^{n^8 k^8} = -\epsilon^{n^8 l^8 m^8} S_{l^8 m^8}^{\cdot\cdot\, k^8} \qquad (79)$$

where $\epsilon^{n^8 l^8 m^8}$ is the permutation tensor defined by

$$\epsilon^{n^8 l^8 m^8} = e^{n^8 l^8 m^8}/\sqrt{g} \qquad (80)$$

and where $e^{n^8 l^8 m^8}$ are the permutation symbols while g is the determinant of the metric tensor $g_{k^8 l^8}$. Since, for the (k^8) state,

$$\underset{k^8}{S}_{12}^{\cdot\cdot 1} = \tfrac{1}{2} \tan\theta\, \delta(x^1) \qquad (81)$$

it follows that

$$\underset{k^8}{\alpha}^{31} = \delta(x^1) \tan\theta \qquad (82a)$$

which in terms of Fig. 5b may be written as

$$\underset{k^8}{\alpha}^{31} = \frac{\Delta x^1_{2'-1'}}{\Delta x^2_{5-5'}} \qquad (82b)$$

For the (k^{10}) state Equations 79 and 74 yield

$$\underset{k^{10}}{\alpha}^{32} = \{\frac{1}{V}\, \delta(x^1)\}_1 + \{-\delta(x^1)\}_2 \qquad (83a)$$

which in terms of Fig. 6b is,

$$\underset{k^{10}}{\alpha^{32}} = \left(\frac{1-V}{V}\right)\delta(x^1) = (\tfrac{1}{4})\delta(x^1) \equiv \frac{\underset{1'-4'}{\Delta x^2}}{\underset{1-1'}{\Delta x^2}} \tag{83b}$$

A free surface density tensor can also be written as

$$\alpha^{n^9 k^9} = \epsilon^{n^9 1^9 m^9}\,\Omega_{\dot{1}^9 \dot{m}^9}{}^{k^9} \tag{84}$$

With the aid of Equation 73 this yields

$$\underset{k^9}{\alpha^{32}} = \underset{k^{10}}{\alpha^{32}} \tag{85}$$

The foundations are thus laid for a complete geometrical theory of phase transformations in solids.

5. Summary and conclusions

The methods of differential geometry have been applied to the analysis of phase transformations in solids. In particular such tensor quantities as distortion, metric, strain, torsion, dislocation density, Burgers vector, and anholonomic object have been developed for such transformations. It is further shown that the interfaces separating the transformed and untransformed regions can be described in terms of a well-defined dislocation array. The present theory applies to all types of transformations and connects the classical, i.e., Reimannian geometries, with the dislocation, i.e., non-Reimannian geometries.

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