Dimensional Changes in Crystals Caused by Dislocations

R. A. Toupin, R. S. Rivlin

Dimensional Changes in Crystals Caused by Dislocations

R. A. TOUPIN, *U. S. Naval Research Laboratory, Washington, D. C.*

AND

R. S. RIVLIN, *Brown University, Providence, Rhode Island*

According to the classical linear elasticity theory, if one or more dislocations are introduced into a body of elastic material, the average value of each of the infinitesimal strain components is zero; in particular, the change in volume is zero. This result seems not to be in accord with experimental data on cold worked metals. In this paper we use nonlinear elasticity theory to show how changes in the average dimensions of elastic bodies, either isotropic or anisotropic, resulting from the introduction of dislocations, can be calculated. In particular, we derive an explicit relation between the resultant change in volume, the stored energy, and the pressure derivatives of the elastic moduli.

1. INTRODUCTION

According to classical elasticity theory, if one or more dislocations are introduced into a body of elastic material, the average value of each of the infinitesimal strain components in a rectangular Cartesian coordinate system is zero. It follows that the change of volume is zero; that in a prism of the material the change of cross-sectional area and the average change of length are zero; that in a rectangular block the average changes in the dimensions parallel to the edges are zero. These results do not, of course, prove that the changes are in fact zero physically. They merely imply that the classical elasticity theory provides an inadequate basis for their calculation.

In the present paper we make use of the second-order elasticity theory to show how changes in the average dimensions of elastic bodies, either isotropic or anisotropic, caused by the introduction of dislocations, can be calculated when the displacement gradients produced by the dislocations are sufficiently small.

It is first shown in Sec. 2 that the average value of each of the stress components, in a rectangular Cartesian coordinate system, is zero. This result is then used, within the framework of the second-order theory, to obtain an expression for the average value of each of the infinitesimal strain components as the average value of an expression of second degree in the displacement gradients, which are associated with the dislocations in the body according to the classical theory. From these results, the dimensional changes can in principle be calculated in a number of cases. In Appendices 1 and 2, it is shown how these formulas may be specialized when the material considered has some particular symmetry, by illustrations from the isotropic case and from the case of cubic symmetry of the hextetrahedral, gyroidal, and hexoctahedral classes.

In Sec. 6 we considered the particular problem of the change in volume, resulting from the introduction of dislocations, of a cubic crystal of one of these classes. The formula derived can be easily specialized to the case when the material is isotropic and the result obtained is in agreement with that which Zener[1] obtained by a very different procedure.

Finally, in Sec. 7 we have employed our result for the cubic case to make certain qualitative predictions regarding the effect of dislocations on the volume of crystals of silver, gold, and copper.

2. AVERAGE STRESS

Consider an elastic body which in the undeformed state has the form shown schematically in Fig. 1. Let R_0 denote the region of space occupied by this body and let S_0 denote the complete boundary of R_0. Let the body be deformed in such a way that certain portions of S_0 are brought into contact with each other and bonded together as shown in Fig. 2, the external forces required to bring the surfaces together then being removed. The body is then in a state of deformation without external forces acting on it.

Let R denote the region occupied by the deformed body. Let S denote the external surface of the deformed

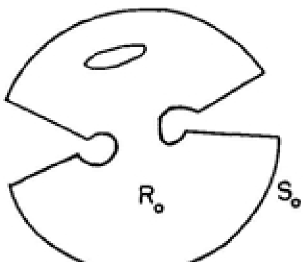

FIG. 1.

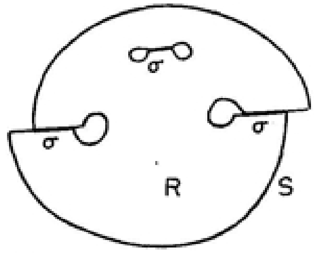

FIG. 2.

[1] C. Zener, Trans. Am. Inst. Mining Met. Engrs. 147, 361 (1942).

body and let σ denote the bonded surfaces in the deformed body, which we may call the *dislocation surfaces*. Then, the displacement and stress fields have discontinuities on σ, while the stress vector acting on σ is continuous across σ.

Let t_{ij} denote the stress components in a rectangular Cartesian coordinate system x at a point x_i of the deformed body. Since no external forces act on the body, we have*

$$\partial t_{ij}/\partial x_j=0 \quad \text{throughout } R, \tag{2.1}$$

and

$$t_{ij}n_j=0 \quad \text{on } S, \tag{2.2}$$

where n_i denotes the unit normal to S at the point considered.

Let $t_{ij}^{(1)}$ and $t_{ij}^{(2)}$ be the limiting values of the stress t_{ij} at a point of the dislocation surface σ as we approach it from its two sides, which we may call sides 1 and 2. Then, since the stress vector is continuous on σ,

$$(t_{ij}^{(2)}-t_{ij}^{(1)})n_j=0 \quad \text{on } \sigma, \tag{2.3}$$

where n_i is the unit vector to σ drawn in the sense from 2 to 1 (say).

We note that, if dV is an element of volume of the deformed body R and dS and $d\sigma$ are elements of area of the surfaces S and σ, using the divergence theorem and the relations (2.2) and (2.3), we have

$$\int_R \frac{\partial}{\partial x_j}(x_k t_{ij})dV=\int_S x_k t_{ij}n_j dS + \int_\sigma x_k(t_{ij}^{(2)}-t_{ij}^{(1)})n_j d\sigma=0. \tag{2.4}$$

We thus have, with (2.1),

$$\int_R \left(t_{ik}+x_k\frac{\partial t_{ij}}{\partial x_j}\right)dV=\int_R t_{ik}dV=0. \tag{2.5}$$

Equation (2.5) expresses the following theorem: *the average value of each of the stress components in a rectangular Cartesian coordinate system in a body, which is held in equilibrium without external forces being applied, is zero.*

We note that in deriving this result no assumption is made regarding the magnitude of the deformation, nor does the elastic nature of the material of the body enter explicitly.

3. SOME BASIC RESULTS IN SECOND-ORDER ELASTICITY THEORY

We consider a deformation of an elastic material, in which a generic particle initially at X_i in the rectangular Cartesian coordinate system x moves to x_i in the same coordinate system. If u_i are the components of the displacement for the particle, then

$$x_i=X_i+u_i. \tag{3.1}$$

The stored elastic energy W per unit of deformed volume, or strain-energy function, then depends on the displacement gradients $u_{i,j}$, and we shall assume that this dependence is polynomial. We use the notation $_{,j}$ to denote partial differentiation with respect to the coordinate X_j. The components of stress t_{ij} are given by

$$t_{ij}=\frac{1}{|\partial x/\partial X|}x_{j,k}\frac{\partial W}{\partial u_{i,k}}. \tag{3.2}$$

If dV and dV_0 denote corresponding elements of volume in the deformed and undeformed states, we have

$$dV/dV_0=|\partial x/\partial X|. \tag{3.3}$$

From (3.2), (3.3), and (2.5), we see that if a body of elastic material is held in a deformed state, without external forces, by the introduction of dislocations, then†

$$\int |\partial x/\partial X|t_{ij}dV_0=\int x_{j,k}\frac{\partial W}{\partial u_{i,k}}dV_0=0. \tag{3.4}$$

W may be expressed in the form,

$$W=W_1+W_2+W_3+\cdots, \tag{3.5}$$

where $W_1, W_2, W_3, \cdots$ are homogeneous polynomials of the first, second, third, $\cdots$ degrees in the displacement gradients. It can be shown that if the stress components are zero when the displacement gradients are zero, $W_1=0$. Then, if the displacement gradients are sufficiently small, $W=W_2$ provides a first approximation to the strain-energy function (that of classical elasticity theory) and $W=W_2+W_3$ provides a second approximation.

If we take $W=W_2$, we are neglecting in W terms of higher degree than the second in the displacement gradients. From (3.2) it is seen that this implies the neglect, in the expressions for the stress components, of terms of higher degree than the first in the displacement gradients. With this approximation, we obtain from (3.4),

$$\int(\partial W_2/\partial u_{i,j})dV_0=0. \tag{3.6}$$

If we take $W=W_2+W_3$, we are neglecting in W terms of higher degree than the third in the displacement gradients. This implies the neglect, in the expressions for the stress components, of terms of higher degree than the second in the displacement gradients. With this

* Here and throughout this paper, lower case Latin indices take the values 1, 2, 3 and the summation convention is applicable to them.

† Here and subsequently integrals with respect to V_0 are considered to be evaluated over the domain R_0.

approximation, we obtain from (3.4),

$$\int\left[\frac{\partial W_2}{\partial u_{i,j}}+u_{j,k}\frac{\partial W_2}{\partial u_{i,k}}+\frac{\partial W_3}{\partial u_{i,j}}\right]dV_0=0. \tag{3.7}$$

4. THE GENERAL ANISOTROPIC CASE

The strain-energy function W cannot have arbitrary dependence on the displacement gradients, but must depend on them through the components E_{ij} of the finite strain tensor defined by

$$E_{ij}=\tfrac{1}{2}(x_{k,i}x_{k,j}-\delta_{ij})=e_{ij}+\alpha_{ij}, \tag{4.1}$$

where

$$e_{ij}=\tfrac{1}{2}(u_{i,j}+u_{j,i}) \quad \text{and} \quad \alpha_{ij}=\tfrac{1}{2}u_{k,i}u_{k,j}. \tag{4.2}$$

e_{ij} are the components of infinitesimal strain of the classical linear elasticity theory, and it is noted that e_{ij} and α_{ij} are homogeneous of first and second degrees, respectively, in the displacement gradients.

By taking W to be a polynomial in the components E_{ij}, we may write

$$W=a_{ijkl}E_{ij}E_{kl}+b_{ijklmn}E_{ij}E_{kl}E_{mn}+\cdots, \tag{4.3}$$

where a_{ijkl} and b_{ijklmn} are constants. From (3.5), (4.1), and (4.3), we obtain

$$W_2=a_{ijkl}e_{ij}e_{kl}, \tag{4.4}$$

and

$$W_3=b_{ijklmn}e_{ij}e_{kl}e_{mn}+a_{ijkl}(e_{ij}\alpha_{kl}+e_{kl}\alpha_{ij}). \tag{4.5}$$

It is easily seen that in (4.4) we may, without loss of generality, take a_{ijkl} to be unaltered by permutation of i and j, of k and l and of ij and kl. Also, in (4.5), we may take b_{ijklmn} to be unaltered by permutation of i and j, of k and l, of m and n, and of ij, kl and mn. We may then write (4.4) as

$$W_2=a_{ijkl}u_{i,j}u_{k,l}, \tag{4.6}$$

and (4.5) as

$$\begin{aligned}W_3&=b_{ijklmn}e_{ij}e_{kl}e_{mn}+2a_{ijkl}e_{ij}\alpha_{kl}\\&=b_{ijklmn}u_{i,j}u_{k,l}u_{m,n}+a_{ijkl}u_{i,j}u_{m,k}u_{m,l}.\end{aligned} \tag{4.7}$$

By introducing (4.4) into (3.6), we obtain

$$a_{ijkl}\int e_{kl}dV_0=0. \tag{4.8}$$

By bearing in mind the symmetry of e_{kl} and of a_{ijkl}, we see that (4.8) represents six simultaneous equations in the six independent quantities $\int e_{kl}dV_0$. From these we readily obtain

$$\int e_{kl}dV_0=0. \tag{4.9}$$

Equations (4.8) and (4.9) are, of course, valid with the approximation that terms of second and higher degrees in the displacement gradients are neglected; i.e., they are valid within the framework of classical elasticity theory.

We obtain a second approximation to $\int e_{kl}dV_0$ from (4.6), (4.7), and (3.7). This yields

$$\begin{aligned}2a_{ijmn}\int e_{mn}dV_0=&-2\int(a_{ikmn}u_{j,k}+a_{jkmn}u_{i,k})u_{m,n}dV_0\\&-a_{ijmn}\int u_{k,m}u_{k,n}dV_0\\&-3b_{ijklmn}\int u_{k,l}u_{m,n}dV_0.\end{aligned} \tag{4.10}$$

This provides six independent equations for the determination of the six quantities $\int e_{mn}dV_0$. These can be calculated in the following manner. Let us denote the pairs of subscripts 11, 22, 33, 23 or 32, 31 or 13, 12 or 21 by 1, 2, 3, 4, 5, 6, respectively. We define the elastic compliances $s_{\alpha\beta}$ $(\alpha,\beta=1,2,\cdots,6)$ by‡

$$2s_{\alpha\beta}a_{\beta\gamma}=\delta_{\alpha\gamma}. \tag{4.11}$$

We therefore have

$$\int e_\alpha dV_0=2s_{\alpha\beta}a_{\beta\gamma}\int e_\gamma dV_0, \tag{4.12}$$

where $2a_{\beta\gamma}\int e_\gamma dV_0$ is given by (4.10). This expression can be used to calculate the average values of the changes in the dimensions of the material due to the introduction of dislocations. For example, suppose the body considered has the shape of a prism with its length parallel to the 1 axis. Then, if A_0 is the initial cross-sectional area of the prism, the average change in length is

$$\frac{1}{A_0}\int e_{11}dV_0=\frac{2}{A_0}s_{1\beta}a_{\beta\gamma}\int e_\gamma dV_0, \tag{4.13}$$

$2a_{\beta\gamma}\int e_\gamma dV_0$ being given by (4.10).

It follows immediately from the result given in Appendix 3 that the total change in volume $V-V_0$ undergone by the body as a result of the introduction of dislocations is given by

$$V-V_0=\int e_{kk}dV_0+\frac{1}{2}\int[(u_{k,k})^2-u_{p,q}u_{q,p}]dV_0, \tag{4.14}$$

with the neglect only of terms of higher degree than the second in the displacement gradients. Again, we may substitute from (4.12) and (4.10) for $\int e_{kk}dV_0$ to obtain an expression for the change in volume which is of the second degree in the displacement gradients.

Each of the expressions obtained from (4.12), (4.13), and (4.14) by substituting for $a_{\beta\gamma}\int e_\gamma dV_0$ from (4.10) is of the second degree in the displacement gradients resulting from the introduction of the dislocations according to the second-order elasticity theory for the

‡ Repetition of a Greek subscript indicates summation over the values 1, 2, $\cdots$, 6 for the subscript. This convention will be employed only in the present section.

material. However, to the order of approximation involved in the calculations, we may replace them by those calculated from the first-order theory for the material, and it is in this sense that we shall understand them.

5. EFFECT OF STRAIN ON THE ELASTIC MODULI

In the expression (3.2) for the stress components we take

$$W=W_2+W_3,$$

where W_2 and W_3 are homogeneous polynomials of the second and third degrees respectively in the displacement gradients. Then, neglecting terms of higher degree than the second in the displacement gradients, we obtain

$$t_{ij}=(1-u_{r,r})\frac{\partial W_2}{\partial u_{i,j}}+u_{j,k}\frac{\partial W_2}{\partial u_{i,k}}+\frac{\partial W_3}{\partial u_{i,j}}. \tag{5.1}$$

Now, let us suppose that the displacement field is increased by an infinitesimal displacement $\bar{u}_i$, and let us calculate the change $\bar{t}_{ij}$ in the stress associated with the new displacement field $u_i+\bar{u}_i$ on the assumption that terms of higher degree than the first in the displacement gradients $\bar{u}_{i,j}$ may be neglected. Then,

$$\bar{t}_{ij}=\frac{\partial t_{ij}}{\partial u_{p,q}}\bar{u}_{p,q}. \tag{5.2}$$

By introducing (5.1) into (5.2), we obtain

$$\begin{aligned}\bar{t}_{ij}=&-\frac{\partial W_2}{\partial u_{i,j}}\bar{u}_{p,p}+\frac{\partial W_2}{\partial u_{i,k}}\bar{u}_{j,k}\\&+\left\{(1-u_{r,r})\frac{\partial^2 W_2}{\partial u_{i,j}\partial u_{p,q}}+u_{j,k}\frac{\partial^2 W_2}{\partial u_{i,k}\partial u_{p,q}}\right.\\&\left.+\frac{\partial^2 W_3}{\partial u_{i,j}\partial u_{p,q}}\right\}\bar{u}_{p,q}.\end{aligned} \tag{5.3}$$

By introducing the expressions (4.6) and (4.7) for W_2 and W_3 into (5.3), we obtain

$$\begin{aligned}\bar{t}_{ij}=&-2a_{ijkl}u_{k,l}\bar{u}_{p,p}+2u_{m,n}(a_{ikmn}\bar{u}_{j,k}+a_{jkmn}\bar{u}_{i,k})\\&+2[3b_{pqijmn}u_{m,n}+(a_{pqil}u_{j,l}+a_{pqjl}u_{i,l})\\&+a_{ijql}u_{p,l}+(1-u_{r,r})a_{ijpq}]\bar{u}_{p,q}.\end{aligned} \tag{5.4}$$

This equation may be rewritten as

$$\bar{t}_{ij}=2(a_{ijrs}+c_{ijrs}^*)\bar{u}_{r,s}, \tag{5.5}$$

where

$$\begin{aligned}c_{ijrs}^*=&-a_{ijkl}u_{k,l}\delta_{rs}+u_{m,n}(a_{ismn}\delta_{jr}+a_{jsmn}\delta_{ir})\\&+(3b_{ijmnpq}u_{m,n}+a_{pqil}u_{j,l}+a_{pqjl}u_{i,l}\\&+a_{ijql}u_{p,l}-u_{r,r}a_{ijpq})\delta_{rp}\delta_{sq}.\end{aligned} \tag{5.6}$$

The relation (5.5) may be rewritten in the form

$$\bar{t}_{ij}=2(a_{ijrs}+c_{ijrs})\partial\bar{u}_r/\partial x_s, \tag{5.7}$$

where

$$c_{ijrs}=c_{ijrs}^*+a_{ijrm}u_{s,m}. \tag{5.8}$$

Then, $2(a_{ijrs}+c_{ijrs})$ are the elastic moduli for infinitesimal deformations of the material which is initially subjected to the displacements u_i. From (5.8) and (5.6), employing the notation

$$3\bar{b}_{pqijrs}=\partial c_{ijrs}/\partial u_{p,q}, \tag{5.9}$$

we obtain immediately

$$\begin{aligned}3\bar{b}_{pqijrs}=&-a_{ijpq}\delta_{rs}-a_{ijrs}\delta_{pq}+a_{ispq}\delta_{jr}\\&+a_{jspq}\delta_{ir}+a_{rsiq}\delta_{jp}+a_{rsjq}\delta_{ip}+a_{ijsq}\delta_{pr}\\&+a_{ijrq}\delta_{ps}+3b_{ijpqrs}.\end{aligned} \tag{5.10}$$

By substituting in (4.10) for $3b_{ijklmn}$ from (5.10), we obtain

$$\begin{aligned}2a_{ijmn}\int e_{mn}dV_0=&-2a_{ijkl}\int u_{m,m}u_{k,l}dV_0\\&+a_{ijmk}\int u_{n,k}u_{m,n}dV_0\\&-3\bar{b}_{pqijrs}\int u_{p,q}u_{r,s}dV_0.\end{aligned} \tag{5.11}$$

If the material has some symmetry, then we must express this fact by determining appropriate forms for a_{ijkl} and b_{ijpqrs}. The manner in which this may be done conveniently is illustrated in Appendices 1 and 2 for the cases when the material is isotropic and when it has cubic symmetry of the hextetrahedral, gyroidal, or hexoctahedral classes. In these appendices we also give the special forms taken, in these cases, by the expression (4.10) and the expression (5.4) for the stress corresponding to an infinitesimal strain superposed on an initial deformation.

Meanwhile, in the next section we shall determine the change of volume, caused by the introduction of dislocations, of cubic crystals of the hextetrahedral, gyroidal, or hexoctahedral classes. The result obtained could have been derived from the more general formalism given in Appendix 2. However, the method employed in Sec. 6 takes advantage of certain algebraic simplifications which are possible for this particular problem.

6. CHANGE OF VOLUME FOR CUBIC CRYSTALS (HEXTETRAHEDRAL, GYROIDAL, AND HEXOCTAHEDRAL CLASSES)

In this section we shall determine the change of volume, caused by the introduction of dislocations, in cubic crystals of the hextetrahedral, gyroidal, and hexoctahedral classes. Before doing so, however, we shall derive certain formulas, which are generally valid, from the results of Secs. 4 and 5.

From (4.10), we obtain, with (4.6),

$$2a_{iimn}\int e_{mn}dV_0=-4\int W_2dV_0-a_{iimn}\int u_{k,m}u_{k,n}dV_0$$
$$-3\bar{b}_{iiklmn}\int u_{k,l}u_{m,n}dV_0. \quad (6.1)$$

By bearing in mind that

$$3\bar{b}_{ijklmn}=\partial c_{klmn}/\partial u_{i,j}, \quad (6.2)$$

we obtain, from (5.10) and (4.6),

$$3b_{iiklmn}u_{k,l}u_{m,n}=3\bar{b}_{iiklmn}u_{k,l}u_{m,n}-W_2+a_{iikl}u_{k,l}u_{m,m}$$
$$-a_{iikn}u_{k,m}u_{m,n}-a_{iiln}u_{k,l}u_{k,n}. \quad (6.3)$$

By introducing (6.3) into (4.10), we obtain

$$2a_{iimn}\int e_{mn}dV_0=-3\int W_2dV_0$$
$$+a_{iikl}\int(u_{k,m}u_{m,l}-u_{k,l}u_{m,m})dV_0$$
$$-3\bar{b}_{iiklmn}\int u_{k,l}u_{m,n}dV_0. \quad (6.4)$$

We may obtain a convenient expression for $\bar{b}_{iiklmn}$ as the rate of change of c_{klmn} with volume, when the material is subjected to a uniform dilatation, in the following manner: We suppose that the fractional extensions undergone by the material in the uniform dilatation are β. Then taking $u_{i,j}=\beta\delta_{ij}$ in (5.6) and (5.8), we obtain

$$c_{ijrs}=\beta(-a_{ijpp}\delta_{rs}+a_{ispp}\delta_{jr}+a_{jspp}\delta_{ir}$$
$$+a_{ijrs}+3b_{ppijrs}). \quad (6.5)$$

By comparing (6.5) and (5.10), we obtain

$$3\bar{b}_{ppijrs}=\partial c_{ijrs}/\partial\beta=3(\partial c_{ijrs}/\partial v), \quad (6.6)$$

where v is the fractional increase of volume of the material in the uniform dilatation.

So far we have made no assumption regarding the symmetry of the material. For cubic crystals of the hextetrahedral, gyroidal, and hexoctahedral classes, it is shown in Appendix 2 that the elastic moduli $2a_{pqrs}$ must be expressible in the form,§

$$2a_{pqrs}=(a_1+2a_2)\delta_{pq}\delta_{rs}-\tfrac{1}{2}a_1(\delta_{sp}\delta_{rq}+\delta_{sq}\delta_{rp})$$
$$+2b_1\sum_{\alpha=1}^{3}\delta_{\alpha p}\delta_{\alpha q}\delta_{\alpha r}\delta_{\alpha s}. \quad (6.7)$$

§ The convention will be used that Greek subscripts take the values 1, 2, 3. The summation convention will not be applied to them.

By introducing this result into (6.4), we obtain

$$2(a_1+3a_2+b_1)\int e_{mm}dV_0$$
$$=-3\int W_2dV_0$$
$$-(a_1+3a_2+b_1)\int[(u_{m,m})^2-u_{m,n}u_{n,m}]dV_0$$
$$-3\bar{b}_{iiklmn}\int u_{k,l}u_{m,n}dV_0. \quad (6.8)$$

By using the result obtained in Appendix 3, we see that neglecting terms of higher degree than the second in the displacement gradients, the change in volume $V-V_0$ of the crystal due to the introduction of dislocations is given by

$$2(a_1+3a_2+b_1)(V-V_0)$$
$$=-3\int W_2dV_0-3\bar{b}_{iiklmn}\int u_{k,l}u_{m,n}dV_0. \quad (6.9)$$

We note that if the cubic crystal undergoes a uniform dilatation, it remains cubic and consequently the elastic moduli $2(a_{pqrs}+c_{pqrs})$ for infinitesimal deformations of this deformed crystal are given by

$$2(a_{pqrs}+c_{pqrs})=(\bar{a}_1+2\bar{a}_2)\delta_{pq}\delta_{rs}-\tfrac{1}{2}\bar{a}_1(\delta_{pr}\delta_{qs}+\delta_{ps}\delta_{qr})$$
$$+2\bar{b}_1\sum_{\alpha=1}^{3}\delta_{\alpha p}\delta_{\alpha q}\delta_{\alpha r}\delta_{\alpha s}, \quad (6.10)$$

where $\bar{a}_1$, $\bar{a}_2$, and $\bar{b}_1$ depend on the fractional increase in volume v, and are equal to a_1, a_2, and b_1, when $v=0$. From (6.10) and (6.6), we obtain

$$2\bar{b}_{ppijrs}\int u_{i,j}u_{r,s}dV_0$$
$$=\left(\frac{\partial\bar{a}_1}{\partial v}+2\frac{\partial\bar{a}_2}{\partial v}\right)\int(u_{k,k})^2dV_0$$
$$-\frac{1}{2}\frac{\partial\bar{a}_1}{\partial v}\int(u_{k,m}u_{k,m}+u_{k,m}u_{m,k})dV_0$$
$$+2\frac{\partial\bar{b}_1}{\partial v}\sum_{\alpha=1}^{3}\int(u_{\alpha,\alpha})^2dV_0. \quad (6.11)$$

On defining $\bar{k}$, $\bar{\mu}$, and $\bar{\nu}$ by

$$\bar{k}=\tfrac{2}{3}(\bar{a}_1+3\bar{a}_2+\bar{b}_1),\quad 2\bar{\mu}=2\bar{b}_1-\bar{a}_1\quad\text{and}\quad\bar{\nu}=-\bar{b}_1, \quad (6.12)$$

and denoting by k, μ and ν the values of $\bar{k}$, $\bar{\mu}$ and $\bar{\nu}$ when

$v=0$, we can rewrite Eq. (6.11) as

$$\bar{b}_{ppijrs}\int u_{i,j}u_{r,s}dV_0$$

$$=\frac{\partial\bar{k}}{\partial v}\frac{1}{k}\int W_D dV_0+\frac{\partial\bar{\mu}}{\partial v}\frac{1}{\mu}\int W_S dV_0+\frac{\partial\bar{\nu}}{\partial v}\frac{1}{\nu}\int W_S' dV_0, \quad (6.13)$$

where

$$W_D=\tfrac{1}{2}k(u_{m,m})^2,$$

$$W_S=\mu[\tfrac{1}{2}(u_{m,n}u_{m,n}+u_{m,n}u_{n,m})-\tfrac{1}{3}(u_{m,m})^2],$$

and

$$W_S'=\nu[\tfrac{1}{2}(u_{m,n}u_{m,n}+u_{m,n}u_{n,m})-\sum_{\alpha=1}^{3}(u_{\alpha,\alpha})^2]. \quad (6.14)$$

Also, we see from (6.7) and (4.6) that, for the cubic crystals considered,

$$W_2=a_{pqrs}u_{p,q}u_{r,s}=\tfrac{1}{2}(a_1+2a_2)(u_{m,m})^2-\tfrac{1}{4}a_1(u_{m,n}u_{m,n}+u_{m,n}u_{n,m})+b_1\sum_{\alpha=1}^{3}(u_{\alpha,\alpha})^2. \quad (6.15)$$

It is then easily seen that

$$W_2=W_D+W_S+W_S'. \quad (6.16)$$

By introducing (6.13) and (6.16) into (6.9), we obtain

$$V-V_0=-\frac{1}{k}\left[\left(1+\frac{1}{k}\frac{\partial\bar{k}}{\partial v}\right)\int W_D dV_0+\left(1+\frac{1}{\mu}\frac{\partial\bar{\mu}}{\partial v}\right)\int W_S dV_0+\left(1+\frac{1}{\nu}\frac{\partial\bar{\nu}}{\partial v}\right)\int W_S' dV_0\right]. \quad (6.17)$$

We can specialize this result to the case of an isotropic material by taking $b_1=\bar{b}_1=0$. We then obtain Zener's result[1]

$$V-V_0=-\frac{1}{k}\left[\left(1+\frac{1}{k}\frac{\partial\bar{k}}{\partial v}\right)\int W_D dV_0+\left(1+\frac{1}{\mu}\frac{\partial\bar{\mu}}{\partial v}\right)\int W_S dV_0\right]. \quad (6.18)$$

7. A QUALITATIVE DEDUCTION

In general, in order to obtain an explicit value for $V-V_0$ from Eqs. (6.17) or (6.18), we need to know the displacement field which is associated with the dislocations according to classical elasticity theory. However, it is easily seen that W_S, W_D, and W_S' are essentially positive. Thus, if for a given material the coefficients of all three of the terms $\int W_S dV_0$, $\int W_D dV_0$, and $\int W_S' dV_0$ in (6.17) have the same signs, we can predict whether a body of the material will increase or decrease in volume when dislocations are introduced.

Daniels and Smith[2] have determined the dependence on applied hydrostatic pressure of the speeds of propagation of plane waves in crystals of copper, silver, and gold. These crystals are all of the type considered in Sec. 6. The wave speeds measured in a crystal are, of course, simply related to the values of $\bar{k}$, $\bar{\mu}$, and $\bar{\nu}$ for the crystal.

If p denotes the applied hydrostatic pressure, we have

$$\frac{\partial}{\partial v}=\frac{\partial p}{\partial v}\frac{\partial}{\partial p}=-k\frac{\partial}{\partial p}. \quad (7.1)$$

We can therefore write (6.17) in the alternative form,

$$V-V_0=\frac{1}{k}\left[\left(\frac{\partial\bar{k}}{\partial p}-1\right)\int W_D dV_0+\left(\frac{k}{\mu}\frac{\partial\bar{\mu}}{\partial p}-1\right)\int W_S dV_0+\left(\frac{k}{\nu}\frac{\partial\bar{\nu}}{\partial p}-1\right)\int W_S' dV_0\right]. \quad (7.2)$$

From the results of Daniels and Smith, the values given in Table I are obtained for the coefficients $\partial\bar{k}/\partial p-1$, $(k/\mu)\partial\bar{\mu}/\partial p-1$ and $(k/\nu)\partial\bar{\nu}/\partial p-1$.

Since these coefficients are all positive, it follows that for each of the metals, the introduction of dislocations should produce an increase in volume.

We easily can establish upper and lower bounds for the change of volume in terms of the total elastic energy $\int W_2 dV_0$ stored in the deformed body in these cases. For example, for copper and silver, we see from the

TABLE I.

	$\frac{\partial\bar{k}}{\partial p}-1$	$\frac{k}{\mu}\frac{\partial\bar{\mu}}{\partial p}-1$	$\frac{k}{\nu}\frac{\partial\bar{\nu}}{\partial p}-1$
Copper	4.59	2.404	3.685
Silver	5.18	3.332	4.611
Gold	5.43	4.139	7.545

[2] W. B. Daniels and C. S. Smith, ONR. Tech. Rept. No. 1, Contract Nonr-1141(05), Project NR017-309 (1958).

table that

$$\frac{\partial\bar{k}}{\partial p}-1>\frac{k}{\nu}\frac{\partial\bar{\nu}}{\partial p}-1>\frac{k}{\mu}\frac{\partial\bar{\mu}}{\partial p}-1. \tag{7.3}$$

With (7.2) and (6.16), we obtain immediately

$$\frac{1}{k}\left(\frac{\partial\bar{k}}{\partial p}-1\right)\int W_2 dV_0 \geq V-V_0 \geq \frac{1}{k}\left(\frac{k}{\mu}\frac{\partial\bar{\mu}}{\partial p}-1\right)\int W_2 dV_0. \tag{7.4}$$

8. APPENDIX 1. ISOTROPIC MATERIALS

For an isotropic material, W must be expressible as a polynomial in J_1, J_2 and J_3 defined by

$$J_1=E_{ii},\quad J_2=\tfrac{1}{2}[(E_{ii})^2-E_{ij}E_{ji}],$$
and
$$J_3=\tfrac{1}{6}[2E_{ik}E_{kj}E_{ji}-3E_{kk}E_{ij}E_{ji}+(E_{ii})^3]. \tag{8.1}$$

Thus retaining terms up to the third degree in E_{ij}, the expression (4.3) for W takes, for an isotropic material, the form,||

$$W=a_1J_2+a_2J_1^2+a_3J_1J_2+a_4J_1^3+a_5J_3. \tag{8.2}$$

From (8.2) and (4.3), we obtain

$$2a_{pqrs}=\frac{1}{4}\left(\frac{\partial}{\partial E_{pq}}+\frac{\partial}{\partial E_{qp}}\right)\left(\frac{\partial}{\partial E_{rs}}+\frac{\partial}{\partial E_{rs}}\right)W\bigg|_{E_{kl}=0}$$
$$=(a_1+2a_2)\delta_{pq}\delta_{rs}-\tfrac{1}{2}a_1(\delta_{pr}\delta_{qs}+\delta_{ps}\delta_{qr}), \tag{8.3}$$

and

$$6b_{mnpqrs}=\frac{1}{8}\left(\frac{\partial}{\partial E_{mn}}+\frac{\partial}{\partial E_{nm}}\right)\left(\frac{\partial}{\partial E_{pq}}+\frac{\partial}{\partial E_{qp}}\right)\times\left(\frac{\partial}{\partial E_{rs}}+\frac{\partial}{\partial E_{sr}}\right)W\bigg|_{E_{kl}=0}$$
$$\begin{aligned}
&=(3a_3+6a_4+a_5)\delta_{mn}\delta_{pq}\delta_{rs}\\
&\quad-\tfrac{1}{2}(a_3+a_5)[\delta_{mn}(\delta_{sp}\delta_{rq}+\delta_{sq}\delta_{rp})\\
&\quad+\delta_{pq}(\delta_{ms}\delta_{nr}+\delta_{mr}\delta_{ns})\\
&\quad+\delta_{rs}(\delta_{mq}\delta_{np}+\delta_{nq}\delta_{mp})]\\
&\quad+\tfrac{1}{4}a_5[\delta_{rq}(\delta_{sm}\delta_{pn}+\delta_{sn}\delta_{pm})\\
&\quad+\delta_{sp}(\delta_{qm}\delta_{rn}+\delta_{qn}\delta_{rm})\\
&\quad+\delta_{rp}(\delta_{sm}\delta_{qn}+\delta_{sn}\delta_{qm})\\
&\quad+\delta_{sq}(\delta_{pm}\delta_{rn}+\delta_{pn}\delta_{rm})].
\end{aligned}$$

By introducing (8.3) into (4.10), we obtain

$$\begin{aligned}
(a_1+2a_2)\delta_{ij}\int e_{mm}dV_0-a_1\int e_{ij}dV_0
&=-\tfrac{1}{2}(2a_1+4a_2-a_3-a_5)\int u_{m,m}(u_{i,j}+u_{j,i})dV_0\\
&\quad+\tfrac{1}{4}(a_3+a_5)\int u_{m,n}u_{n,m}\delta_{ij}dV_0\\
&\quad-\tfrac{1}{2}(3a_3+6a_4+a_5)\int(u_{m,m})^2\delta_{ij}dV_0\\
&\quad+\tfrac{1}{4}(2a_1-a_5)\int(u_{i,m}u_{m,j}+u_{j,m}u_{m,i}+u_{m,i}u_{m,j})dV_0\\
&\quad+\tfrac{1}{4}(4a_1-a_5)\int u_{i,m}u_{j,m}dV_0\\
&\quad-\tfrac{1}{4}(2a_1+4a_2-a_3-a_5)\int u_{m,n}u_{m,n}\delta_{ij}dV_0.
\end{aligned} \tag{8.4}$$

Introducing (8.3) into (5.4), we obtain

$$\begin{aligned}
\bar{t}_{ij}=&(a_1+2a_2)\bar{u}_{p,p}\delta_{ij}-\tfrac{1}{2}a_1(\bar{u}_{i,j}+\bar{u}_{j,i})\\
&-(2a_1+4a_2-3a_3-6a_4-a_5)\delta_{ij}u_{k,k}\bar{u}_{p,p}\\
&+(\tfrac{3}{2}a_1+2a_2-\tfrac{1}{2}a_3-\tfrac{1}{2}a_5)[(u_{i,j}+u_{j,i})\bar{u}_{p,p}\\
&+u_{p,p}(\bar{u}_{i,j}+\bar{u}_{j,i})]\\
&+(a_1+2a_2-\tfrac{1}{2}a_3-\tfrac{1}{2}a_5)\delta_{ij}u_{m,n}\bar{u}_{m,n}\\
&-\tfrac{1}{2}(a_3+a_5)\delta_{ij}u_{m,n}\bar{u}_{n,m}\\
&-\tfrac{1}{2}(a_1-\tfrac{1}{2}a_5)[(u_{j,k}+u_{k,j})(\bar{u}_{i,k}+\bar{u}_{k,i})\\
&+(u_{i,k}+u_{k,i})(\bar{u}_{j,k}+\bar{u}_{k,j})]\\
&-\tfrac{1}{2}a_1(u_{j,k}\bar{u}_{i,k}+u_{i,k}\bar{u}_{j,k}).
\end{aligned} \tag{8.5}$$

9. APPENDIX 2. CUBIC CRYSTALS (HEXTETRAHEDRAL, GYROIDAL, AND HEXOCTAHEDRAL CLASSES)

For cubic crystals of the hextetrahedral, gyroidal, and hexoctahedral classes, the axes of which are in the directions of the axes of the coordinate system x, it has been shown[3] that the strain-energy function may be expressed as a polynomial in J_1, J_2, and J_3, defined by (8.1), and I_1, I_2, and I_3, defined by

$$I_1=E_{11}^2+E_{22}^2+E_{33}^2,\quad I_2=E_{11}E_{22}E_{33},$$
and
$$I_3=E_{11}E_{23}^2+E_{22}E_{31}^2+E_{33}E_{12}^2, \tag{9.1}$$

together with certain further invariants of higher degree than the third in E_{ij}. Retaining terms up to the third degree in E_{ij}, the strain-energy function W then takes the form

$$W=W'+b_1I_1+b_2J_1I_1+b_3I_2+b_4I_3, \tag{9.2}$$

where W' denotes the expression for W given in (8.2).

|| This is substantially the result given by F. D. Murnaghan, Am. J. Math. 59, 235 (1937).

[3] G. F. Smith and R. S. Rivlin, Trans. Am. Math. Soc. 88, 175 (1958).

We obtain immediately

$$\frac{1}{4}\left(\frac{\partial}{\partial E_{pq}}+\frac{\partial}{\partial E_{qp}}\right)\left(\frac{\partial}{\partial E_{rs}}+\frac{\partial}{\partial E_{sr}}\right)\bigg|_{E_{kl}=0} W=2a_{pqrs}$$

$$=2a_{pqrs}'+2b_1\sum_{\alpha=1}^{3}\delta_{\alpha p}\delta_{\alpha q}\delta_{\alpha r}\delta_{\alpha s},$$

and

$$\frac{1}{8}\left(\frac{\partial}{\partial E_{mn}}+\frac{\partial}{\partial E_{nm}}\right)\left(\frac{\partial}{\partial E_{pq}}+\frac{\partial}{\partial E_{qp}}\right)$$

$$\times\left(\frac{\partial}{\partial E_{rs}}+\frac{\partial}{\partial E_{sr}}\right)W\bigg|_{E_{kl}=0}=6b_{mnpqrs}$$

$$\begin{aligned}
&=6b_{mnpqrs}'+2b_2\sum_{\alpha=1}^{3}(\delta_{mn}\delta_{\alpha p}\delta_{\alpha q}\delta_{\alpha r}\delta_{\alpha s}\\
&\quad+\delta_{pq}\delta_{\alpha r}\delta_{\alpha s}\delta_{\alpha m}\delta_{\alpha n}+\delta_{rs}\delta_{\alpha m}\delta_{\alpha n}\delta_{\alpha p}\delta_{\alpha q})\\
&\quad+b_3\sum_{\alpha,\beta,\gamma=1}^{3}\pi_{\alpha\beta\gamma}\delta_{\alpha m}\delta_{\alpha n}\delta_{\beta p}\delta_{\beta q}\delta_{\gamma r}\delta_{\gamma s}\\
&\quad+\tfrac{1}{4}b_4\sum_{\alpha,\beta,\gamma=1}^{3}\pi_{\alpha\beta\gamma}[\delta_{\alpha m}\delta_{\alpha n}(\delta_{\beta p}\delta_{\gamma q}+\delta_{\gamma p}\delta_{\beta q})\\
&\quad\times(\delta_{\beta r}\delta_{\gamma s}+\delta_{\gamma r}\delta_{\beta s})\\
&\quad+\delta_{\alpha p}\delta_{\alpha q}(\delta_{\beta r}\delta_{\gamma s}+\delta_{\gamma r}\delta_{\beta s})(\delta_{\beta m}\delta_{\gamma n}+\delta_{\gamma m}\delta_{\beta n})\\
&\quad+\delta_{\alpha r}\delta_{\alpha s}(\delta_{\beta m}\delta_{\gamma n}+\delta_{\gamma m}\delta_{\beta n})(\delta_{\beta p}\delta_{\gamma q}+\delta_{\gamma p}\delta_{\beta q})],
\end{aligned}\tag{9.3}$$

where $\pi_{\alpha\beta\gamma}$ is the permutation symbol defined by $\pi_{\alpha\beta\gamma}=1$ if $\alpha\beta\gamma$ is a permutation of 1, 2, 3 and $\pi_{\alpha\beta\gamma}=0$ otherwise¶; a_{pqrs}' and b_{mnpqrs}' are used to denote the values of a_{pqrs} and b_{mnpqrs} given by (8.3).

On introducing (9.3) into (4.10) and using e_{ij}' to denote e_{ij} in Eq. (8.4), we obtain

$$\begin{aligned}
&(a_1+2a_2)\delta_{ij}\int e_{mm}dV_0-a_1\int e_{ij}dV_0\\
&\qquad+2b_1\sum_{\alpha=1}^{3}\delta_{\alpha i}\delta_{\alpha j}\int e_{\alpha\alpha}dV_0\\
&=(a_1+2a_2)\delta_{ij}\int e_{mm}'dV_0-a_1\int e_{ij}'dV_0\\
&\quad-\sum_{\alpha=1}^{3}\int\{2b_1(\delta_{\alpha i}u_{j,\alpha}u_{\alpha,\alpha}+\delta_{\alpha j}u_{i,\alpha}u_{\alpha,\alpha})\\
&\quad+b_1\delta_{\alpha i}\delta_{\alpha j}u_{k,\alpha}u_{k,\alpha}+b_2[\delta_{ij}(u_{\alpha,\alpha})^2\\
&\quad+2\delta_{\alpha i}\delta_{\alpha j}u_{\alpha,\alpha}u_{p,p}]+\tfrac{1}{2}b_3\pi_{\alpha\beta\gamma}\delta_{\alpha i}\delta_{\alpha j}u_{\beta,\beta}u_{\gamma,\gamma}\\
&\quad+\tfrac{1}{8}b_4\pi_{\alpha\beta\gamma}[\delta_{\alpha i}\delta_{\alpha j}(u_{\beta,\gamma}+u_{\gamma,\beta})^2\\
&\qquad+2u_{\alpha,\alpha}(\delta_{\beta i}\delta_{\gamma j}+\delta_{\gamma i}\delta_{\beta j})(u_{\beta,\gamma}+u_{\gamma,\beta})]\}dV_0.
\end{aligned}\tag{9.4}$$

¶ We note that Greek subscripts are assumed to take the values 1, 2, 3, and the summation convention is not applied to them.

Introducing (9.3) into (5.4) and using $\bar{t}_{ij}'$ to denote the expression for $\bar{t}_{ij}$ given in (8.5), we obtain

$$\begin{aligned}
\bar{t}_{ij}=\bar{t}_{ij}'&+2b_1\sum_{\alpha=1}^{3}\delta_{\alpha i}\delta_{\alpha j}\bar{u}_{\alpha,\alpha}\\
&+\sum_{\alpha=1}^{3}[-2(b_1-b_2)\delta_{\alpha i}\delta_{\alpha j}(u_{\alpha,\alpha}\bar{u}_{p,p}+u_{p,p}\bar{u}_{\alpha,\alpha})\\
&+2b_1(\delta_{\alpha i}u_{j,\alpha}+\delta_{\alpha j}u_{i,\alpha})\bar{u}_{\alpha,\alpha}\\
&+2b_1u_{\alpha,\alpha}(\delta_{\alpha i}\bar{u}_{j,\alpha}+\delta_{\alpha j}\bar{u}_{i,\alpha})+2b_1\delta_{\alpha i}\delta_{\alpha j}u_{p,\alpha}\bar{u}_{p,\alpha}\\
&+2b_2\delta_{ij}u_{\alpha,\alpha}\bar{u}_{\alpha,\alpha}]+\sum_{\alpha,\beta,\gamma=1}^{3}\{b_3\pi_{\alpha\beta\gamma}\delta_{\alpha i}\delta_{\alpha j}u_{\beta,\beta}\bar{u}_{\gamma,\gamma}\\
&+\tfrac{1}{4}b_4\pi_{\alpha\beta\gamma}\delta_{\alpha i}\delta_{\alpha j}(u_{\beta,\gamma}+u_{\gamma,\beta})(\bar{u}_{\beta,\gamma}+\bar{u}_{\gamma,\beta})\\
&+\tfrac{1}{4}b_4\pi_{\alpha\beta\gamma}(\delta_{\alpha i}\delta_{\beta j}+\delta_{\beta i}\delta_{\alpha j})[(u_{\alpha,\beta}+u_{\beta,\alpha})\bar{u}_{\gamma,\gamma}\\
&\qquad+u_{\gamma,\gamma}(\bar{u}_{\alpha,\beta}+\bar{u}_{\beta,\alpha})]\}.
\end{aligned}\tag{9.5}$$

10. APPENDIX 3

If $\mathbf{A}$ is any 3×3 matrix, then

$$\det\mathbf{A}=\tfrac{1}{6}[(tr\mathbf{A})^3-3tr\mathbf{A}\,tr\mathbf{A}^2+2tr\mathbf{A}^3].\tag{10.1}$$

If in a deformation of a body, a point initially at X_i in a rectangular Cartesian coordinate system x moves to x_i in the same system, the ratio between the volume dV of an element in the deformed state to its volume dV_0 in the undeformed state is given by

$$dV/dV_0=|x_{i,j}|.\tag{10.2}$$

With (10.1), we obtain

$$\frac{dV}{dV_0}=\tfrac{1}{6}[(x_{r,r})^3-3x_{r,r}x_{p,q}x_{q,p}+2x_{p,q}x_{q,r}x_{r,p}].\tag{10.3}$$

Writing $x_i=X_i+u_i$ and assuming that the displacement gradients $u_{i,j}$ are sufficiently small so that we may neglect terms of higher degree than the second in them, we obtain, from (10.3),

$$\frac{dV}{dV_0}=1+u_{r,r}+\tfrac{1}{2}(u_{r,r})^2-\tfrac{1}{2}u_{p,q}u_{q,p}.\tag{10.4}$$

ACKNOWLEDGMENT

The work described in this paper was started in 1952–53 when both of the authors were members of the staff of the Naval Research Laboratory, Washington, D. C. As far as one of the authors (R.S.R.) is concerned, its completion was sponsored by the Office of Naval Research under Contract Nonr-562(10) with Brown University.