Archives of Mechanics • Archiwum Mechaniki Stosowanej • 25, 6, pp. 911-922, Warszawa 1973

Foundations of the theory of disclinations

R. W. LARDNER (BURNABY)

THE THEORY of continuous distributions of disclinations in non-linear elastic solids is derived. It is shown that the spatial strain tensor and the coefficients of connection are well defined state quantities, and the relationships between these quantities and the densities of dislocations and disclinations are obtained. For a linear elastic material, an expression is given for the stresses produced in an infinite medium by an arbitrary distribution of these two kinds of defects.

W pracy wyprowadzono teorię ciągłych rozkładów dysklinacji w ośrodkach stałych nieliniowo-sprężystych. Wykazano, że przestrzenny tensor odkształcenia oraz współczynniki koneksji są dobrze określonymi wielkościami stanu; wyprowadzono ponadto związki między tymi wielkościami oraz gęstościami dyslokacji i dysklinacji. Dla materiału liniowo-sprężystego podano wzory na naprężenia wywołane w ośrodku nieograniczonym przez dowolne rozkłady tych dwóch rodzajów defektów.

Предлагается теория континуального распределения дисклинаций в нелинейных упругих средах. Показано, что пространственный тензор деформаций и коэффициенты связности являются хорошо определенными параметрами состояния. Выведены соотношения, связывающие эти величины с плотностями дислокаций и дисклинаций. Получена формула для напряжений в неограниченном линейно-упругом теле, вызванных произвольным распределением в пространстве дефектов одного и другого рода.

1. Introduction

THERE has recently been some discussion and a certain amount of controversy relating to the theory of disclinations (i.e. rotation dislocations), particularly by MURA [1] and de WIT [2]. One point at issue is whether, in a body containing disclinations, it is permissible to use quantities such as the elastic and plastic distortion tensors. In this paper we shall give a foundation for the theory of disclinations based on nonlinear continuum mechanics which will, we hope, provide an answer to this and other questions. The main discussion will be applicable to both linear and non-linear elastic materials, although in the last two sections of the paper we shall specialize to the linear theory to obtain certain further results.

We shall show that, for any material containing disclinations, the fundamental quantities which remain well-defined are the elastic strain tensor and the coefficients of connection, introduced for the theory of dislocations by KONDO [3] and BILBY, BULLOUGH and SMITH [4]. The usual relationship is found between the dislocation density and this connection, while its curvature tensor is shown to be essentially the same as the density of disclinations. In the special case of linear materials, this allows us to relate the incompatibility of the elastic strain tensor to the two defect densities. In the final section of the paper we shall derive the stress and strain fields produced by arbitrary distributions of dislocations and disclinations, obtaining results which have previously been derived [1, 2] by other methods. One feature of the derivation presented here is that no use is made of such redundant quantities as "total displacement field" and "plastic strain".

2. Elastic strain tensor

Consider an elastic body containing dislocations and disclinations, whose particles occupy positions $\mathbf{x}$ in space with components (x_1, x_2, x_3) with respect to some Cartesian frame. Usually in continuum mechanics a second state of the body, called a reference configuration, is introduced, and the current configuration is viewed as a distortion from the reference configuration. In particular, for homogeneous elastic solids, the theory becomes considerably simplified if we choose as reference configuration the natural state of the body — that is the state in which the stresses vanish identically. However, if the body contains dislocations or disclinations, this becomes impossible, since no configuration of the whole body exists for which the stresses are zero.

In order to overcome this problem, NOLL and TRUESDELL [5] construct what they term a local reference configuration in the following way. Let $\mathbf{x}_0$ be any particle of the body and $N(\mathbf{x}_0)$ a small neighbourhood of that particle. If $N(\mathbf{x}_0)$ were to be cut out of the body and the stresses in it allowed to relax, then this small element would assume its natural state. Such a configuration, which can be found for each sufficiently small neighbourhood of the body, is called the local reference configuration (LRC) of $N(\mathbf{x}_0)$. The LRC's of all the elements of the body cannot of course be joined continuously together to give a reference configuration for the whole body.

We shall denote the position which the particle $\mathbf{x}$ in $N(\mathbf{x}_0)$ occupies in the LRC of that neighbourhood by $\boldsymbol{\xi}$ with components (ξ_k). We can then construct the deformation gradients between these two configurations, which we denote by $\mathbf{M}$ and $\mathbf{m}$, with components

$$M_{ki} = \frac{\partial x_i}{\partial \xi_k}, \quad m_{jk} = \frac{\partial \xi_k}{\partial x_j}, \tag{2.1}$$

where

$$m_{ik} M_{kj} = M_{jk} m_{ki} = \delta_{ij}. \tag{2.2}$$

In the usual way we construct the two Cauchy-Green tensors, defined by $\mathbf{B} = \mathbf{M}\mathbf{M}^t$ and $\mathbf{C} = \mathbf{M}^t\mathbf{M}$, where $\mathbf{M}^t$ denotes the transpose of $\mathbf{M}$. In terms of these, the spatial strain tensor $\mathbf{e}$ and the material strain tensor $\mathbf{E}$ are defined by writing $\mathbf{B} = \mathbf{I}+2\mathbf{E}$ and $\mathbf{C}^{-1} = \mathbf{I}-2\mathbf{e}$. In terms of components therefore

$$E_{ik} = \frac{1}{2}\{M_{il} M_{kl} - \delta_{ik}\}, \quad e_{ik} = \frac{1}{2}\{\delta_{ik} - m_{il} m_{kl}\}. \tag{2.3}$$

So far we have been concerned with the LRC of each neighbourhood $N(\mathbf{x}_0)$ of the body considered separately, and we would like to impose some connection between these configurations for different neighbourhoods. First of all, let $N(\mathbf{x}_0)$ and $N(\mathbf{x}_1)$ be two neighbourhoods which overlap, and let $\mathcal{I}$ denote their intersection. Then the particles in $\mathcal{I}$ will in general have two LRC's, one coming from $N(\mathbf{x}_0)$ and one from $N(\mathbf{x}_1)$. However, if we suppose that the natural state of the material is unique apart from orientation in space, it follows that the two LRC's of $\mathcal{I}$ differ only by a rigid rotation. Consequently, by rotating the LRC of one of the neighbourhoods, say $N(\mathbf{x}_1)$, we can arrange that the two LRC's coincide in the overlap region.

Now suppose that $N(\mathbf{x}_0)$ and $N(\mathbf{x}_1)$ do not overlap. In this case we construct a path from $\mathbf{x}_0$ to $\mathbf{x}_1$ in the body and choose a sequence of points $\mathbf{y}_1 = \mathbf{x}_0, \mathbf{y}_2, \ldots, \mathbf{y}_n = \mathbf{x}_1$ on the path with neighbourhoods $N(\mathbf{y}_1), N(\mathbf{y}_2) \ldots N(\mathbf{y}_n)$ such that each neighbourhood overlaps the previous one in the sequence. Then the orientation of the LRC of each neighbourhood of the sequence is fixed in turn in such a way that it coincides with the LRC of the previous neighbourhood in the overlap region. By means of this construction, a continuous local reference configuration is found for the whole path from $\mathbf{x}_0$ to $\mathbf{x}_1$, and in particular a connection is established between the LRC's of $N(\mathbf{x}_0)$ and $N(\mathbf{x}_1)$.

A natural question now arises. Suppose that we choose a complete circuit $\mathscr{C}$, starting and finishing at $\mathbf{x}_0$, and suppose we construct a continuous LRC in the above manner for the whole path $\mathscr{C}$, will we end up with the same LRC for $N(\mathbf{x}_0)$ as the one we started out with? The answer to this is negative if the material contains disclinations: after completing the circuit, the LRC of $N(\mathbf{x}_0)$ will be rotated with respect to its original orientation.

Let $\mathbf{dx}$ be a small material element at $\mathbf{x}_0$ which corresponds to an element $\mathbf{d\xi}$ with components $(d\xi_k)$ in the original LRC of $N(\mathbf{x}_0)$. After continuing round $\mathscr{C}$, $\mathbf{dx}$ corresponds to an element $(d\xi'_k)$, say, where

$$d\xi'_k = R_{kl}(\mathscr{C})d\xi_l.$$

$R_{kl}(\mathscr{C})$ are the components of an orthogonal matrix which measures the rotation of LRC's corresponding to $\mathscr{C}$. This matrix is directly related to the number of disclination lines threading $\mathscr{C}$ and, as we shall see later, provides a definition of disclination density.

From (2.1) we see that the deformation gradients $\mathbf{M}$ and $\mathbf{m}$ are changed to

$$M'_{ki} = \frac{\partial x_i}{\partial \xi'_k} = R_{kl}(\mathscr{C})M_{li}, \qquad m'_{jk} = \frac{\partial \xi'_k}{\partial x_j} = m_{jl}R_{lk}(\mathscr{C}). \tag{2.4}$$

It follows from (2.3) therefore, since $R_{kl}(\mathscr{C})$ is orthogonal, that the spatial strain tensor is unchanged: $e'_{ik} = e_{ik}$. Thus we have the very important result that, even in a body containing disclinations, the spatial strain tensor is a uniquely defined quantity. Clearly from (2.4), the elastic deformation gradients are not uniquely defined in such a material. For a linear material, this means that the elastic distortion is not well-defined. We see also from (2.3) that the material strain tensor changes and is therefore not a well-defined quantity.

3. Coefficients of connection

Let $\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3\}$ be the orthonormal basis for the Cartesian coordinates (x_i), and let us define a triad of vectors $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ at $\mathbf{x}$ as

$$\mathbf{e}_k = M_{kp}\,\mathbf{u}_p. \tag{3.1}$$

This triad forms a basis, since we always assume the deformation gradients (2.1) to be non-singular. Initially $\{\mathbf{e}_k\}$ can be constructed via (3.1) only for the single neighbourhood $N(\mathbf{x})$. However, using the construction in Sec. 2 of a continuous LRC for a neighbourhood of any simple curve through $\mathbf{x}$, we can define $\{\mathbf{e}_k\}$ at all points along such a curve. Let

$\mathbf{x}+\mathbf{dx}$ be a neighbouring point on the curve under consideration. We set $\mathbf{de}_k = \mathbf{e}_k(\mathbf{x}+ +\mathbf{dx})-\mathbf{e}_k(\mathbf{x})$. Then, since $\{\mathbf{e}_k(\mathbf{x})\}$ is a basis, we may expand

$$\mathbf{de}_k = J_{klm}\ \mathbf{e}_l(\mathbf{x})\,dx_m,$$

where J_{klm} are certain coefficients. Substituting from (3.1), therefore,

$$dM_{kp} = J_{klm} M_{lp} dx_m. \tag{3.2}$$

We have seen in (2.4) that the gradients M_{kp} cannot be globally defined when disclinations are present. These quantities are only defined along paths in the body, and the differential equations (3.2) may only be integrated along paths. If, however, the body contains no disclinations, (3.2) may be integrated to give a single field M_{kp}, and using (2.2) we have that

$$J_{klm} = \frac{\partial M_{kp}}{\partial x_m} m_{pl}. \tag{3.3}$$

It is possible to define a linear connection or parallelism along any simple curve $\mathscr{C}$ in the body in the following way. Let the triad $\{\mathbf{e}_k(\mathbf{x})\}$ be constructed at each point of $\mathscr{C}$. Let $\mathbf{v} = v_l \mathbf{u}_l$ and $\mathbf{v}' = v'_l \mathbf{u}_l$ be two vectors at points $\mathbf{x}$ and $\mathbf{x}'$ of $\mathscr{C}$, respectively. Then we say that $\mathbf{v}$ and $\mathbf{v}'$ are "parallel" if they have the same components with respect to the triads $\{\mathbf{e}_k(\mathbf{x})\}$ and $\{\mathbf{e}_k(\mathbf{x}')\}$, i.e. if $\mathbf{v} = w_l \mathbf{e}_l(x)$ and $\mathbf{v}' = w_l \mathbf{e}_l(\mathbf{x}')$, for some set of coefficients $\{w_l\}$. Using (2.2) and (3.1), the condition of parallelism becomes that

$$v'_l = v_k M_{pl}(\mathbf{x}') m_{kp}(\mathbf{x}).$$

Now, taking $\mathbf{x}' = \mathbf{x}+\mathbf{dx}$ and writing $v'_l - v_l = dv_l$, this takes the form (to first order)

$$dv_l = -L_{ljm} v_j dx_m, \tag{3.4}$$

where

$$L_{ljm} = -m_{jk} J_{kpm} M_{pl}. \tag{3.5}$$

Equation (3.4) is the usual form for a linear connection, and the quantities L_{ljm} are called the coefficients of the connection.

When there are no disclinations present, substitution from (3.3) gives

$$L_{ljm} = -m_{jk}\frac{\partial M_{kl}}{\partial x_m},$$

which is the familiar form for the connection found in the theory of dislocations [4].

It is apparent from (3.2) that the coefficients J_{klm} cannot be uniquely determined throughout the body. If after completing a closed circuit in the body, M_{ki} become changed to $M'_{ki} = R_{kl} M_{li}$, then from (3.2) it follows that J_{klm} become changed to J'_{klm}, where $J'_{klm} = R_{kp} R_{ln} J_{pnm}$. However, from (3.5) it is easily seen that $L'_{ljm} = -m'_{jk} J'_{kpm} M'_{pl} = L_{ljm}$. This gives the second important result that the coefficients of the connection form a uniquely defined field throughout the body, even when disclinations are present. The significance of this result lies in the fact, as we shall show, that the dislocation and disclination densities are directly related to these coefficients.

From (2.3) we obtain that

$$(3.6)\qquad \frac{\partial e_{ik}}{\partial x_m}dx_m = -\frac{1}{2}\{dm_{il}m_{kl}+m_{il}dm_{kl}\}$$

$$= \frac{1}{2}\{m_{ip}J_{plm}m_{kl}+m_{il}m_{kp}J_{plm}\}dx_m = -\frac{1}{2}\{L'_{ikm}+L'_{kim}\}dx_m,$$

where

$$L'_{ikm} = L_{jkm}[\delta_{ij}-2e_{ij}].$$

In the second step here we have used the fact that

$$(3.7)\qquad dm_{il} = -m_{ik}J_{klm}dx_m,$$

which may easily be derived from (2.2) and (3.2). In the third step we have used (2.3) and (3.5). From (3.6) it follows therefore that

$$(3.8)\qquad L'_{ikm}+L'_{kim} = -2\frac{\partial e_{ik}}{\partial x_m}.$$

Let us introduce the following definitions

$$(3.9)\qquad e_{kij} = \frac{1}{2}\left\{\frac{\partial e_{jk}}{\partial x_i}+\frac{\partial e_{ik}}{\partial x_j}-\frac{\partial e_{ij}}{\partial x_k}\right\},$$

$$(3.10)\qquad T_{jlm} = \frac{1}{2}\{L_{jlm}-L_{jml}\},\qquad T'_{ikm} = T_{jkm}[\delta_{ij}-2e_{ij}].$$

The quantities e_{kij} are the Christoffel symbols derived from the strain tensor, while T_{jlm} is the torsion tensor associated with the connection L_{jlm}. Now, let us rotate the indices in (3.8) cyclically to obtain two further equations, add one of these to (3.8) and subtract the other. The result is easily seen to be that

$$(3.11)\qquad L'_{kij} = 2e_{kij}+T'_{kij}+T'_{ijk}-T'_{jki}.$$

We shall make use of this result in Sec. 5. Let us simply remark here that it shows that the strain and the coefficients of connection may not be specified independently. Once e_{ik} and the torsion are given — the second of these being simply the antisymmetric part of the connection — then the complete connection may be determined from (3.11).

4. Defect density tensors

Let $\mathscr{C}$ be a closed circuit in the body, starting and finishing at the spatial point **x**, and let us construct a continuous local reference configuration for the points of $\mathscr{C}$. As we have seen, upon completing the circuit, the orientation of the reference configuration of $N(\mathbf{x})$ is rotated from its original orientation if $\mathscr{C}$ encloses any disclinations. In addition, the curve $\mathscr{C}$ in its local reference configuration (i.e. the curve consisting of the same material particles as $\mathscr{C}$) will not in general be a closed curve. We may use the closure failure of $\mathscr{C}$ in its LRC to define the dislocation density tensor in the usual way. (In this context, $\mathscr{C}$ will be called a Burgers circuit.)

The closure failure of $\mathscr{C}$ is caused both by dislocations and disclinations. However, if $\mathscr{C}$ is of infinitesimal dimension l, the dislocation contribution to the closure failure is of order l^2, proportional to the area of surface spanned by $\mathscr{C}$, while the disclination contribution is of order l^3. The additional factor l arises since the displacement discontinuity induced by a disclination is proportional to distance from the disclination line. Thus in the limit as $\mathscr{C}$ shrinks to zero, the closure failure to leading order of magnitude is produced entirely by dislocations.

For simplicity, we take $\mathscr{C}$ to be an infinitesimal parallelogram $ABCDA$, where A is $\mathbf{x}$, B is $\mathbf{x}+\mathbf{dx}^{(1)}$, C is $\mathbf{x}+\mathbf{dx}^{(1)}+\mathbf{dx}^{(2)}$ and D is $\mathbf{x}+\mathbf{dx}^{(2)}$. In the LRC, $\overrightarrow{AB} = dx_k^{(1)}\mathbf{u}_k$ becomes an element $d\xi_l^{(1)}\mathbf{u}_l = dx_k^{(1)}m_{kl}(\mathbf{x})\mathbf{u}_l$. Similarly $\overrightarrow{BC}$ becomes an element

$$dx_k^{(2)}m_{kl}(\mathbf{x}+\mathbf{dx}^{(1)})\mathbf{u}_l = dx_k^{(2)}[m_{kl}(\mathbf{x})-m_{kn}(\mathbf{x})J_{nlm}dx_m^{(1)}]\mathbf{u}_l,$$

where we have used (3.7) in writing this second step. Similar expressions are obtained for the elements in the LRC corresponding to $\overrightarrow{AD}$ and $\overrightarrow{DC}$. The difference between the two legs $\overrightarrow{ABC}$ and $\overrightarrow{ADC}$ in the LRC gives the closure failure in the reference configuration,

$$\mathbf{B} \equiv -[\overrightarrow{ABC}-\overrightarrow{ADC}]_{(\mathrm{LRC})} = -m_{kn}J_{nlm}(dx_k^{(1)}dx_m^{(2)}-dx_m^{(1)}dx_k^{(2)})\mathbf{u}_l. \tag{4.1}$$

This quantity is often termed the true Burgers vector of the circuit. The minus sign is a matter of convention.

Setting $\mathbf{n}dS = \mathbf{dx}^{(1)}\wedge\mathbf{dx}^{(2)}$ as the vector element of area, we have

$$\mathbf{B} = -\varepsilon_{kmj}m_{kn}J_{nlm}n_j dS\mathbf{u}_l.$$

The element of material in the current configuration which corresponds to $\mathbf{B}$ in the LRC is usually called simply the Burgers vector of the circuit, and is given by

$$\mathbf{b} = -\varepsilon_{kmj}m_{kn}J_{nlm}n_j dS\, M_{lp}\mathbf{u}_p = \varepsilon_{kmj}L_{pkm}n_j dS\mathbf{u}_p.$$

The dislocation density tensor a_{pj} is defined by setting

$$\mathbf{b} = a_{pj}n_j dS\mathbf{u}_p, \tag{4.2}$$

so that

$$a_{pj} = L_{pkm}\varepsilon_{kmj} = T_{pkm}\varepsilon_{kmj}$$

after using the definition (3.10) of the torsion. This result reproduces the familiar relationship between torsion and dislocation density which is found when disclinations are absent [3, 4]. It may be inverted to read

$$T_{pkm} = \frac{1}{2}a_{pj}\varepsilon_{jkm}. \tag{4.3}$$

Let $\mathscr{C}$ again be a closed curve in the body, starting and finishing at $\mathbf{x}$ and let $\mathbf{v}$ be any vector at $\mathbf{x}$. We can construct a corresponding vector at each point around $\mathscr{C}$ by parallel displacement of $\mathbf{v}$, using the connection (3.4). When we arrive at $\mathbf{x}$ again, after parallel displacement all around $\mathscr{C}$, the resulting final vector will be $\mathbf{v}'$, say, in general different from $\mathbf{v}$. If $\mathscr{C}$ is the above parallelogram, we have in fact the following well-known formula for the difference between $\mathbf{v}$ and $\mathbf{v}'$:

$$v'_l = v_l - L_{lnim}v_n dx_i^{(1)}dx_m^{(2)}, \tag{4.4}$$

where

$$L_{lnim} = \frac{\partial L_{lnm}}{\partial x_i} - \frac{\partial L_{lni}}{\partial x_m} + L_{lji} L_{jnm} - L_{ljm} L_{jni}. \tag{4.5}$$

These quantities form the components of the Riemann-Christoffel curvature tensor belonging to the connection (3.5).

Now let $\mathbf{v}$ be one of the vectors $\{\mathbf{e}_k\}$, so that $v_l = M_{kl}$. From (4.4) therefore

$$M'_{kl} = M_{kl} - L_{lnim} M_{kn} dx_i^{(1)} dx_m^{(2)}.$$

But the change in M_{kl} on completing any circuit is given by (2.4), and comparing these two gives the following expression for the amount of rotation associated with the parallelogram circuit:

$$R_{kq}(\mathscr{C}) = M_{kn}[\delta_{ln} - L_{lnim} dx_i^{(1)} dx_m^{(2)}] m_{lq}.$$

It is clear from the definition (4.5) that L_{lnim} is antisymmetric between the pair of indices (i, m), so that we may replace $dx_i^{(1)} dx_m^{(2)}$ in this expression in favour of the element of area $n_q dS = \varepsilon_{qim} dx_i^{(1)} dx_m^{(2)}$, to obtain that

$$m_{nk} R_{kq}(\mathscr{C}) M_{ql} = \delta_{ln} - \frac{1}{2} \varepsilon_{imq} L_{lnim} n_q dS.$$

Let the infinitesimal rotation $R_{kq}(\mathscr{C})$ correspond to a small angular rotation vector $\omega_j(\mathscr{C})$. Then $R_{kq}\mathscr{C}) = \delta_{kq} + \varepsilon_{kqj} \omega_j(\mathscr{C})$. Therefore we have that

$$m_{lk} \varepsilon_{kqj} M_{ql} \omega_j(\mathscr{C}) = -\frac{1}{2} \varepsilon_{imq} L_{lnim} n_q dS.$$

We now use the left-hand side of this equation to define the density of disclination tensor d_{lnq} in the following way (see Sec. 5 for a discussion of this definition):

$$m_{nk} \varepsilon_{kqj} M_{ql} \omega_j(\mathscr{C}) = d_{lnq} n_q dS. \tag{4.6}$$

Thus finally the density of disclinations is connected with the curvature by the following equivalent equations,

$$d_{lnq} = -\frac{1}{2} \varepsilon_{imq} L_{lnim}, \qquad L_{lnim} = -d_{lnq} \varepsilon_{qim}. \tag{4.7}$$

Equation (3.11) expresses the coefficients L_{lnm} in terms of the strain tensor and dislocation density, after noting from (4.3) that the torsion may be written in terms of dislocation density. Substituing this expression into (4.5) and the result into (4.7) then gives a relation between the strain tensor and the two densities of dislocations and disclinations. For a non-linear medium with large strains, this relation is very complicated when expanded in full. For this reason, we shall in the next section consider the case of small strains, for which the curvature condition (4.7) takes on a very transparent form.

5. Infinitesimal strains

Let us now assume that the strain tensor e_{kl} and the densities of dislocations and disclinations, a_{jm} and d_{lnq} , are all small, and let us keep only terms of first order in these quantities. The torsion tensor is also small, and therefore, from (3.11), so are the connection coefficients. To first order we may set $L'_{kij} = L_{kij}$ and $T'_{kij} = T_{kij}$, so that (3.11) becomes

$$(5.1)\qquad L_{kij} = 2e_{kij}+\frac{1}{2}(a_{kp}\varepsilon_{pjk}+a_{ip}\varepsilon_{pjk}-a_{jp}\varepsilon_{pki}$$
$$= \varepsilon_{kiq}\left[-a_{jq}+\frac{1}{2}a\delta_{jq}+\varepsilon_{nrq}\frac{\partial e_{jr}}{\partial x_n}\right]-\frac{\partial e_{ik}}{\partial x_j},$$

after substituting from (4.3) and manipulating the permutation symbols. Here $a = a_{pp}$.

In this approximation, from (4.5),

$$L_{lnim} = \frac{\partial L_{lnm}}{\partial x_i} - \frac{\partial L_{lni}}{\partial x_m}.$$

Upon substituting from (5.1), the final term in this equation will not make any contribution to the curvature tensor. Because of the factor ε_{kiq} therefore, L_{lnim} is antisymmetric between the pair of indices (ln) as well as between (im). Consequently it suffices to consider the related Einstein tensor

$$(5.2)\qquad L_{pq} = -\frac{1}{4}\varepsilon_{pln}\varepsilon_{qim}L_{lnim},$$

since this definition may be inverted to express the curvature in terms of L_{pq}:

$$(5.3)\qquad L_{lnim} = -\varepsilon_{lnp}\varepsilon_{imq}L_{pq}.$$

Combining (4.7) and (5.2) now gives

$$(5.4)\qquad L_{pq} = \frac{1}{2}\varepsilon_{pln}d_{lnq} = -\frac{1}{2}\varepsilon_{pln}\varepsilon_{qim}\frac{\partial L_{lnm}}{\partial x_i}$$
$$= \varepsilon_{qim}\frac{\partial a_{mp}}{\partial x_i}-\frac{1}{2}\varepsilon_{pqi}\frac{\partial a}{\partial x_i}-\varepsilon_{pkr}\varepsilon_{qim}\frac{\partial^2 e_{rm}}{\partial x_k\,\partial x_i}$$

after substituting from (5.1). It is most transparent if we separate this equation into symmetric and antisymmetric parts. For the latter, multiply by ε_{pqr} and contract over p, q. This result becomes

$$(5.5)\qquad \frac{\partial a_{rp}}{\partial x_p} = -\varepsilon_{rpq}L_{pq}.$$

For the symmetric part, we note that the second term on the right is antisymmetric in p and q, while the third term is symmetric, so that we have

$$(5.6)\qquad \varepsilon_{pkr}\varepsilon_{qim}\frac{\partial^2 e_{rm}}{\partial x_k\,\partial x_i} = \left[\varepsilon_{qim}\frac{\partial a_{mp}}{\partial x_i}-L_{pq}\right]^{(s)}.$$

Here, the (s) indicates symmetrization over the two free indices.

Equation (5.6) provides an equation for the incompatibility of the strain tensor in terms of the densities of dislocations and disclinations. In this context we note that for small strains the Einstein tensor is essentially equivalent to the density of disclinations, since from (4.7) and (5.3) we have that

$$(5.7)\qquad d_{lnq} = \varepsilon_{lnp}L_{pq},\qquad L_{pq} = \frac{1}{2}\varepsilon_{lnp}d_{lnq}.$$

Substituting from the second of these expressions into (5.5), this latter condition takes the simpler form

$$\frac{\partial a_{rp}}{\partial x_p} = d_{rpp}. \tag{5.8}$$

Here, we have used the fact that $d_{lnq} = -d_{nlq}$ for the small strain case. The left-hand side of this equation physically measures the rate per unit volume at which dislocation lines terminate within the material, so that this rate is given in terms of the disclination density by (5.8).

Finally, in this section let us return to the definition (4.4) of d_{lnq}. We can introduce the polar decomposition $\mathbf{m} = \mathbf{UQ}$ of the matrix $\mathbf{m} = (m_{kl})$, where $\mathbf{U}$ is a symmetric matrix and $\mathbf{Q}$ an orthogonal matrix. From (2.3) it follows that $\mathbf{U}^2 = 1-2\mathbf{e}$ and so to first order $\mathbf{U} \approx \mathbf{1}-\mathbf{e}$. Therefore from (2.2), to first order $\mathbf{M} \approx \mathbf{Q}^t(\mathbf{1}+\mathbf{e})$, where $\mathbf{M} = (M_{jk})$. If we substitute these expressions into the left-hand side of (4.6), we may drop the terms involving $\mathbf{e}$ to first order, and obtain that

$$d_{lnq} n_q dS = \varepsilon_{kqj} Q_{nk} Q_{lq} \omega_j(\mathscr{C}) = \varepsilon_{lnp} Q_{pj} \omega_j(\mathscr{C}).$$

In the last step we have used the orthogonality of $\mathbf{Q}$. We observe again that for small strains, d_{lnq} is antisymmetric in its first two indices.

The matrix $\mathbf{Q}$ measures the average rotation between the reference configuration and the material at the point $\mathbf{x}$ in question. Generally we shall choose the orientation of the reference configuration in such a way that at $\mathbf{x}$, $\mathbf{Q}$ reduces to the identity. (This can only be done for one point at a time, of course.) In this case

$$d_{lnq} n_q dS = \varepsilon_{lnp} \omega_p(\mathscr{C}). \tag{5.9}$$

Now let us consider a single dislocation-disclination line, Γ. Γ is a closed curve bounding an open surface S inside the body across which a displacement discontinuity has occurred. According to a theorem of Weingarten, this displacement discontinuity must be a rigid motion of the type

$$u_i^+(\mathbf{x}) - u_i^-(\mathbf{x}) = b_i + \varepsilon_{ijk} \Omega_j (x_k - x_k^0), \tag{5.10}$$

i.e. a translation b_i and a rotation Ω_j about $\mathbf{x}^0$. Now, if $\mathscr{C}$ is any Burgers circuit, the rotation $\omega_j(\mathscr{C})$ of the reference frames associated with $\mathscr{C}$ is zero unless $\mathscr{C}$ links Γ and is given by $\omega_j(\mathscr{C}) = -\Omega_j$ if $\mathscr{C}$ links Γ in the positive sense. (The sign convention here is indicated in Fig. 1: Γ is given a sense positive with respect to vectors pointing from the $+$side to the $-$side of S; and $\mathscr{C}$ is positive with respect to Γ.) This then gives, from (5.9),

$$d_{lnq}(\mathbf{x}) = -\varepsilon_{lnp} \Omega_p \oint_\Gamma \delta(\mathbf{x} - \boldsymbol{\xi}) d\xi_q,$$

where $\boldsymbol{\xi}$ is a point on Γ. From (5.7) therefore,

$$L_{pq}(\mathbf{x}) = -\Omega_p \oint_\Gamma \delta(\mathbf{x} - \boldsymbol{\xi}) d\xi_q. \tag{5.11}$$

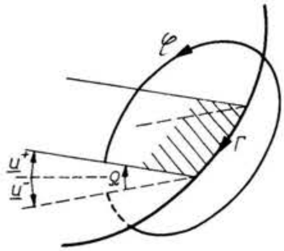

FIG. 1.

The Burgers vector of the circuit $\mathscr{C}$, as defined in (4.1) and the related discussion, is again zero unless $\mathscr{C}$ links Γ, and is given by the displacement discontinuity (5.10) at the point, where $\mathscr{C}$ crosses S in the event that $\mathscr{C}$ does link Γ. From (4.2) therefore, the dislocation density tensor is given by

$$a_{pj}(\mathbf{x}) = \oint_{\Gamma} [b_p + \varepsilon_{pqr}\Omega_q(x_r - x_r^0)]\delta(\mathbf{x}-\boldsymbol{\xi})d\xi_j. \tag{5.12}$$

It may be verified [2] that the two densities given by (5.11) and (5.12) satisfy the conservation equation (5.5).

6. Internal stresses

In this section we shall investigate the stress-field produced by a given distribution of dislocations and disclinations in a linear elastic medium. For the case of continuous distributions of these defects, we shall assume that the two density tensors a_{pj} and d_{lnq} (or equivalently L_{pq}) are specified. Denoting the stress tensor by σ_{ij}, we then have the equations,

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0, \quad \sigma_{ij} = c_{ijkl} e_{kl}, \tag{6.1}$$

where c_{ijkl} is the elastic modulus tensor. In addition, e_{ij} is related to the densities of dislocations and disclinations by the equations of Sec. 5.

It is convenient to introduce the following definition,

$$\lambda_{pm} = -\frac{1}{2}\varepsilon_{pln} L_{lnm}.$$

From (5.4) we then have that

$$L_{pq} = \varepsilon_{qim}\frac{\partial \lambda_{pm}}{\partial x_i}. \tag{6.2}$$

Furthermore, from (5.1) we obtain that

$$\lambda_{sj} = a_{js} - \frac{1}{2} a\delta_{js} + \varepsilon_{nrs}\frac{\partial e_{jr}}{\partial x_n}.$$

Contracting this equation over s and j gives that $\lambda = -\frac{1}{2}a$, where $\lambda = \lambda_{jj}$, and therefore

$$\varepsilon_{nrs}\frac{\partial e_{jr}}{\partial x_n} = \lambda_{sj} - \lambda\delta_{sj} - a_{js}. \tag{6.3}$$

The elastic Greens function $G_{kj}(\mathbf{x}-\mathbf{x}')$ for an infinite medium satisfies the differential equations

$$c_{ijkl}\frac{\partial^2}{\partial x_i \partial x_l} G_{km}(\mathbf{x}-\mathbf{x}') = \delta_{jm}\delta(\mathbf{x}-\mathbf{x}').$$

Therefore

$$\begin{aligned} e_{mr}(\mathbf{x}) &= \int c_{ijkl}\frac{\partial^2}{\partial x_i \partial x_l} G_{km}(\mathbf{x}-\mathbf{x}')e_{jr}(\mathbf{x}')dV' \\ &= \int c_{ijkl}\frac{\partial}{\partial x_l} G_{km}(\mathbf{x}-\mathbf{x}')\left[\frac{\partial e_{jr}(\mathbf{x}')}{\partial x_i'} - \frac{\partial e_{ji}(\mathbf{x}')}{\partial x_r'}\right]dV'. \end{aligned} \tag{6.4}$$

In obtaining this second form we have integrated by parts to switch $\partial/\partial x_i'$ from the Greens function to e_{jr}. The second term which has been introduced on the right vanishes identically, since another integration by parts switches $\partial/\partial x_l'$ over to act on e_{ji}, and, from(6.1) together with the symmetry properties of the modulus tensor it follows that $c_{ijkl}\frac{\partial e_{ji}(x')}{\partial x_l'} = 0$. Equation (6.4) may then be written as

$$\begin{aligned} e_{mr}(\mathbf{x}) &= -\int c_{ijkl}\frac{\partial}{\partial x_l} G_{km}(\mathbf{x}-\mathbf{x}')\varepsilon_{sri}\varepsilon_{nts}\frac{\partial e_{jt}(\mathbf{x}')}{\partial x_n'}dV' \\ &= -\int \varepsilon_{sri}c_{ijkl}\frac{\partial}{\partial x_l} G_{km}(\mathbf{x}-\mathbf{x}')\left[\lambda_{sj}(\mathbf{x}') - a_{js}(\mathbf{x}')\right]dV' \end{aligned} \tag{6.5}$$

after using (6.3). (Note that the term $\lambda\delta_{sj}$ gives a contribution which vanishes identically).

This result bears a strong resemblance to Eq. (W. 4.12) in de Wit's paper. The dislocation density terms in the two equations are in fact identical, since we have the relationship $a_{js} = \alpha_{sj}$ between our density tensor and de Wit's. The λ-term is not precisely the same as de Wit's second term, since λ_{sj} is not in general equal to the "plastic bend-twist tensor" $\varkappa_{js}^p$ which appears in de Wit's theory. However, equation (6.2) relating λ_{sj} to the density of disclinations is the same as de Wit's equation (W. 4.2) between $\varkappa_{js}^p$ and the quantity θ_{nh} which he terms the density of disclinations. (To be precise, θ_{nh} coincides with $-L_{hn}$.) This fact enables us to apply exactly the argument of de Wit's paper leading from his Eq. (W. 4.12) to (W. 4.15), and to obtain therefore that

$$e_{mr}(\mathbf{x}) = \left\{\int \varepsilon_{sri}c_{ijkl}\frac{\partial}{\partial x_l} G_{km}(\mathbf{x}-\mathbf{x}')a_{js}(\mathbf{x}')dV' - \int I_{mrbs}(\mathbf{x}-\mathbf{x}')L_{sb}(\mathbf{x}')dV'\right\}^{(s)}, \tag{6.6}$$

where

$$I_{mrbs}(\mathbf{x}) = \int \varepsilon_{abi}\varepsilon_{srj}c_{ijkl}\frac{\partial^2 G_{km}(\mathbf{x}')}{\partial x_l' \partial x_a'}\frac{dV'}{4\pi|\mathbf{x}-\mathbf{x}'|}.$$

In (6.6), the symbol (s) denotes that the two terms on the right must be symmetrized with respect to the two free indices. [This symmetrization is not necessary in (6.5).]

The result (6.6) can now be used to find the stress and strain fields caused by a single dislocation-disclination loop by substituting (5.11) and (5.12) for the two density tensors. Since (5.11) coincides with de Wit's equation (W. 5.23) and (5.12) with his (W. 5.21), the result so obtained will simply reproduce that given in de Wit's paper, which in turn coincides with Mura's result [1].

Finally, we should like to comment on the formalism used by de Wit in deriving his result (W. 4.12) corresponding to (6.5). The basis of this approach is the introduction of a displacement field u_i between the current configuration and some arbitrary reference configuration. A corresponding plastic strain, e^p_{ij} is introduced through the definition: $\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right) = e_{ij}+e^p_{ij}$. Since the reference configuration for the displacement is arbitrary, it is clear that neither u_i nor e^p_{ij} can enter any expressions relating, say, the stress field and the defect densities. This has turned out to be the case in Eq. (6.6), and an interesting feature of this equation is that it has been derived here without introducing the redundant concepts of a displacement field and a plastic strain.

References

1. T. MURA, Arch. Mech. Stos., **24**, 449, 1972.
2. R. de WIT, Arch. Mech. Stos., **24**, 499, 1972.
3. K. KONDO, Proc. 2nd. Japan Congr. Appl. Mechs. (Science Council of Japan), p. 41.
4. B. A. BILBY, R. BULLOUGH, and E. SMITH, Proc. Roy. Soc. **A231**, 263, 1955.
5. C. TRUESDELL, and W. NOLL, Handbuch d. Physik III/3, Springer, 1965, Sections 34, 44.

MATHEMATICS DEPARTMENT
SIMON FRASER UNIVERSITY
BURNABY, B. C., CANADA

Received November 11, 1972.