The Continuum Theory of Lattice Defects

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I. Introduction

1. Relation between Lattice Defects and Continuum Theory

Among the imperfections to which a crystal is subject,[1] some (interstitial and impurity atoms, vacant lattice sites, dislocations . . .) are relatively permanent. The introduction of one of them generally alters the

[1] F. Seitz, *in* "Imperfections in Nearly Perfect Crystals" (W. Shockley, ed.), Chapter 1. Wiley, New York, 1952.

position of every lattice point. Obviously in calculation we cannot take every lattice point into account explicitly in a crystal of any size, and must be content to treat the greater part of the crystal as a continuum. In favorable cases the exact behavior in the regions where the continuum approximation is inappropriate is unimportant and can be taken into account by giving suitable values to certain parameters appearing in the continuum solution.

The continuum analog of a crystal containing imperfections is an elastic body in a state of stress not produced by surface and body forces. The appropriate tool for handling the "continuum theory of lattice defects" is thus the usual theory of elasticity modified to include internal stress. Unlike the residual stresses encountered in engineering practice, these internal stresses have to be considered as capable of moving about in the medium. Such mobile "strain figures" were discussed by Burton[2] and Larmor[3] when elastic models of the ether were in vogue. Recent interest in solid state physics has stimulated further development. It is the object of the present review to emphasize some of the background principles and to illustrate them by specific examples chosen to bring out the peculiar features involved. Naturally the continuum theory can hardly be expected to answer questions of current interest about the more intimate behavior of lattice defects (e.g., the binding energy of two adjacent point defects). On the other hand, the theory perhaps suffers from the disadvantage that its limitations are more immediately obvious than are those of other approximate methods which have to be used in dealing with the solid state, for it sometimes gives good results even in what appear to be extreme cases.

2. Basic Ideas and Survey of Topics

Of the properties of lattice defects, only some can be expected to survive and still be describable in the continuum idealization. The theory of elasticity is concerned with the relation between the deformation of a body and the energy content of itself and its surroundings. Thus we are effectively limited to a discussion of the deformations and energy changes associated with the presence of defects.

The first problem is to find a way of transcribing defects into their continuum analog. This can usually be done in a plausible *ad hoc* way for particular types of defect (Section a). It is also possible to develop a general theory based on an internal stress "source function" bearing the same relation to the internal strain as charge does to electric field in electrostatics (Section 4b). Closely related to this is the description of

[2] C. V. Burton, *Phil. Mag.* [5] **33**, 191 (1892).

[3] J. Larmor, *Phil. Trans. Roy. Soc.* **A190**, 205 (1897).

internal stress in terms of a continuous distribution of dislocations (Section 9d).

Figure 1 shows a body containing a number of defects S, T, and interacting with its surroundings, typified by a weight W and a spring P. If S moves about, the deformation and elastic energy of the body change. At the same time the changes of shape of its outer surface communicate themselves to W and P and alter their potential energy.

The shape of the body is related to the position of a defect in a rather complicated way. When the defect is moved its elastic field is not simply transported with it bodily, since this would usually violate whatever boundary conditions may have been imposed at its surface. It is often convenient to divide the elastic field into a part which *is* transported bodily with the defect ("field in an infinite medium") and a remainder ("image field") which adjusts itself so that the boundary conditions are

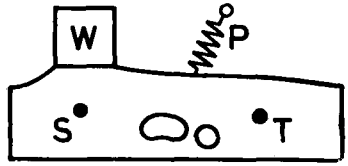

FIG. 1. To illustrate Section 2.

satisfied. We shall see that the image field often plays an unexpectedly important role. There is an analogy with electrostatic problems involving charges in a finite medium whose dielectric constant is large enough to confine the field effectively to its interior, as opposed to the case of charges in free space, where inconvenient surface integrals can be relegated to infinity.

Generally it will not be enough to describe a defect by its position alone; for example, a dislocation loop may change its shape. Let $\alpha, \beta \ldots$ be a (possibly infinite) set of parameters sufficient to characterize the configuration of the defects. Both the elastic energy of the body E_{el} and the potential energy E_{ext} of any external mechanism connected with it will depend on the parameters. Rather than E_{el} and E_{ext} individually, the quantity of physical interest is their sum, the total energy[4,5,6]

$$E_{tot} = E_{el}(\alpha,\beta \ldots) + E_{ext}(\alpha,\beta \ldots).$$

If the parameters are able to vary (subject to certain constraints), it is E_{tot} and not E_{el} or E_{ext} which must be minimized with respect to them to

[4] B. A. Bilby, *Proc. Phys. Soc.* (*London*) **A63,** 3 (1950).
[5] M. O. Peach, *J. Appl. Phys.* **22,** 1359 (1951).
[6] J. D. Eshelby, *Phil. Trans. Roy. Soc.* **A244,** 87 (1951).

find the equilibrium state. In fact the distinction between internal and external energy is artificial, though convenient. Consider, for example, a dislocation in a specimen strained in a tensile testing machine by tightening a screw. We may regard this as a case of a defect in a body (the specimen) acted on by external forces, or as a defect in a complicated self-stressed body (specimen plus machine).

From a thermodynamic point of view E_{tot} is likewise the important quantity. The properties of a nonisolated system may be derived from a knowledge of its enthalpy or Gibbs free energy under adiabatic or isothermal conditions. Although we shall usually regard E_{el} as "purely mechanical" it is strictly the body's internal energy in the adiabatic case, or its Helmholtz free energy in the isothermal case.[7,8] It follows that E_{tot} is its enthalpy or Gibbs free energy, for these quantities are introduced precisely to give an account of the internal energy or Helmholtz free energy of the body plus the energy of its environment under the guise of considering a property of the body alone. If we take this wider point of view we may also derive thermodynamic information from the temperature variation of E_{tot}. (On the elastic model this variation will be determined by thermal expansion and the change of elastic constants with temperature.)

In the infinitesimal theory of elasticity two or more elastic fields may be superimposed. The expression for E_{tot} will then be made up of "self-energy" terms quadratic in the individual fields together with interaction terms involving products of pairs of fields. It is often convenient to deal with the interaction energies rather than with E_{tot}, particularly when the self-energy terms are formally infinite. Even when there are such infinite terms it is possible to "subtract them out" and find a simple expression for the interaction terms (Section 6).

In accordance with usage in analytical mechanics and thermodynamics we may call

$$F(\alpha) = -\partial E_{tot}/\partial \alpha$$

the generalized force associated with the parameter α. Equilibrium is determined by equating to zero the generalized forces corresponding to those parameters which are supposed to be freely variable. In nonequilibrium problems the generalized forces, being derivatives of the free energy, are the driving forces which provide the raw material for a kinetic calculation of the rate of approach to equilibrium by arguments outside the scope of a continuum theory.

[7] I. S. Sokolnikoff, "Mathematical Theory of Elasticity." McGraw-Hill, New York, 1946.

[8] A. E. Green and W. Zerner, "Theoretical Elasticity," p. 72. Oxford Univ. Press, London and New York, 1954.

If it is sufficient to give the Cartesian coordinates x, y, z specifying the position of a defect, we may call

$$\mathbf{F} = -(\partial/\partial x, \partial/\partial y, \partial/\partial z)E_{\text{tot}} \tag{2.1}$$

the force on the defect in the narrower sense. It is often convenient to subdivide $\mathbf{F}$ along the following lines. Consider the force on the defect S in Fig. 1.

(i) If S is the only defect in the body and W and P are absent, $E_{\text{tot}} = E_{\text{el}}$ will vary with the position of the defect. Because in a homogeneous body the existence of $\mathbf{F}$ is evidently related to the presence of the surface, we may speak of it as an image force $\mathbf{F}^I$, in analogy with the nomenclature in electrostatics. The surface of an internal cavity O will make a contribution to the image force. The cavity will still make a contribution even if it is filled with material, provided its elastic constants differ from those of the remainder of the body. More generally, inhomogeneities of the medium will contribute to $\mathbf{F}^I$. In fact we may simply say that $\mathbf{F}^I$ is due to inhomogeneities if we regard the body as part of an infinite body whose elastic constants are zero outside a certain region.

(ii) If the defect T is introduced, the force on S will have a different value, say $\mathbf{F} = \mathbf{F}^I + \mathbf{F}^T$, and we may call $\mathbf{F}^T$ the force which T exerts on S.

(iii) If surface tractions are next applied (as by W and P), $\mathbf{F}$ becomes, say, $\mathbf{F}^I + \mathbf{F}^T + \mathbf{F}^E$. Then $\mathbf{F}^E$ can be regarded as the force exerted on S by the surface tractions, or the external mechanism responsible for them.

(iv) If x, y, z now refer to the position of the cavity or region of elastic inhomogeneity O, E_{tot} will depend on x, y, z and we may speak of $\mathbf{F}$ as the force on the inhomogeneity.

The results of Section 5a lead at once to simple expressions for $\mathbf{F}^E$ and $\mathbf{F}^T$ (Section 5b), while in Section 6 we find an expression for the force on an inhomogeneity. In Section 7 we develop a general expression for the force on a singularity or inhomogeneity which embraces the foregoing results but which is not limited to infinitesimal deformations. In the infinitesimal case it completes the results of Section 5b by giving a formula for $\mathbf{F}^I$ analogous to the expressions for $\mathbf{F}^E$ and $\mathbf{F}^T$.

As a first illustration we take the familiar misfitting sphere model for a point defect. Image effects play an important part here. They make a large contribution to the volume change produced by the defect, and their retention is essential if we are to reach formally the intuitively obvious result that a uniform density of defects produces a uniform macroscopic dilatation of the body containing them (Section 8a). In Section 8b we take up the effect of point defects on the x-ray diffraction pattern of a crystal in relation to its macroscopic deformation. Image terms again make themselves felt in the elastic theory of the energy of solid solutions

(Section 8c). In Section 8d we refine the model of a point defect by including the effect of anisotropy, and in Section 8e we consider a defect as a lattice inhomogeneity.

In Section 9 we consider some particular topics in the theory of dislocations. (There are several excellent accounts of the general theory.[9,10,11]) Section 9a gives a formal derivation of the interaction energy of a dislocation loop with a stress-field. Section 9b deals with image effects, in particular the problem of a screw dislocation in a rod. This presents unexpected features and is of some interest in connection with the properties of metallic "whiskers." Dislocations in motion (Section 9c) present some intriguing theoretical problems, but at present they do not appear to be of much practical significance. Finally in Section 10 we gather together a few points relating to the behavior of lattice inhomogeneities on a large scale.

II. Formal Theory

3. Elements of Elasticity

The clearest approach to the usual infinitesimal theory, with which we shall be chiefly concerned, is by way of the general theory of finite deformation. Moreover, since some of our results hold in the general case, we give first a simple formulation of the theory of finite strain in a medium with an arbitrary stress-strain relation.

Throughout we use the convention that a repeated suffix is to be summed over the values 1, 2, 3 and that suffixes following a comma denote differentiation:

$$e_{ii} = e_{11} + e_{22} + e_{33}, \qquad u_{i,j} = \partial u_i/\partial x_j, \qquad u_{i,jk} = \partial^2 u_i/\partial x_j \partial x_k,$$
$$p_{ij,j} = p_{i1,1} + p_{i2,2} + p_{i3,3}.$$

The symbol δ_{ij} has the value 1 or 0 according to whether i and j are or are not equal. The symbol ϵ_{ijk} has the value 1 if ijk is an even permutation of 123, -1 if it is an odd permutation and is zero otherwise.

The state of finite strain produced in a medium (conveniently visualized as a transparent jelly) by body and surface forces may be described most vividly thus. Imagine space partitioned into small cubes by the network of a rectangular coordinate system x_i. Within the body we embed a network of threads coinciding with the coordinate net. When the medium is strained, the embedded net becomes a curvilinear coordinate system $\bar{x}_i$ (Fig. 2a), and the shape and size of any small mesh (cubic before

[9] F. R. N. Nabarro, *Advances in Phys.* 1, 269 (1952).
[10] W. T. Read, Jr., "Dislocations in Crystals." McGraw-Hill, New York, 1953.
[11] A. Seeger, "Handbuch der Physik," 3rd ed., p. 383. Springer, Berlin, 1955.

deformation) gives an immediate picture of the deformation in its neighborhood.

The vector $\mathbf{u}$ joining a point x_i of the undeformed coordinate net to a point $\bar{x}_i$ of the deformed net with $\bar{x}_1 = x_1$, $\bar{x}_2 = x_2$, $\bar{x}_3 = x_3$ is evidently the finite displacement undergone by the particle of material originally

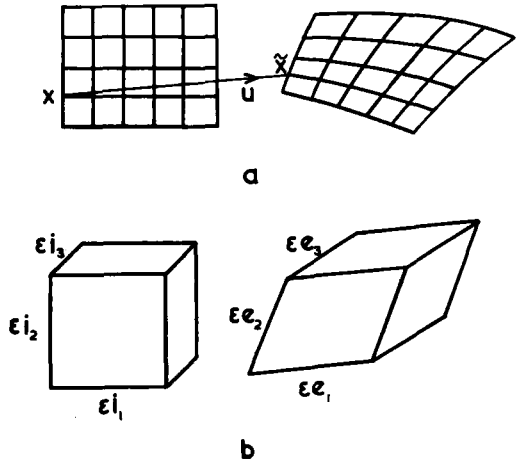

FIG. 2. Finite deformation.

at x_i. As a vector field, the displacement may be considered to be a function of the rectilinear x_i or the curvilinear $\bar{x}_i$. Let $\mathbf{u}(x_i)$ denote the vector arrow whose tail is at x_i, $\mathbf{u}(\bar{x}_i)$ the arrow whose head is at $\bar{x}_i$. The relations

$$\mathbf{u}(x_i) = \mathbf{u}(\bar{x}_i), \qquad \partial \mathbf{u}(x_i)/\partial x_j = \partial \mathbf{u}(\bar{x}_i)/\partial \bar{x}_j$$

if

$$x_i = \bar{x}_i$$

merely expresses the fact that every $\mathbf{u}$-arrow joins the points x_i, $\bar{x}_i$ with identical coordinate numbers. Thus, mathematically, we need not distinguish the x_i (Lagrangian coordinates) from the $\bar{x}_i$ (embedded coordinates). Let u_i be the components of $\mathbf{u}$ along the unit vectors $\mathbf{i}_1$, $\mathbf{i}_2$, $\mathbf{i}_3$ of the undeformed coordinate system:

$$\mathbf{u} = u_m \mathbf{i}_m = u_1 \mathbf{i}_1 + u_2 \mathbf{i}_2 + u_3 \mathbf{i}_3.$$

A small cube with edges $\epsilon \mathbf{i}_1$, $\epsilon \mathbf{i}_2$, $\epsilon \mathbf{i}_3$ (Fig. 2b) before deformation becomes a parallelepipedal mesh of the deformed coordinate system with edges $\epsilon \mathbf{e}_1$, $\epsilon \mathbf{e}_2$, $\epsilon \mathbf{e}_3$ where

$$\mathbf{e}_i = \frac{\partial}{\partial x_i}(x_m \mathbf{i}_m + \mathbf{u}) = (\delta_{mi} + u_{m,i})\mathbf{i}_m. \tag{3.1}$$

For the purposes of the theory of elasticity we need to disentangle from the $\mathbf{e}_i$ (or the $u_{m,i}$) a measure of deformation free from any reference to the *orientation* of the elementary mesh. The six scalar products

$$g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j = u_{i,j} + u_{j,i} + u_{m,i}u_{m,j} + \delta_{ij}$$

evidently provide such a measure, for they give the lengths of the edges ($\epsilon g_{11}^{\frac{1}{2}}$ . . .) and the angles between them ($\cos^{-1} g_{12}/g_{11}^{\frac{1}{2}}g_{22}^{\frac{1}{2}}$ . . .) and so enable us to reconstruct the mesh the correct size and shape without telling us how to orientate it. In place of the g_{ij}, the strain components

$$e_{ij} = \tfrac{1}{2}(g_{ij} - \delta_{ij}) \tag{3.2}$$

are generally used.

Let the material all round the elementary mesh be cut away and let such forces be applied to its free surfaces that it retains its shape, size, and orientation. Let $\epsilon^2\mathbf{p}_j$ be the force on the face which, before deformation, had the positive x_j axis normal to it. Then the p_{ij} defined by resolving $\mathbf{p}_j$ along $\mathbf{i}_1$, $\mathbf{i}_2$, $\mathbf{i}_3$,

$$\mathbf{p}_j = p_{ij}\mathbf{i}_i = p_{1j}\mathbf{i}_1 + p_{2j}\mathbf{i}_2 + p_{3j}\mathbf{i}_3,$$

are the (unsymmetrical) Boussinesq[12] stress components. The equation of equilibrium of the mesh is easily shown to be

$$\frac{\partial p_{ij}}{\partial x_j} + f_i = 0 \tag{3.3}$$

where

$$\mathbf{f} = f_m\mathbf{i}_m$$

is the body force per unit mesh of the deformed (or equally well, the undeformed) coordinate net. Consideration of the work done in a small additional deformation of the body shows that

$$p_{ij} = \frac{\partial W}{\partial u_{i,j}} \tag{3.4}$$

where W is the density of elastic energy per unit mesh.

In the infinitesimal linear theory,[7] which we shall use unless otherwise stated, second-order terms in the strain tensor are neglected,

$$e_{ij} = \tfrac{1}{2}(u_{i,j} + u_{j,i}) \tag{3.5}$$

and W is taken to be a general quadratic expression in the e_{ij}:

$$W = \tfrac{1}{2}c_{ijkl}e_{ij}e_{kl}. \tag{3.6}$$

[12] L. Brillouin, "Les Tenseurs en Méchanique et en Élasticité," p. 246. Masson, Paris, 1949.

The suffixes of the elastic constants c_{ijkl} have the same symmetry as those of $e_{ij}e_{kl}$, that is, i and j or k and l or (ij) and (kl) may be interchanged without altering c_{ijkl}. The stress tensor is now symmetrical,

$$p_{ij} = p_{ji} = c_{ijkl}e_{kl} = c_{ijkl}u_{k,l}. \tag{3.7}$$

Moreover, in an isotropic medium

$$p_{ij} = \lambda e_{mm}\delta_{ij} + 2\mu e_{ij}. \tag{3.8}$$

The equilibrium equation is

$$p_{ij,j} = 0 \tag{3.9}$$

in the absence of body forces and

$$p_{ij,j} + f_i = 0 \tag{3.10}$$

in their presence. In the isotropic case (3.10) may be written in terms of the displacement:

$$\mu\nabla^2\mathbf{u} + (\lambda + \mu)\ \text{grad div}\ \mathbf{u} + \mathbf{f} = 0. \tag{3.11}$$

For finite strain, the problem of finding a rotation which when combined with the deformation e_{ij} will send the cube with edges $\epsilon\mathbf{i}_1$, $\epsilon\mathbf{i}_2$, $\epsilon\mathbf{i}_3$ into the parallelepiped with edges $\epsilon\mathbf{e}_1$, $\epsilon\mathbf{e}_2$, $\epsilon\mathbf{e}_3$ is rather complex. In the linear theory, however, we may define the rotation to be half the curl of the displacement,

$$\tilde{\omega}_i = -\tfrac{1}{2}\epsilon_{ijk}u_{j,k}$$

or more conveniently as the antisymmetric tensor

$$\tilde{\omega}_{ij} = \tfrac{1}{2}(u_{i,j} - u_{j,i}). \tag{3.12}$$

We have

$$\tilde{\omega}_{ij} = -\epsilon_{ijk}\tilde{\omega}_k, \qquad \tilde{\omega}_k = -\tfrac{1}{2}\epsilon_{kij}\tilde{\omega}_{ij}.$$

With an eye to later application, it is convenient to have a definition of the rotation directly in terms of the $\mathbf{e}_i$ and $\mathbf{i}_i$ without reference to the $u_{i,j}$. If $\mathbf{e}_i$ and $\mathbf{i}_i$ differ only infinitesimally, the magnitude of the vector $\mathbf{i}_1 \times \mathbf{e}_1$ is the angle through which $\mathbf{i}_1$ must be rotated to coincide with $\mathbf{e}_1$. Its direction is the axis about which the rotation must be performed. Then $\frac{1}{2}(\mathbf{i}_1 \times \mathbf{e}_1 + \mathbf{i}_2 \times \mathbf{e}_2) \cdot \mathbf{i}_3$ is the x_3 component of the averages of the rotations of the edges $\epsilon\mathbf{i}_1$, $\epsilon\mathbf{i}_2$ of that face of the elementary cube of Fig. 2b which has $\mathbf{i}_3$ for normal. In fact we may put

$$\tilde{\omega} = \tfrac{1}{2}(\mathbf{i}_1 \times \mathbf{e}_1 + \mathbf{i}_2 \times \mathbf{e}_2 + \mathbf{i}_3 \times \mathbf{e}_3) \tag{3.13}$$

for then

$$\tilde{\omega}_3 = -\tilde{\omega}_{12} = \tfrac{1}{2}(\mathbf{i}_1 \times \mathbf{e}_1 + \mathbf{i}_2 \times \mathbf{e}_2) \cdot \mathbf{i}_3 = \tfrac{1}{2}(u_{2,1} - u_{1,2})$$

by (3.1), in agreement with (3.12).

From (3.5) and (3.12), we have

$$\tilde{\omega}_{ij,k} = e_{ki,j} - e_{kj,i} \qquad \text{or} \qquad \tilde{\omega}_{l,k} = -\epsilon_{lij}e_{ki,j}. \tag{3.14}$$

The two tensor fields e_{ij}, $\tilde{\omega}_{ij}$ cannot be strain and rotation in an elastic field with a displacement function unless they satisfy (3.14). But this is not enough to ensure the existence of a displacement, for the line integral

$$\tilde{\omega}_l(Q) - \tilde{\omega}_l(P) = -\int_P^Q \epsilon_{lij}e_{ki,j}dx_k \tag{3.15}$$

giving the difference in the rotation at points P, Q must be independent of the path joining them. The curl of the integrand must be zero, that is we must have

$$S_{ij} = 0 \tag{3.16}$$

where

$$S_{ij}(e_{pq}) = -\epsilon_{ikm}\epsilon_{jln}e_{kl,mn}. \tag{3.17}$$

It is shown directly in works on the theory of elasticity that the vanishing of S_{ij} in a region is the necessary and sufficient condition for the existence of a displacement there.

Consider a narrow tube in the unstrained material with its axis parallel to the x_3 axis. In the strained state $\tilde{\omega}_{3,3}dx_3$ is the relative rotation of two of its cross sections separated by dx_3, while $\tilde{\omega}_{3,1}$, $\tilde{\omega}_{3,2}$ are its curvatures about the x_1 and x_2 axes. We may call $\tilde{\omega}_{i,j}$ the curvature tensor.

It will be convenient to summarize here some elementary theorems and manipulations which will be needed later.

If (u_i,e_{ij},p_{ij}) and (u_i',e_{ij}',p_{ij}') are two sets of quantities, each related by (3.5), (3.7), and satisfying (3.9), we obviously have

$$p_{ij}e_{ij}' = p_{ij}'e_{ij} = p_{ij}u_{r,j}' = p_{ij}'u_{i,j} = (p_{ij}u_i')_{,j} = (p_{ij}'u_i)_{,j}. \tag{3.18}$$

Thus the vector

$$v_j = p_{ij}u_i' - p_{ij}'u_i \tag{3.19}$$

has zero divergence, and so by Gauss's theorem

$$\int_{\Sigma_1} v_j dS_j = \int_{\Sigma_2} v_j dS_j \tag{3.20}$$

for any two surfaces Σ_1, Σ_2 which can be deformed into one another without encountering singularities of v_j. (We use dS_j as an abbreviation for $n_j dS$, where n_j is the normal to the surface and dS is the surface element.) In particular if Σ contains no singularities of v_j,

$$\int_\Sigma v_j dS_j = 0. \tag{3.21}$$

If the material is homogeneous ($c_{ijkl,m} = 0$), the difference between the elastic field u_i', p_{ij}' and the same field advanced bodily a short distance

along the x_l axis satisfies the elastic equations. Thus in (3.19), (3.20), (3.21) we may replace u_i', p_{ij}' by $u_{i,l}'$, $p_{ij,l}'$.

If p_{ij}, p_{ij}' satisfy (3.10) instead of (3.9), we have

$$\int_\Sigma (p_{ij}u_i' - p_{ij}'u_i)dS_j = \int (f_i'u_i - f_iu_i')dv$$

(Betti's reciprocal theorem[13,14]).

We also have

$$\int p_{ij}e_{ij}'dv = \int p_{ij}u_{i,j}'dv = \int \{(p_{ij}u_i')_{,j} + f_iu_i'\}dv = \int p_{ij}u_i'dS_j + \int f_iu_i'dv$$

provided only that

$$p_{ij,j} + f_i = 0 \qquad \text{and} \qquad e_{ij}' = \tfrac{1}{2}(u_{i,j}' + u_{j,i}'). \tag{3.22}$$

Here p_{ij} and e_{ij}' need satisfy no other conditions and need not be related in any way. In particular they need not be possible stress and strain tensors in the same material. With $u_i' = x_i$, (3.22) gives

$$\int p_{ii}dv = \int_\Sigma p_{ij}x_idS_j + \int f_ix_idv. \tag{3.23}$$

In a homogeneous isotropic or cubic medium, $p_{ii} = 3Ke_{ii}$, where K is the bulk modulus. We have then the expression

$$\Delta V = \frac{1}{3K}\int \mathbf{r}\cdot\mathbf{T}dS + \frac{1}{3K}\int \mathbf{r}\cdot\mathbf{f}dv \tag{3.24}$$

for the volume change produced by a body force density $\mathbf{f}$ and surface tractions $\mathbf{T}$. If $\mathbf{f}$ and $\mathbf{T}$ are zero, $\Delta V = 0$ even if the body is in a state of self-stress in which p_{ij} does not vanish throughout the interior.

We shall also need Stokes's theorem in the relatively unfamiliar form

$$\int_\Sigma w_{\ldots j,l}dS_j = \int_\Sigma w_{\ldots m,m}dS_l \tag{3.25}$$

for a closed surface. This follows by applying Stokes's theorem in its usual form to the quantity $\epsilon_{lij}w_{\ldots}$, or by applying Gauss's theorem to the body generated by giving the surface a small displacement parallel to the x_l axis (see Fig. 7).

4. Specification of Internal Stress

a. Somigliana Dislocations

To pass from the crystal lattice with defects to its elastic analog, we must be able to associate with each type of defect a suitable state of

[13] A. E. H. Love, "Mathematical Theory of Elasticity." Cambridge U. P., London, 1952.

[14] S. Timoshenko and J. N. Goodier, "Theory of Elasticity." McGraw-Hill, New York, 1951.

internal stress in the continuum. For brevity we shall refer to these states of internal stress as "singularities."

Most of the singularities of physical interest are particular cases of a general type of dislocation described by Somigliana.[15] To construct a Somigliana dislocation, mark out in the elastic body a surface C bounded by a curve c and make a cut coinciding with C. Give each pair of points adjacent to one another on opposite sides of the cut a relative displacement $\mathbf{d}$ (Fig. 3), scraping away material where there would be interpenetration. Fill in the remaining gaps with additional material and cement together. This evidently leaves the material in a state of internal stress. The stress $p_{ij}n_j$ (where n_j is the normal to C) is continuous across

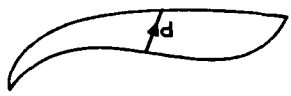

FIG. 3. A Somigliana dislocation.

the surface of discontinuity, but the various components of stress and strain p_{ij}, e_{ij} in general are not. It is physically obvious, and can be proved mathematically[15,16] that a knowledge of $\mathbf{d}$ as a function of position over C, together with the boundary conditions at the surface of the body, completely determines the resulting state of internal stress. If $\mathbf{d}$ is a reasonably smooth function, stress and strain will be finite everywhere except possibly at c.

If $\mathbf{d}$ has a constant value, we have the usual dislocations of solid state theory, the dislocations of types 1, 2, 3, of Volterra.[17] If $\mathbf{d} = \mathbf{r} \times \boldsymbol{\omega}$, where $\mathbf{r}$ is the position vector and $\boldsymbol{\omega}$ a constant, we have Volterra's dislocations of types 4, 5, 6. Physically we may take them to represent twist and tilt boundaries made up of an array of dislocations which, in the spirit of the continuum approximation, have been replaced by a continuous distribution of infinitesimal dislocations.

To make a model of a point defect, we take for C a small sphere with a suitable distribution of $\mathbf{d}$ over the surface. If we let the radius of the sphere tend to zero and, at the same time, increase $\mathbf{d}$ in such a way that the displacement at a fixed distance from the sphere remains finite, we obtain a point singularity in the mathematical sense. For many purposes it is an adequate representation of a physical point defect.

As a simple example we might take $\mathbf{d}$ constant in magnitude and directed radially. Somigliana's recipe is then equivalent to the following.

[15] C. Somigliana, *Atti accad. nazl. Lincei Rend. Classe sci. fis. mat. e nat.* **23**(1) 463 (1914); **24**(1) 655 (1915).

[16] M. Gebbia, *Ann. Mat. Pura Appl.* **7**, 141 (1902).

[17] V. Volterra, *Ann. Éc. Norm. Sup.* **24**, 400 (1907).

Cut a sphere out of the matrix, alter its radius by adding or removing material, and reinsert in the matrix. This is just the familiar misfitting-sphere model for a substitutional or interstitial atom.

It is convenient to divide the elastic field of the singularity into two parts, u_i^∞ and p_{ij}^∞, the value it would have in an infinite medium and an "image field" u_i^I, p_{ij}^I chosen so that $u_i^\infty + u_i^I$, $p_{ij}^\infty + p_{ij}^I$ satisfy the conditions imposed at the surface of the actual finite body containing the singularity. Then if we give Somigliana's surface of discontinuity a displacement ξ, the elastic field will change from

$$u_i = u_i^\infty(x_k) + u_i^I(x_k), \qquad p_{ij} = p_{ij}^\infty(x_k) + p_{ij}^I(x_k) \tag{4.1}$$

to

$$u_i = u_i^\infty(x_k - \xi_k) + u_i^I(x_k, \xi_k), \qquad p_{ij} = p_{ij}^\infty(x_k - \xi_k) + p_{ij}^I(x_k, \xi_k) \tag{4.2}$$

The ∞ field undergoes a rigid displacement, but the image field changes in a more complicated way which can only be found by solving a boundary-value problem. The exact form of u_i^∞, p_{ij}^∞ can be fixed by requiring that p_{ij}^∞ shall approach zero at large distances, at least as r^{-2} in three-dimensional problems and at least as r^{-1} in two dimensions.

b. The Incompatibility Tensor

The way in which we introduced the stress field associated with a given defect is analogous to a development of electrostatics which begins by postulating that the field of a point-charge is er/r^3. Electrostatics may alternately be developed starting from the concept of a charge density which is the "source" of the field and determines it by way of Poisson's equation. The field of a point charge is then found by specializing the density to have the form of a delta function. Something analogous can be done in the elastic case. We start with a body in a state of internal stress and find a "source function of internal stress" which, when prescribed, determines the internal stress if suitable boundary conditions are given.

In engineering practice, the state of internal stress of a body is investigated by cutting a piece off and seeing how it or the remainder deforms. We may idealize this process as follows.[14,6] Let a small cubical element be marked out in the body and then cut out of it. Its shape and size will alter; in other words, it will spontaneously undergo a certain strain, say e_{ij}. By repeating this process for every point we obtain a field $e_{ij}(x_k)$ which serves to specify the state of internal strain. (Evidently this e_{ij} is minus the strain derived from the internal stress using Hooke's law.) Unlike a strain field arising from external forces, e_{ij} will not, in general, satisfy the compatibility conditions (3.16). We can see this most clearly by reversing the foregoing argument. Cut a stress-free body into elemen-

tary cubes and give each one a permanent strain e_{ij}^* so that the field $e_{ij}^*(x_k)$ has continuous first and second derivatives but is otherwise arbitrary. Then, in general, $S_{ij}(e_{mn}^*) \neq 0$. Now pull the elements back to their original cubical form and size by suitable forces applied to their surfaces and cement them together. Then remove the distribution of body forces resulting from the building-in of these surface forces. This induces in the body an additional strain e_{ij}' for which $S_{ij}(e_{mn}') = 0$. The internal stresses are now those derived from $e_{ij}^* + e_{ij}'$ by Hooke's law. If now the body is redissected, each element will undergo a spontaneous strain $e_{ij} = e_{ij}^* + e_{ij}'$ for which $S_{ij}(e_{mn}) = S_{ij}(e_{mn}^*) \neq 0$.

Evidently if to the internal strain there is added a strain produced by external forces, and therefore derivable from a displacement, the value of S_{ij} is unaltered. Thus in a sense the "incompatibility tensor" S_{ij} separates the internal from the external strain. It is in fact a suitable source function for internal stress. In other words, given $S_{ij}(\mathbf{r})$ as a function of position, we can in principle solve the relation

$$-\epsilon_{ikm}\epsilon_{jln}e_{kl,mn} = S_{ij}(\mathbf{r}) \tag{4.3}$$

for the e_{kl}. A solution is

$$e_{ij}(\mathbf{r}) = \frac{1}{4\pi}\int \frac{S_{ij}(\mathbf{r}') - S_{mm}(\mathbf{r}')\delta_{ij}}{|\mathbf{r} - \mathbf{r}'|}\,dv$$

if S_{ij}, or less restrictively its normal component $S_{ij}n_j$, vanishes at the boundary of the body. (This follows from the solution of a similar problem in the general theory of relativity.[18]) If this boundary condition is not satisfied, less elegant solutions are still possible.

To any such solution we can add the general solution of $S_{ij} = 0$, namely $e_{ij}^0 = \frac{1}{2}(u_{i,j}^0 + u_{j,i}^0)$ with arbitrary u_i^0. The complete determination of the state of internal stress when $S_{ij}(\mathbf{r})$ is prescribed thus goes as follows. Find any solution e_{ij} of (4.3). With the aid of Hooke's law, find the stresses p_{ij} and hence the body-forces $f_i = -p_{ij,j}$ and surface tractions $p_{ij}n_j$ necessary to maintain them. By standard elastic theory determine the compatible strain e_{ij}^0 arising from equal and opposite forces. Then the stress in the body is that derived from $e_{ij} + e_{ij}^0$ by Hooke's law.

Such calculations are simplified by introducing a stress function $\chi_{ij} = \chi_{ji}$ related to p_{ij} in the same way as e_{ij} is to S_{ij}:

$$p_{ij} = -\epsilon_{ikm}\epsilon_{jln}\chi_{kl,mn}. \tag{4.4}$$

Clearly for any χ_{kl} we have $p_{ij,j} = 0$. Southwell[19] and Kuzmin[20] have

[18] A. S. Eddington, "Mathematical Theory of Relativity," p. 128. Cambridge U. P., New York, 1923.

[19] R. V. Southwell, *Phil. Mag.* [7] **30**, 253 (1940).

[20] R. O. Kuzmin, *Compt. rend. acad. sci. U.R.S.S.* **49**, 326 (1945).

shown directly that any symmetric tensor with vanishing divergence can, conversely, be represented in the form (4.4), and indeed with one or other of the restrictions $\chi_{12} = \chi_{23} = \chi_{31} = 0$ (Maxwell's form) or

$$\chi_{11} = \chi_{22} = \chi_{33} = 0$$

(Morera's form).[13] Kröner[21] has reduced the problem to manageable form for the isotropic case and obtains the direct relation

$$\nabla^4 \chi_{ij} = 2\mu \left(S_{ij} + \frac{\sigma}{1-\sigma} S_{mm} \delta_{ij} \right) \qquad (\sigma = \text{Poisson's ratio})$$

between incompatibility tensor and stress function. He has also discussed the anisotropic case.[22] The elastic energy of a self-stressed body can be expressed in the form

$$\tfrac{1}{2} \int \chi_{ij} S_{ij} dv$$

plus certain surface terms which vanish if $S_{ij} n_j$ vanishes at its surface.[23,21]

From a given state of incompatible strain, e_{ij}, we can construct a tensor

$$g_{ij} = \delta_{ij} + 2e_{ij} \tag{4.5}$$

on the pattern of (3.2). If we take the g_{ij} as a metric tensor associated with our ordinary Euclidean coordinate system, we thereby define a geometry which is in general not Euclidean but Riemannian. The test for this is whether the Riemann tensor formed from the g_{ij} vanishes or not. In three dimensions, where the four-suffixed Riemann tensor R_{prst} has only six independent components, we may equally well use the two-component tensor $S_{ij} = \epsilon_{ipr} \epsilon_{jst} R_{prst}$[24] which, with (4.5), can be shown to be identical with the S_{ij} of (3.17). Eckart[25] has shown that this Riemannian geometry has a simple physical meaning. The non-Euclidean arc length

$$s = \int_c (g_{ij} dx_i dx_j)^{\frac{1}{2}} \tag{4.6}$$

along any curve c drawn in the body is the actual length of a thin curved rod with c as axis when it has been cut out and allowed to relax its internal stresses. If we take a rectangular closed path $ABCD$ (Fig. 4a) and calculate (4.6) along each of the four sides we shall find in general that $s_{AB} \neq s_{CD}$, $s_{BC} \neq s_{DA}$. Thus when a filamentary loop enclosing $ABCD$ is cut out,

[21] E. Kröner, *Z. Physik* **139**, 175 (1954).
[22] E. Kröner, *Z. Physik* **141**, 386 (1955).
[23] R. V. Southwell, *Proc. Roy. Soc.* **A154**, 4 (1936).
[24] A. J. McConnell, "Applications of the Absolute Differential Calculus," p. 154. Blackie, London, 1936.
[25] C. Eckart, *Phys. Rev.* **73**, 373 (1948).

it must be cut through (say at A) in order to relax its stresses completely. Moreover, the cut will define the two ends of a vector AA' (Fig. 4b). We may relate this to Frank's[26] discussion of the Burgers circuit in a dislocated crystal. We traverse a circuit in a region of "good" crystal surrounding "bad" crystal. For each interatomic step we make in the real crystal, we make a corresponding step in a perfect "comparison" crystal. When we have come back to the starting point in the real crystal, we are still a certain vector distance (closure failure) from the starting point in the comparison crystal. If we desire, we may dispense with a separate comparison crystal and have the work of traversing the comparison circuit done for us automatically. Dissect out a thin loop enclosing the circuit in the real crystal and cut through the loop. We are left with a perfect crystal, admittedly with an odd shape, which can serve as a

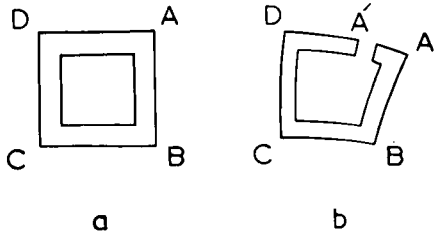

FIG. 4. To illustrate Section 4b.

comparison crystal, in which the Burgers circuit is already marked out and the closure failure is directly indicated by the gap AA'.

The physical significance of S_{ij} can be seen as follows. Equation (3.15) gives the difference of the rotation at the ends of a path drawn in a region where $S_{ij} = 0$. Consider a closed path c embracing a region where $S_{ij} \neq 0$. The integral will not in general vanish. In fact Stokes's theorem and (3.17) give for its value

$$\Delta\tilde{\omega}_l = -\int_C S_{lm} dS_m$$

where C is any cap bounded by c. Consider first a state of plane strain where S_{33} is the only nonvanishing component of S_{ij}, and let S_{33} vanish everywhere except in a small patch near the origin, so that we may write $S_{33} = \omega\delta(x_1)\delta(x_2)$. Then

$$\Delta\tilde{\omega}_3 = -\int_C S_{33} dS_3 = -\omega.$$

This describes the state of internal strain resulting from cutting out a wedge of material of angle ω and cementing the faces of the cut together

[26] F. C. Frank, *Phil. Mag.* [7] **42**, 809 (1951).

(Fig. 5a). In physical terms, this represents a tilt grain boundary of angle ω terminating at the origin. Thus S_{33} is a measure of the number of terminations of tilt boundaries per unit area. More generally, S_{ij} measures the flux of Volterra dislocations of types 4, 5, 6 or, in other words, the number of tilt and twist boundaries which terminate in unit area. The exact relation can be developed in detail, but it is evident that S_{ij} is not an adequate measure of the density of physical dislocations which give rise to a discontinuity of displacement, not of rotation. The Bianchi identity $S_{ij,j} = 0$ expresses the fact that a Volterra dislocation of general type cannot end in the medium.

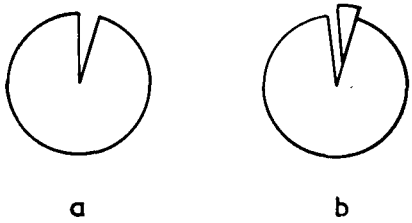

FIG. 5. Relation between edge and "wedge" dislocations.

An edge dislocation can be made by cutting out a parallel-sided fissure and closing the gap. This can be done by removing a wedge and inserting a wedge of the same angle at an adjacent point (Fig. 5b). Thus to describe an edge dislocation at the origin we should have to take $S_{33} = \text{const}\ \partial\{\delta(x_1)\delta(x_2)\}/\partial x_2$. More generally, if we take Volterra tilt and twist dislocations to be analogous to current-carrying wires, edge and screw dislocations are analogous to closely-spaced wires carrying opposite currents.[27] We shall treat the description of internal stress in terms of dislocations in Section 9d.

5. ELASTIC INTERACTION ENERGIES

a. Interaction Energies between Stress Systems

Suppose that in the body whose surface is Σ_0 we have one system of internal stress S whose sources lie entirely within the surface Σ (Fig. 6) and another system T whose sources lie entirely outside Σ. If E_S and E_T are the values of the total elastic energy when S or T alone exists in the body, we may write the total energy when they coexist in the form $E_S + E_T + E_{\text{int}}(S,T)$. Here

$$E_{\text{int}}(S,T) = \tfrac{1}{2}\int(p_{ij}{}^S e_{ij}{}^T + p_{ij}{}^T e_{ij}{}^S)dv$$

is, by definition, the interaction energy between S and T. According to

[27] E. Kröner, *Proc. Phys. Soc.* (*London*) **A421**, 55 (1955).

(3.18) the two terms in the integral are equal. The volume integral can be reduced to a surface integral if we note that one or other of the strains can be written in terms of displacements inside and outside Σ. In fact $e_{ij}{}^S$ can

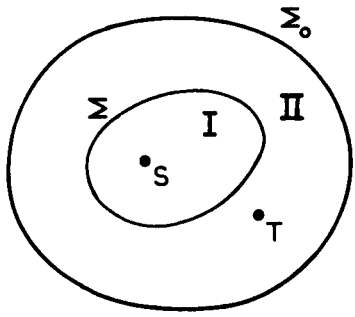

FIG. 6. To illustrate Section 5.

be written as $\frac{1}{2}(u_{i,j}{}^S + u_{j,i}{}^S)$ in region II and $e_{ij}{}^T$ as $\frac{1}{2}(u_{i,j}{}^T + u_{j,i}{}^T)$ in region I, but not conversely. Hence we have

$$E_{\text{int}}(S,T) = \int_{\text{I}} p_{ij}{}^S u_{i,j}{}^T dv + \int_{\text{II}} p_{ij}{}^T u_{i,j}{}^S dv.$$

Because of the equilibrium equations (3.9) $p_{ij}{}^S u_{i,j}{}^T = (p_{ij}{}^S u_i{}^T)_{,j}$. Gauss's theorem converts the first term into

$$\int_\Sigma p_{ij}{}^S u_i{}^T dS_j.$$

Similarly the second term becomes

$$\int_{\Sigma_0} p_{ij}{}^T u_i{}^S dS_j - \int_\Sigma p_{ij}{}^T u_i{}^S dS_j.$$

The minus sign is correct if in $dS_j = n_j dS$, n_j is supposed to be the outward normal to Σ. The integral over Σ_0 vanishes since $p_{ij}{}^T n_j = 0$ on Σ_0. Thus we have an expression[6]

$$E_{\text{int}}(S,T) = \int_\Sigma (p_{ij}{}^S u_i{}^T - p_{ij}{}^T u_i{}^S) dS_j \tag{5.1}$$

for the interaction energy between S and T in the form of an integral over a surface separating them. From the derivation it is clear that the choice of Σ is arbitrary so long as it lies in a region where both $u_i{}^S$ and $u_i{}^T$ exist; analytically, the divergence of the integrand vanishes in the region between two such surfaces.

Now let $p_{ij}{}^T$ and $u_i{}^T$ be the stress and displacement produced by surface tractions $p_{ij}{}^T n_j$ instead of by a source of internal stress; $u_i{}^T$ exists

throughout the body. Thus for the interaction term in the elastic energy we have

$$E_{\text{int}}^*(S,T) = \int p_{ij}^S u_{i,j}^T dv = \int (p_{ij}^S u_i^T)_{,j} dv = \int_{\Sigma_0} p_{ij}^S u_i^T dS_j.$$

This vanishes however, since $p_{ij}^S n_j = 0$ at the surface of the body. Thus

the interaction term in the elastic energy between a system of internal stress and a system of external stress is zero. (5.2)

The response of a body to external forces can be derived from its elastic energy by Castigliano's and related theorems.[14] Hence (5.2) says physically that the response of a body to external forces is the same whether it is self-stressed or not.[28]

This does not, of course, mean that there is no interaction energy between the internal and external stresses, since we must include the potential energy of the external mechanism giving rise to the latter. We can in fact show that (5.1) is still a good measure of the interaction energy when T refers to an external stress. The requirement that Σ separate S from T evidently means now that Σ shall lie within Σ_0 but outside the sources of S. In particular we may put $\Sigma = \Sigma_0$. Then

$$E_{\text{int}}(S,T) = -\int_{\Sigma_0} p_{ij}^T u_i^S dS_j.$$

To be a sensible interaction energy $E_{\text{int}}(S,T)$ must have the following property: $E_{\text{int}}(S'',T) - E_{\text{int}}(S',T)$ is the difference of the energy of the whole system for two different states of internal stress S'' and S' and the same external stress T, insofar as it depends on cross terms between S'' and T or S' and T. The energy of the system is made up of the elastic energy of the body and the potential energy of the mechanism producing the surface traction. We have just seen that the former makes no contribution to the interaction energy. The change of the potential energy is the negative of the work done by the external forces in passing from S' to S'', that is

$$-\int_\Sigma p_{ij}^T (u_i^{S''} - u_i^{S'}) dS_j.$$

This is just $E_{\text{int}}(S'',T) - E_{\text{int}}(S',T)$ as calculated from (5.1). Hence, quite generally, (5.1) gives the interaction energy between S and an elastic field produced by internal or external stress, or, by an easy generalization, a combination of both. In place of (5.1) we may write

$$E_{\text{int}}(S,T) = \int_\Sigma \{(p_{ij}^S + p_{ij}^U) u_i^T - p_{ij}^T (u_i^S + u_i^U)\} dS_j$$

[28] R. V. Southwell, "Theory of Elasticity." Oxford Univ. Press, London and New York, 1936.

where u_i^U, p_{ij}^U is any elastic field free of singularities within Σ, for, by (3.21), the additional terms give no contribution. In other words, in place of u_i^S we can use any "wrong" elastic field which has the same singularities inside Σ. In particular we may put $u_i^U = -u_i^I$ and obtain the result

$$E_{\text{int}}(S,T) = \int_\Sigma (p_{ij}^\infty u_i^T - p_{ij}^T u_i^\infty) dS_j \tag{5.3}$$

which is the most generally useful. Here u_i^∞ and u_i^I are the displacement in an infinite medium and the image displacement discussed in Section 4.

It may happen that a fictitious distribution of body force f_i^S inside Σ can be found which produces the same stress on and outside Σ as does the actual source of internal stress within Σ. Then Gauss's theorem reduces (5.1) to the volume integral

$$E_{\text{int}}(S,T) = -\int \mathbf{f}^S \cdot \mathbf{u}^T dv \tag{5.4}$$

taken over the interior of Σ.

These results are closely connected with the Green's function for the boundary-value problems of elasticity.[13] Suppose that for some point singularity at P we can evaluate the interaction energy explicitly in the form

$$E_{\text{int}}(S,T) = \varphi(u_i^T, p_{ij}^T \text{ at } P). \tag{5.5}$$

Combining this with (5.1) we have a formula for evaluating φ at P from the applied surface tractions. Evidently u_i^S is the appropriate Green's function. Similarly, combining (5.5) with (5.3) we see that merely with the help of the "Green's function for an infinite medium," u_i^∞, we can find φ only if we know both surface traction and displacement. Thus, for example, the result (8.9) gives McDougall's[13] formula for dilatation in terms of surface traction, while the interaction energy for an infinitesimal dislocation loop (see Section 9a) gives effectively Lauricella's[13] relation for determining shear stress in terms of surface data.

b. The Force on a Singularity

From the foregoing we can easily find an expression for the force on the singularity S due to another stress system T, in the sense explained in Section 2. Evidently the force in the x_l direction is

$$F_l = \lim_{\epsilon \to 0} \epsilon^{-1}\{E_{\text{int}}(S',T) - E_{\text{int}}(S,T)\}$$

where S' stands for the singularity S after it has been advanced a distance ϵ along the x_l axis. To find the elastic field of S', we may shift the field of S bodily and make an adjustment to ensure that the boundary condi-

tions are still satisfied. Thus

$$u_i^{S'} = u_i^S - \epsilon u_{i,l}^S + u_i'$$
$$p_{ij}^{S'} = p_{ij}^S - \epsilon p_{ij,l}^S + p_{ij}'.$$

The field u_i', p_{ij}' is free of singularities within Σ, and, by (3.21), makes no contribution to $E_{\text{int}}(S,T)$. Thus from (5.1) we have at once

$$F_l = \int_\Sigma (p_{ij,l}^S u_i^T - p_{ij}^T u_{i,l}^S) dS_j \tag{5.6}$$

or, splitting this into ∞ field and image field terms and applying (3.21) to the latter, we obtain

$$F_l = \int_\Sigma (p_{ij,l}^\infty u_i^T - p_{ij}^T u_{i,l}^S) dS_j. \tag{5.7}$$

These results are still true if the affixes S, T or ∞, T are interchanged:

$$F_l = \int_\Sigma (p_{ij,l}^T u_i^S - p_{ij}^S u_{i,l}^T) dS_j \tag{5.8}$$
$$= \int_\Sigma (p_{ij,l}^T u_i^\infty - p_{ij}^\infty u_{i,l}^T) dS_j \tag{5.9}$$

for the difference between (5.6) and (5.8) is

$$\int_\Sigma (p_{ij}^T u_i^S - p_{ij}^S u_i^T)_{,l} dS_j = \int_\Sigma (p_{ij}^T u_i^S - p_{ij}^S u_i^T)_{,j} dS_l$$
$$= \int_\Sigma (p_{ij}^T u_{i,j}^S - p_{ij}^S u_{i,j}^T) dS_l = 0$$

by (3.25) and (3.18). (We have assumed that u_i^S is single-valued on Σ; the case where this is not so is discussed in reference 6.) Equation (5.9) follows from (5.8) on rejecting the image field as before. Any of these expressions for F_l give the image force if u_i^T, p_{ij}^T are replaced by the image field u_i^I, p_{ij}^I. This follows by a rather tedious extension of the present argument[6] or more simply from the results of Section 7.

6. Interaction Energies between Stresses and Inhomogeneities

Suppose that a body is subject to prescribed surface tractions over its surface Σ_0 and that the elastic constants c_{ijkl} are functions of position. Let the elastic constants change to some other function of position c_{ijkl}' and let the new values of the elastic quantities be distinguished by primes, the prescribed surface tractions remaining unaltered. The increase of elastic energy is

$$\delta E_{\text{el}} = \tfrac{1}{2}\int (p_{ij}' e_{ij}' - p_{ij} e_{ij}) dv \tag{6.1}$$
$$= \tfrac{1}{2} \int_{\Sigma_0} p_{ij} (u_i' - u_i) dS_j. \tag{6.2}$$

The work done by the external forces during the alteration, $-\delta E_{\text{ext}}$, is clearly just twice (6.2). Thus

$$\delta(E_{\text{el}} + E_{\text{ext}}) = -\delta E_{\text{el}} = \tfrac{1}{2}\delta E_{\text{ext}}. \tag{6.3}$$

Of the work done by the external forces, half disappears and half goes to increase the internal energy of the body.

Equation (6.1) can be written in the form

$$\delta E_{\text{el}} = \tfrac{1}{2}\int(p_{ij}e_{ij}' - p_{ij}'e_{ij})dv = \tfrac{1}{2}\int(c_{ijkm}' - c_{ijkm})e_{ij}'e_{km}dv \tag{6.4}$$

for the difference between (6.1) and (6.4) can be transformed by (3.18) into

$$\tfrac{1}{2}\int_{\Sigma_0}(p_{ij}' - p_{ij})(u_i' - u_i)dS_j$$

which vanishes in view of the boundary condition $p_{ij}n_j = p_{ij}'n_j$. We may also write

$$\delta E_{\text{el}} = \tfrac{1}{2}\int(s_{ijkm}' - s_{ijkm})p_{ij}'p_{km}dv \tag{6.5}$$

where the coefficients are those giving e_{ij} in terms of p_{ij}, $e_{ij} = s_{ijkm}p_{km}$.

The x_1 component of the effective force on the elastic inhomogeneity is evidently given by taking $c_{ijkm}'(x_1,x_2,x_3) = c_{ijkm}(x_1 - \epsilon, x_2,x_3)$ calculating (6.4), dividing by $-\epsilon$, and letting ϵ tend to zero. Thus

$$F_l = \tfrac{1}{2}\int c_{ijkm,l}e_{ij}e_{km}dv = \tfrac{1}{2}\int\{(c_{ijkm}e_{ij}e_{km})_{,l} - 2c_{ijkm}e_{ij,l}e_{km}\}dv$$
$$= \int(W_{,l} - p_{ij}e_{ij,l})dv$$

where W is the elastic energy-density. The second term may be written as $-p_{ij}u_{i,jl} = -(p_{ij}u_{i,l})_{,j}$ since $p_{ij,j} = 0$. Gauss's theorem then gives[6]

$$F_l = \int_{\Sigma_0}(W\delta_{jl} - p_{ij}u_{i,l})dS_j. \tag{6.6}$$

It follows from the discussion in Section 7 that (6.8) also gives the force on an inhomogeneity due to a system of internal stress provided Σ_0 is taken to be a surface separating the inhomogeneity from the source of internal stress.

According to the discussion in Section 2, Eq. (6.3) states that in an adiabatic change the changes of enthalpy and internal energy are equal and opposite, or that in an isothermal change the changes of the Gibbs and Helmholtz free energies are equal and opposite. For a thermodynamic system in which the deformation is described sufficiently by giving the specific volume V, there is the adiabatic relation

$$H = E - V(\partial E/\partial V)_S$$

between enthalpy H and internal energy E and the isothermal relation

$$G = F - V(\partial F/\partial V)_T$$

between Gibbs free energy G and Helmholtz free energy F. If E or F is a quadratic function of V we have $H = -E$, $G = -F$. Equation (6.3) is just the generalization of this to the more complex elastic case. It depends on the energy density being quadratic in the strains.

7. The Energy-Momentum Tensor of the Elastic Field

It is possible to develop a general expression[6] for the force on an elastic singularity or inhomogeneity which embraces the foregoing results and which, moreover, is valid for finite strain and an arbitrary stress-strain relation. If the latter is to be true, we must use the total displacement and stress throughout, since, in a nonlinear system, the division of elastic quantities into parts due to image terms, internal and external stress systems and the like no longer has any meaning.

We begin with the simple case of a body whose free surface Σ_0 is subject to surface tractions and which contains some singularity S, that is, a source of internal stress or an elastic inhomogeneity. For the moment, we suppose that the displacements are infinitesimal.

We first find the change in the elastic energy of the body E_{el} on moving S a small distance ϵ in the direction of the positive x_1 axis. We can do this in two stages: (i) at each point (x_1,x_2,x_3) we replace the value $\varphi(x_1,x_2,x_3)$ of any quantity associated with the elastic field by $\varphi(x_1 - \epsilon, x_2,x_3)$, and (ii) we adjust the surface values of φ, as thus changed, so that they again conform with the boundary conditions. In stage (i) the change of elastic energy evidently is

$$\begin{aligned} \delta E_{el}^{(i)} &= -\epsilon \int \frac{\partial W}{\partial x_1}\, dv + O(\epsilon^2) \\ &= -\epsilon \int_{\Sigma_0} W dS_1 + O(\epsilon^2) \end{aligned} \tag{7.1}$$

where W is the energy density. If we suppose that for some reason W or its derivative cannot be defined throughout the interior of Σ_0, we may evaluate $\delta E_{el}^{(i)}$ by keeping the φ fixed and shifting Σ_0 by ϵ in the direction of the negative x_1 axis. Evidently $\delta E_{el}^{(i)}$ is the volume integral of W over the unshaded area of Fig. 7 with due regard for sign; this again gives (7.1). The figure also makes it clear that the shaded area contributes nothing. Thus, in the case of singularities for which W becomes formally infinite, we have managed to "subtract out the infinities."

If the displacement at the surface is u_i before stage (i), it will be $u_i - \epsilon u_{i,1} + O(\epsilon^2)$ at its conclusion. Let its value at the conclusion of stage

(ii) be u_i^{final}. Similarly, if the surface traction is $p_{ij}n_j$ initially, it will be $(p_{ij} - \epsilon p_{ij,1})n_j + O(\epsilon^2)$ at the end of stage (i). During the course of stage (ii), it will be $(p_{ij} - \epsilon p_{ij,1})n_j + p_{ij}'n_j$, where p_{ij}' will vary during the adjustment in a way depending on the degree of "hardness" of the external mechanism. In any case it will be of order ϵ. Thus the energy entering the body during stage (ii) is

$$\delta E_{\text{el}}^{(ii)} = \int_{\Sigma_0} p_{ij}(u_i^{\text{final}} - u_i + \epsilon u_{i,1})dS_j + O(\epsilon^2). \tag{7.2}$$

Consider next the change of E_{ext}. The surface traction has changed from

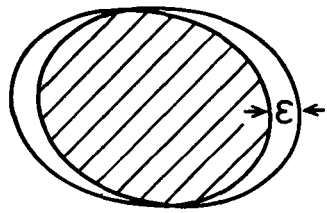

FIG. 7. To illustrate Section 7.

$p_{ij}n_j$ to $p_{ij}n_j + O(\epsilon)$ and the surface has moved through a distance $u_i^{\text{final}} - u_i$ (of order ϵ) at each point. Thus

$$\delta E_{\text{ext}} = -\int_{\Sigma_0} p_{ij}(u_i^{\text{final}} - u_i)dS_j + O(\epsilon^2) \tag{7.3}$$

and so

$$\delta(E_{\text{el}} + E_{\text{ext}}) = \epsilon \int_{\Sigma_0} (p_{ij}u_{i,1} - W\delta_{1j})dS_j + O(\epsilon^2).$$

Fortunately the expression $u_i^{\text{final}} - u_i$ which is generally incalculable and which would contribute non-negligible terms of order ϵ to (7.2) and (7.3), disappears from their sum. For the force in the x_1 direction we thus have

$$F_1 = -\lim_{\Sigma \to 0} \epsilon^{-1}\delta(E_{\text{el}} + E_{\text{ext}}) = \int_{\Sigma_0} (W\delta_{1j} - p_{ij}u_{i,1})dS_j.$$

We could, of course, equally well have displaced the singularity parallel to the x_2 or x_3 axis. Thus

$$F_l = \int_{\Sigma} (W\delta_{jl} - p_{ij}u_{i,l})dS_j \tag{7.4}$$

taking for Σ the surface Σ_0 of the body. By expressing W and p_{ij} in terms of c_{ijkl} and $u_{k,l}$, it is easy to show that the divergence of the integrand, $W_{,l} - (p_{ij}u_{i,l})_{,j}$ vanishes wherever $c_{ijkl,m} = 0$, that is wherever the material is homogeneous. Thus the integral (7.4) can be taken over any surface Σ into which Σ_0 can be deformed without entering a region in which u_i

cannot be defined or where the elastic constants vary with position. Thus Σ can be any surface embracing, but not cutting, inhomogeneities or sources of internal stress.

The extension to the case where there is a force on S arising from sources of internal stress which are outside Σ (Fig. 6), in addition to or instead of those arising from surface tractions, is immediate. No difference is made in $E_{el} + E_{ext}$ if we redefine E_{el} to be the elastic energy within Σ and re-define E_{ext} to be the sum of the elastic energy between Σ and Σ_0 and the energy of the external mechanism. We can then repeat the previous calculation, now taking Σ as the surface of the "body" and regarding everything outside Σ as the mechanism producing surface tractions on Σ. This is quite legitimate since we were careful, in the original derivation of (7.4), to impose no limitation on the external mechanism, beyond the continuity requirement that a change of order ϵ in any one of the quantities $p_{ij}n_j$, u_i, E_{ext} involve a change of the same order in the other two. Evidently we arrive at (7.4) again, with Σ being any surface separating the singularity S from the surface tractions and the sources of internal stress which we regard as exerting a force on it.

When there is no source of internal stress outside Σ and E_{ext} vanishes, (7.4) gives the image force on S arising from the imposed boundary conditions and any inhomogeneities in II (Fig. 6), since nothing in the argument excludes the latter. Boundary conditions for which $E_{ext} = 0$ are: surface traction zero over some regions of Σ_0, displacement constant over the remainder. When the boundary condition is $p_{ij}n_j = 0$ all over Σ_0, (7.4) reduces to

$$F_l = \int_{\Sigma_0} W dS_l$$

and we may say that the energy change in a small displacement simply arises from the movement of the peripheral elastic field of S into and out of Σ_0 in stage (i) (Fig. 7). The adjustment in stage (ii) makes no further contribution.

In stage (i) the whole elastic field was supposed to be shifted. This means, in particular, that the elastic contents underwent the change $c_{ijkl}(x_1,x_2,x_3) \rightarrow c_{ijkl}(x_1 - \epsilon, x_2,x_3)$. Thus even if there are no sources of internal stress within Σ, F_l will not be zero if there are elastic inhomogeneities within Σ_0 Eq. (7.4) then gives the force on them in agreement with (6.6). When there are both sources of internal stress and inhomogeneities within Σ, F_l gives the combined force on them. There is no way of separating the two contributions.

Equation (7.4) is also valid for finite strain and for an arbitrary stress-strain relation if the x_i are interpreted as the Lagrangian x_i of Section 3

and u_i, p_{ij} are the finite displacement and Boussinesq stress components there defined. dS_j is to be taken as the surface element before deformation. The proof is the same word for word except that the vanishing of the divergence of the integrand of (7.4) now follows from the relation

$$\frac{\partial W(u_{m,n})}{\partial x_l} = \frac{\partial W}{\partial u_{i,j}} u_{i,jl}$$

which is valid wherever W depends only on the $u_{i,j}$ and not explicitly on the x_i.

To sum up, the integral

$$F_l = \int_\Sigma P_{jl} dS_j \tag{7.5}$$

with

$$P_{jl} = W\delta_{jl} - p_{ij}u_{i,l}$$

gives the force on all sources of stress and elastic inhomogeneities in I (Fig. 6) arising from surface stresses on Σ_0, from sources of internal stress in II and from the image effects associated with the boundary conditions and elastic inhomogeneities in II.

In the linear infinitesimal case, we may split the elastic field into terms relating to S in an infinite medium (∞), the corresponding image term (I), the field arising from other sources of internal stress (T) and from external forces (E):

$$u_i = u_i^\infty + u_i^I + u_i^T + u_i^E, \qquad p_{ij} = p_{ij}^\infty + p_{ij}^I + p_{ij}^T + p_{ij}^E.$$

Then

$$F_l = F_l^I + F_l^T + F_l^E$$

where

$$F_l^X = \int_\Sigma (u_i^X p_{ij,l}^\infty - p_{ij}^X u_{i,l}^\infty) dS_j, \qquad X = I, E, T.$$

To see this one need only verify with the help of (3.18) and (3.25) that a typical cross term in (7.5), say

$$(X,Y) = \int_\Sigma (\tfrac{1}{2} p_{mn}^X e_{mn}^Y \delta_{jl} - p_{ij}^X u_{i,l}^Y) dS_j, \qquad X, Y = I, E, T, \infty$$

is equal to (Y,X) and to

$$\tfrac{1}{2} \int_\Sigma (u_i^X p_{ij,l}^Y - p_{ij}^X u_{i,l}^Y) dS_j.$$

This expression vanishes by (3.21) unless one or other of the quantities X, Y stands for ∞. The term (∞, ∞) vanishes in view of the limitations imposed on u_i^∞ in Section 4. We have thus recovered the results of Section 5 with the extension to the case of the image force, as promised there.

The spatial part of the canonical energy-momentum tensor of the time-independent elastic field is P_{jl}. It is interesting to set up the complete four-dimensional tensor for the general time-dependent field. The equation of motion in the embedded coordinates of Fig. 2a is found by replacing the force f_i by $f_i - \rho\ddot{u}_i$ in (3.3). With (3.4) this gives

$$-\frac{\partial}{\partial x_j}\frac{\partial W}{\partial u_{i,j}} + \frac{\partial}{\partial t}\rho\dot{u}_i = f_i. \tag{7.6}$$

This is the equation of motion derived from the Lagrangian density

$$L = \tfrac{1}{2}\rho\dot{\mathbf{u}}^2 - W(u_{i,j})$$

for the free elastic field together with an external force density f_i not taken account of in the Lagrangian. The methods of field theory[29] enable us to derive an energy-momentum tensor

$$T_{\eta\lambda} = (\partial L/\partial u_{i,\eta})u_{i,\lambda} - L\delta_{\eta\lambda}$$
$$(\eta,\lambda = 1, 2, 3, 4;\ x_4 = t;\ u_4 = 0).$$

Its components are

$$\begin{aligned} T_{jl} &= P_{jl} - \tfrac{1}{2}\rho\dot{\mathbf{u}}^2\delta_{jl}, \qquad & T_{44} &= W + \tfrac{1}{2}\rho\dot{\mathbf{u}}^2 \\ s_j &= T_{j4} = -p_{ij}\dot{u}_i, & g_l &= T_{4l} = \rho\dot{u}_i u_{i,l}. \end{aligned} \tag{7.7}$$

If the medium is homogeneous, there is the conservation law

$$\partial T_{jl}/\partial x_j + \partial g_l/\partial t = f_i u_{i,l}. \tag{7.8}$$

Here T_{44} is the energy density and s_j the energy flux vector.[18] The "field momentum" density g_l differs from the true momentum density $G_l = \rho\dot{u}_l$. We may give the following formal interpretation. Consider an imaginary particle able to move through the medium, and take for its generalized coordinates $x_i(t)$ the values of x_1, x_2, x_3 associated with the point of the embedded coordinate net of Fig. 2a with which it coincides at time t. (The shape of the coordinate net changes, of course, with time.) Its equation of motion will be

$$\frac{d}{dt}\frac{\partial T}{\partial \dot{x}_l} - \frac{\partial T}{\partial x_l} = Q_l \tag{7.9}$$

where $T(x_i,\dot{x}_i)$ is its kinetic energy and Q_l is the generalized force acting on it. In particular, we can identify the particle with a small element of the elastic medium, say the elementary mesh of Fig. 2b. Throughout its motion $\dot{x}_l = 0$. This does not mean, however, that its generalized momentum $\partial T(x_i,\dot{x}_i)/\partial\dot{x}_l$ vanishes. In fact the momentum is easily shown to be $\epsilon^3\rho(\dot{u}_l + \dot{u}_i u_{i,l})$, that is, $\epsilon^3(G_l + g_l)$. Thus the field momentum density

[29] G. Wenzel, "Quantum Theory of Fields." Interscience, New York, 1949.

is the difference between the true momentum and the generalized momentum per unit mesh when the motion of the medium is referred to the coordinate system deforming with it. Equation (7.8) becomes, term for term

$$\epsilon^3 \partial(G_i + g_i)/\partial t - \epsilon^3 \rho \dot{u}_n u_{n,j} = \epsilon^3 \{f_n + p_{nj,j}\}[\delta_{ni} + u_{n,i}]. \qquad (7.10)$$

The $\epsilon^3\{\ \}$ are the Cartesian components of the force on the element, made up of the applied force and the force exerted on it by its neighbors. The factor $[\ ]$ converts this to the generalized force. Equation (7.10) can be transformed into

$$\frac{\partial}{\partial t}(G_i + g_i) - \frac{\partial}{\partial x_j}(p_{ij} - T_{ji}) = f_n(\delta_{ni} + u_{n,i})$$

which is just the result of adding (7.6) and (7.8). If there is a region v outside which the disturbance is zero, integration gives

$$\frac{d}{dt}\int_v (G_i + g_i)dv = \int_v f_n(\delta_{ni} + u_{n,i})dv \qquad (7.11)$$

that is, the rate of change of true plus field momentum is equal to the sum of the generalized external forces acting on all the elementary meshes. This takes a more interesting form if f_n is derivable from a potential depending only on the absolute position of the element (and on time), so that $f_n = \partial V/\partial(x_i + u_i)$. The integrand on the right of (7.10) is simply $\partial V/\partial x_i$ and hence the integral vanishes if V vanishes outside v. Thus if the elastic field is varying as a result of an interaction with, say, electrified particles which move within it, changes in momentum may be calculated correctly by assuming a fictitious momentum density $-g_i$ in place of the true G_i.[30]

A number of points in the theory of fields receive a simple interpretation in the case of the elastic field when it is realized that the x_i are embedded (Lagrangian) coordinates. In other words, the u_i have the dual role of field variables and components of an actual displacement of the material. Thus, for example, the fact that certain "spin" terms have to be introduced to obtain conservation of angular momentum is closely related to the circumstance that $x_i + u_i$ and not x_i is the appropriate lever arm for taking moments.

These results refer to a homogeneous medium where L does not depend explicitly on x_i. In a medium with internal stress and elastic inhomogeneities, we have

$$P_{jl,j} = \partial W(x_k, u_{i,k})/\partial x_l \qquad (7.12)$$

[30] W. Brenig, *Z. Physik* **143**, 168 (1955).

for the static case in the absence of body forces. The right-hand side denotes the explicit dependence on x_l when W is regarded as a function of the independent variables x_k and the $u_{i,k}$. Equation (7.11) is closely related to our derivation of (7.4). However, there are certain difficulties connected with the direct use of (7.12) which our method by-passes. In the simplest cases it is possible to extend the methods of the present section to dynamical problems (see Section 9c).

III. Applications

8. Point Defects

a. Distortion of Crystals

As the simplest elastic model of a substitutional or interstitial atom we take a sphere ("inclusion") forced into a spherical hole of slightly different size in an infinite block ("matrix") of elastic material.

It is clear that $\mathbf{u}^\infty$ must be spherically symmetric and must not increase with distance outside the inclusion. In fact

$$\mathbf{u}^\infty = c\mathbf{r}/r^3 = -c \operatorname{grad} (1/r) \tag{8.1}$$

where the constant c is a measure of the "strength" of the defect. Equation (8.1) is of the same form as the field around a charged particle. Thus $\operatorname{div} \mathbf{u}^\infty = 0$, $\nabla^2\mathbf{u}^\infty = 0$ and (3.11) is obviously satisfied with $\mathbf{f} = 0$. A second solution $\mathbf{u} = \text{const} \cdot \mathbf{r}$ also satisfies (3.11) since $\operatorname{div} \mathbf{u}$ is constant and $\nabla^2\mathbf{u} = 0$. The sum of these solutions is the general solution of the second-order equation in r to which (3.11) reduces for spherical symmetry. Hence (8.1) is the only solution which satisfies our conditions. The corresponding stress is simply

$$p_{ij}^\infty = 2\mu u_{i,j}^\infty. \tag{8.2}$$

This follows from (3.8) and the fact that both the divergence and curl of the displacement vanish. When a defect is introduced at any point within a closed surface Σ_0 in the infinite matrix, a surface element dS with normal $\mathbf{n}$ moves and sweeps out a volume $\mathbf{u}^\infty \cdot \mathbf{n}dS$. The volume enclosed by Σ_0 increases by

$$\Delta V^\infty = \int_{\Sigma_0} \mathbf{u}^\infty \cdot \mathbf{n}dS = c \int_{\Sigma_0} \frac{\mathbf{r} \cdot \mathbf{n}}{r^3} dS = 4\pi c \tag{8.3}$$

the integral being simply the total solid angle subtended by Σ_0 at the defect. We note that there is a volume change even though $\operatorname{div} \mathbf{u}^\infty$ is zero in the matrix.

Consider (8.1) for a moment as a solution of the elastic equations valid for all $\mathbf{r}$, even though in our application it does not hold inside the

inclusion. Formally we have

$$\text{div } \mathbf{u}^\infty = -c\nabla^2(1/r) = 4\pi c\delta(\mathbf{r})$$

and

$$\nabla^2\mathbf{u}^\infty = -c \text{ grad } \nabla^2(1/r) = 4\pi c \text{ grad } \delta(\mathbf{r}).$$

Then (3.11) shows that $\mathbf{u}^\infty$ can be produced by a density of body force

$$\mathbf{f} = -4\pi c(\lambda + 2\mu) \text{ grad } \delta(\mathbf{r}). \tag{8.4}$$

In Cartesian coordinates, grad $\delta(\mathbf{r})$ has components

$$\left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\right)\delta(\mathbf{r})$$

and (8.4) formally represents three equal "double forces without moment"[13] at right angles (Fig. 8a).

If we wish Σ_0 to be a free surface, we must add to $\mathbf{u}^\infty$ the image displacement $\mathbf{u}^I$ produced by surface tractions $-p_{ij}^\infty n_j$ distributed over Σ_0. A complete solution is possible only in the simplest cases, but we can always find the volume change ΔV^I due to $\mathbf{u}^I$. According to (3.24) and (8.2)

$$\Delta V^I = -\frac{2\mu}{3K}\int_{\Sigma_0} x_i \frac{\partial}{\partial x_i} u_k^\infty dS_k. \tag{8.5}$$

Since u_k^∞ is homogeneous of degree -2, the integral in (8.5) is -2 times the integral in (8.3) and

$$\Delta V^I = 4\pi c \frac{2(1-2\sigma)}{1+\sigma}$$

(σ is Poisson's ratio). The total volume change is

$$\Delta V = \Delta V^\infty + \Delta V^I = 4\pi c\gamma \tag{8.6}$$

where

$$\gamma = 3\frac{1-\sigma}{1+\sigma} = \frac{3K+4\mu}{3K}. \tag{8.7}$$

We may also find ΔV directly from (3.24), inserting the body forces (8.4) and zero surface tractions and using the result

$$\int \mathbf{r}\cdot\{\text{grad } \delta(\mathbf{r})\}dv = \int x_i \frac{\partial}{\partial x_i}\delta(\mathbf{r})dv = -\int \delta(\mathbf{r})\frac{\partial x_i}{\partial x_i}dv = -3.$$

Here ΔV^I is quite a substantial fraction of ΔV^∞, being one-half if σ is $\frac{1}{3}$, $\frac{4}{5}$ if σ is $\frac{1}{4}$. Unlike ΔV^∞, it arises from an actual dilatation of the matrix, although we cannot, in general, calculate how this dilatation is distributed.

The interaction energy of the point defect with another system of internal or external stress T may be found by using any of the results in Section 5. For example, noting that (8.4) may be written

$$\mathbf{f} = -\Delta V K \operatorname{grad} \delta(\mathbf{r}) \tag{8.8}$$

(5.2) gives

$$\begin{aligned} E_{\text{int}} &= \Delta V K \int \mathbf{u}^T \cdot \operatorname{grad} \delta(\mathbf{r}) dv = -\Delta V K \int \delta(\mathbf{r}) \operatorname{div} \mathbf{u}^T dv \\ &= \Delta V p^T \end{aligned} \tag{8.9}$$

where p^T is the hydrostatic pressure produced at the defect by the field T. In particular two point defects of the type considered here interact only through their image fields, since div $\mathbf{u}^\infty = 0$.[31]

If there are N defects in the body, its volume change will be $4\pi\gamma cN$. We can also say something about the change of *shape* of a body containing a large number of defects if we are prepared to admit a lack of rigor of the kind involved in the transition from the theory of a set of point charges to the electrostatics of a continuous charge distribution.[32] Let the defects be uniformly scattered throughout the body with a mean density of n defects per unit volume.

Consider first a sphere. The following results are almost obvious from the foregoing discussion and considerations of symmetry. If the sphere forms part of an infinite medium, introduction of the defects increases its volume by a fraction $4\pi cn$ and leaves its surface a sphere, apart from small ripples whose scale is set by the mean distance between defects, namely about $n^{-\frac{1}{3}}$. The dilatation is zero between the defects. When the sphere is cut out of its matrix it undergoes an additional fractional change of volume $4\pi cn(\gamma - 1)$, associated this time with a uniform dilatation of the material. Its surface remains a sphere, again apart from ripples. We may summarize these results thus:

(i) $\mathbf{u}^\infty$ alone or $\mathbf{u}^I$ alone produces a change of size without change of shape. (8.10)

(ii) $\mathbf{u}^\infty$ and $\mathbf{u}^I$ together produce a change of size without change of shape. The fractional change in volume is $4\pi c\gamma n$. (8.11)

(iii) Between the defects there is a uniform dilatation $4\pi c(\gamma - 1)n$, which is less by a factor $(\gamma - 1)/\gamma$ than that suggested by the change in the volume enclosed by the surface of the body. (8.12)

We now try to show that (ii) and (iii) remain valid for a body of arbitrary shape, but that (i) does not. If the body whose surface is Σ_0 is

[31] F. Bitter, *Phys. Rev.* **37**, 1526 (1931).

[32] J. D. Eshelby, *J. Appl. Phys.* **25**, 255 (1954).

embedded in an infinite matrix we have

$$\mathbf{u}^{\infty}(\mathbf{r}) = c \sum_{m} \frac{\mathbf{r} - \mathbf{r}_m}{|\mathbf{r} - \mathbf{r}_m|^3}. \tag{8.13}$$

At a point outside Σ_0, and sufficiently far from Σ_0 for the distance to the nearest defect to be large compared with the mean distance between defects, the displacement is approximately

$$\bar{\mathbf{u}}^{\infty}(\mathbf{r}) = cn \int \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} dv. \tag{8.14}$$

In accordance with the spirit of the usual discrete-to-continuous transition, we shall suppose that this is valid right up to Σ_0. Equation (8.14) has the same form as the electric field due to a uniform change density $4\pi cn$ filling Σ_0, so that the deformation of Σ_0 on introducing the defects is certainly not a uniform expansion. A direct calculation of the image traction $-p_{ij}^{\infty} n_j$ at each point of Σ_0, followed by a calculation of the field it would produce in the body with Σ_0 as free surface evidently is impossible. Thus we shall use an indirect approach. According to (8.4), (8.1) may be written

$$u_i^{\infty} = -4\pi\gamma K \frac{\partial}{\partial x_j} \sum_{m} U_{ij}(\mathbf{r} - \mathbf{r}_m)$$

where $U_{ij}(\mathbf{r})$ is the value of $u_i(\mathbf{r})$ when a unit point force acts at the origin parallel to the x_j axis. Thus

$$\begin{aligned} \bar{u}_i^{\infty} &= 4\pi c\gamma n K \int_V \frac{\partial}{\partial x_j'} U_{ij}(\mathbf{r} - \mathbf{r}')dv \\ &= 4\pi c\gamma n K \int_{\Sigma_0} U_{ij}(\mathbf{r} - \mathbf{r}')n_j dS. \end{aligned}$$

This shows that outside Σ_0 $\bar{\mathbf{u}}^{\infty}$ can be considered to be caused by a layer of body force on each element dS of Σ_0 of amount $4\pi\gamma cnK dS$ and directed along its normal.

We now carry out the following sequence of operations:

(i) Mark out the surface Σ_0 of the proposed body in an infinite medium.

(ii) Introduce the distribution of defects inside Σ_0. A change of size and shape is undergone by Σ_0.

(iii) Apply a body force $-4\pi\gamma cnK\mathbf{n}dS$ to each element of Σ_0. Now Σ_0 is restored to its size and shape in stage (i) and the displacement in the matrix is everywhere zero.

(iv) Cut away this unstrained matrix, scraping right up to the layer of body force, but not removing it. Nothing is altered within Σ_0. Now Σ_0 is the actual surface of the body, but is subject to a hydrostatic pressure $4\pi\gamma cnK$, since the layer of body force has now become a surface traction; Σ_0 still has the shape and size it had in stage (i).
(v) Remove the hydrostatic pressure. The body undergoes a uniform dilatation $4\pi\gamma cn$.

The displacement due to the layer of body force is clearly given by $-\bar{\mathbf{u}}^\infty$ inside Σ_0 as well as in the matrix. The displacement after stage (iii) or (iv) is thus $\mathbf{u}^\infty - \bar{\mathbf{u}}^\infty$ and is $\mathbf{u}^\infty + \mathbf{u}^I$ after stage (v). Since these differ by a uniform expansion $\mathbf{u} = \frac{4}{3}\pi\gamma cn\mathbf{r}$, we have

$$\mathbf{u}^I = \tfrac{4}{3}\pi\gamma cn\mathbf{r} - \bar{\mathbf{u}}^\infty \tag{8.15}$$

showing that $\mathbf{u}^I$ is not uniform. Its dilatation, however, is constant, for $\bar{\mathbf{u}}^\infty$ is $-$ grad φ, where φ is the potential of a uniform charge density cn filling Σ_0. Thus div $\bar{\mathbf{u}}^\infty = -\nabla^2\varphi = 4\pi cn$ and div $\mathbf{u}^I = 4\pi cn(\gamma - 1)$. The expression (8.14) also provides a reasonable value for the "macroscopic" displacement (excluding the image term) for points within the body. We define the macroscopic displacement at a point as the actual microscopic displacement averaged over a sphere of radius R large compared with the distance between defects. From the fact that (8.14) is a potential function, it is easy to show[32] that the macroscopic displacement so defined is

$$\mathbf{u}^\infty = \frac{c}{R^3}\sum_{r_m<R}\mathbf{r}_m + c\sum_{r_m>R}\frac{\mathbf{r}_m}{r_m^3}$$

where $\mathbf{r}_m$ is the position vector from the point we are interested in to the defect. When R is large enough, the first term, being proportional to the position vector of the center of gravity of a large number of points taken at random in a sphere, should approach zero. The second term may be replaced by an integral, since the distance between the defects is small compared with any of the r_m. This integral is just (8.14) with the sphere R omitted from the volume of integration; however, the omitted part of the integral is proportional to the gravitational attraction at the center of a homogeneous sphere, that is, zero. Thus for points within the body, (8.14) gives the macroscopic displacement omitting image terms.

Since the image displacement defined by (8.15) is derived from the smoothed $\bar{\mathbf{u}}^\infty$, it needs no averaging to give its macroscopic value. Indeed we can go further. If we were to deduce the image traction $-p_{ij}^\infty n_j$ from the exact (8.13) instead of the smoothed (8.14), the results would differ only by terms fluctuating on the scale of the interdefect distance. According to

St. Venant's principle this difference would make itself felt only to a depth of the same order; the smoothed and unsmoothed $\mathbf{u}^I$ would agree in the bulk of the material.

Adding the macroscopic image and ∞ displacements and using (8.15), we have finally, for the total macroscopic displacement, the uniform expansion

$$\bar{\mathbf{u}} = \bar{\mathbf{u}}^\infty + \mathbf{u}^I = \tfrac{4}{3}\pi\gamma c n \mathbf{r}. \tag{8.16}$$

Thus we have verified that for shapes other than spherical (8.11) and (8.12) remain true, although (8.10) does not.

The more general case in which the density of defects is a non-uniform function of position $n(\mathbf{r})$ is now easily disposed of. Let the body be dissected into elementary cubes in each of which n is nearly constant. Each will undergo a uniform dilatation $4\pi\gamma c n(\mathbf{r})$. In the undissected body these expansions are inhibited and lead to distortion and internal stress. The problem is thus identical with the determination of the elastic state of a nonuniformly heated body if we identify the temperature T with n and the linear coefficient of thermal expansion α with one-third of the volume change produced by one defect. Thus

$$T(\mathbf{r}) = n(\mathbf{r}), \qquad \alpha = \tfrac{4}{3}\pi\gamma c.$$

For particular problems, we can draw on the methods already developed for calculating thermal stress.[14] Here we consider a simple problem of some physical interest.[33] Suppose that a thin surface layer of a massive body has been filled with defects (for example by irradiation), so that n is a function of depth which has fallen effectively to zero in a distance small compared with the dimensions of the body. Let n have the value n_s at the surface. The expansion of an element at the surface is unhindered perpendicular to the surface, but cannot take place parallel to it. Thus the free expansion $e_{11} = e_{22} = e_{33} = 4\pi\gamma c n_s$ must be supplemented by an additional deformation e_{ij}' in which $e_{11}' = e_{22}' = -e_{33}$ and $p_{33}' = 0$. (We take the x_3 axis along the normal to the surface.) An easy calculation gives a total expansion perpendicular to the surface

$$e_{33} + e_{33}' = e_{33}(1 + \sigma)/(1 - \sigma)$$

and a stress (compressive if $c > 0$) of magnitude $4\pi\gamma c n_s E/3(1 - \sigma)$ across any plane perpendicular to the surface (E is Young's modulus). Thus an x-ray determination of the spacing of lattice planes parallel to the surface would give $(1 + \sigma)/(1 - \sigma) \sim 2$ times the change of lattice constant that would be observed for a body uniformly filled with n_s defects per unit volume. If the x-ray beam penetrates to a depth where

[33] D. Binder and W. J. Sturm, *Phys. Rev.* **96**, 1519 (1954).

$n(\mathbf{r})$ departs appreciably from n_s, or if the defects are distributed down to a depth which is not small compared with the dimensions of the body, a detailed calculation using the theories of thermal stress and x-ray diffraction is necessary. For a cylinder in which n depends only on distance from the axis or for a plate in which n depends only on depth and is symmetric about the midplane, we have

$$\frac{e_s}{\bar{e}} = \frac{1+\sigma}{1-\sigma}\frac{n_s}{\bar{n}} - \frac{2\sigma}{1-\sigma}. \tag{8.17}$$

Here e_s is the expansion normal to the surface at the surface, $\bar{e}$ is the fractional change of radius or thickness, n_s is the concentration of defects at the surface, and $\bar{n}$ is the average concentration of defects. The ratio (8.17) has the value deduced above for $n_s \gg \bar{n}$ and approaches unity as n_s approaches $\bar{n}$.

b. Effect on X-Ray Diffraction

In Section 8a we took it as obvious that the change of x-ray lattice parameter in a crystal uniformly expanded by lattice defects would be just what one would infer from its change of macroscopic dimensions. Doubt was thrown on this[34] at one time but apparently the intuitive result is true.[35,36,32] This is confirmed by Huang's[37] results. He considered a spherical crystal containing a uniform random distribution of defects and took the expression (8.13) for the displacement of the lattice points. He found a change in the positions of x-ray reflections consistent with a volume change equal to the ΔV^∞ of (8.3) per defect. Huang omitted image effects, but his results may be taken to apply to a sphere subjected to a uniform hydrostatic pressure just sufficient to annul the image terms, which for a sphere are equivalent to a uniform hydrostatic tension. Removal of this pressure evidently would affect the change of x-ray lattice constant and the geometrical dimensions in the same way; both would be multiplied by a factor γ. For a shape of crystal other than spherical, the conditionally convergent sums of the type (8.13) involved in Huang's calculation are dependent on the shape of the crystal, and omission of the image terms would involve more complex errors than the mere omission of a factor γ. His method cannot be extended easily to the general case, since it rests on the fact that the displacement of the atom at $\mathbf{r}_m$ arising from the defect at $\mathbf{r}_n$ depends only on $\mathbf{r}_m - \mathbf{r}_n$. This is no longer true when

[34] P. H. Miller, Jr. and B. R. Russell, *J. Appl. Phys.* **23,** 1163 (1952).
[35] P. H. Miller, Jr. and B. R. Russell, *J. Appl. Phys.* **24,** 1248 (1953).
[36] J. Teltow, *Ann. Physik* **12,** 111 (1953).
[37] K. Huang, *Proc. Roy. Soc.* **A190,** 102 (1947).

image terms are included. We shall give an alternative argument based on a result of Miller and Russell.[34]

Suppose that the base vectors of the perfect crystal lattice are $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ and that those of the corresponding reciprocal lattice are $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$. The atoms of the crystal are taken to be situated at the points $\mathbf{r} = L_i\mathbf{a}_i$ with integral L_i, and the maxima of scattering power in reciprocal space are at the points $\mathbf{k} = h_i\mathbf{b}_i$ with integral h_i. If the crystal is distorted, the lattice points move to the neighboring points $(L_i + \Delta L_i)\mathbf{a}_i$, while the maxima of scattering power move to $(h_i + \Delta h_i)\mathbf{b}_i$. Miller and Russell derive the following relation between Δh_i and ΔL_i,

$$\Delta h_i \Sigma L_i L_j + h_i \Sigma \Delta L_i L_j = 0 \tag{8.18}$$

valid for small integral h_i. The summations are over all points of the crystal lattice and the origin of coordinates is at the center of gravity of the crystal. If we assume that we may take the macroscopic displacement (8.16) for the displacement of the lattice points, we have

$$\Delta L_i = \tfrac{4}{3}\pi\gamma cnL_i.$$

Equation (8.18) shows at once that the reciprocal lattice undergoes a uniform contraction equal and opposite to the uniform dilatation of the crystal lattice; in other words the fractional change of lattice constant is in fact equal to the fractional change in the linear dimensions of the crystal. The replacement of sums by integrals involved in using (8.14) in place of (8.13) seems justified in this particular application. It would be inadequate in calculating the influence of the defects on line profiles or the scattering power between the points of the reciprocal lattice. Omission of the image terms would lead to a nonuniform deformation of the reciprocal lattice. There would not be a simple relation between the change of x-ray lattice constant and macroscopic deformation. Their retention, here as elsewhere, in addition to being physically correct, makes the solution much simpler.

If a spherical crystal of radius R contains one defect at a distance ξ from its center, it can be shown[32] that

$$\Delta V_X^{\infty} = \tfrac{5}{2}(1 - \xi^2/R^2)\Delta V_G^{\infty}$$

where ΔV_G^{∞} is the geometrical change of volume and ΔV_X^{∞} is the change that would be inferred from x-ray measurements. To avoid an awkward elastic calculation, image effects are neglected. When $\xi = 0$,

$$\Delta V_X^{\infty} = 2{\cdot}5\Delta V_G^{\infty}.$$

Miller and Russell based their original argument on this result. However, if the defect is more than about three-quarters of the way from the center

to the surface of the sphere, ΔV_X^∞ is less than ΔV_G^∞. In fact if ξ^2 is given its mean value over the sphere, $\frac{3}{5}R^2$, we have $\Delta V_X^\infty = \Delta V_G^\infty$. Hence a uniform density of defects in the sphere would give equal x-ray and geometrical expansions. Clearly the equality will not be affected by reintroducing the image terms.

c. Solid Solutions

So far we have been able to treat a point defect simply as a center of dilatation. To discuss solid solutions we must relate the strength c of the center of dilatation to the details of the sphere-in-hole model. This is simple when the sphere and matrix have the same elastic constants. Let $V_{\text{mis}} = V_i - V_h$ be the excess of the volume of the sphere V_i over the volume of the hole V_h before the one is inserted in the other. It is easier to visualize the state of affairs if V_{mis} is negative, for then we may start by putting the sphere loosely into the hole. We can take this configuration as an unstrained body to which (3.24) may be applied. When we draw the surfaces of sphere and hole together and cement them we have the same body in a state of internal stress. According to (3.24), however, the volume of material is unchanged. Hence the empty volume eliminated, V_{mis}, must be balanced by an equal decrease in the volume enclosed by the bounding surface of the matrix.[13,38] Thus when inclusion and matrix have the same elastic constants we have simply

$$\Delta V = V_{\text{mis}}, \qquad c = V_{\text{mis}}/4\pi\gamma.$$

When the matrix and inclusion are of different materials, (3.23) tells us only that the volume integral of the hydrostatic pressure is zero in the assembled system, and a more explicit calculation is necessary. We could solve the general elastic equations, matching surface traction and displacement at the boundary between matrix and inclusion. The following method is less tedious, however, and also gives directly the information we shall need below concerning the elastic energy of a defect.

When the inclusion is put into the hole, their common boundary will evidently take up some intermediate position. Let ΔV_h, ΔV_i be the changes of volume of hole and inclusion. The inclusion will evidently be subject to a uniform hydrostatic pressure; its elastic energy will be

$$E_i = \tfrac{1}{2}K_i(\Delta V_i)^2/V_i. \tag{8.19}$$

In the infinite matrix the displacement will be given by (8.1). A direct calculation using (8.2), (3.8), (3.6) shows that the energy density at distance r is

$$\mu e_{ij}e_{ij} = 6\mu c^2/r^6.$$

[38] F. Seitz, *Revs. Mod. Phys.* **18**, 384 (1946).

Hence, by integration, the energy exterior to a sphere of volume V_h is $E_m = 32\pi^2c^2/3V_h$. But ΔV_h is just the ΔV^∞ associated with c by Eq. (8.3). Hence

$$E_m = \tfrac{2}{3}\mu_m(\Delta V_h)^2/V_h. \tag{8.20}$$

We may imagine the hole to have been blown up by an internal pressure. Comparison of (8.19) and (8.20) shows that the change of volume of the hole and the internal pressure are related just as are the change of volume and external pressure for a solid sphere, provided the "effective bulk modulus for expanding a hole" is taken to be $\frac{4}{3}\mu_m$.[39] Since the internal pressure in the hole must equal the external pressure on the inclusion, we have

$$\tfrac{4}{3}\mu_m\Delta V_h/V_h = -K_i\Delta V_i/V_i$$

or, to the first order, simply

$$\tfrac{4}{3}\mu_m\Delta V_h + K_i\Delta V_i = 0.$$

However, we also have the relation $\Delta V_h - \Delta V_i = V_{\text{mis}}$, whence

$$\Delta V_h = \Delta V^\infty = 4\pi c = V_{\text{mis}}/\gamma'. \tag{8.21}$$

Here

$$\gamma' = \frac{3K_i + 4\mu_m}{3K_i}$$

is formed on the pattern of (8.7) but from the bulk modulus of the inclusion and the shear modulus of the matrix. We shall suppose that the relation (8.6) is not affected appreciably by the presence of the inhomogeneous inclusion. Then (8.21) gives

$$\Delta V = \gamma V_{\text{mis}}/\gamma'.$$

From (8.19) and (8.20) we find for the total energy of the defect

$$E_s = E_i + E_m = \tfrac{2}{3}\mu_m\gamma'(4\pi c)^2/V_h. \tag{8.22}$$

We shall refer to E_s as the "self-energy" of the defect to distinguish it from its interaction energy with any other stress system, in particular that arising from other defects.

Consider a dilute substitutional solid solution of a metal M_1 in a metal M_2. Let Ω_1, Ω_2 be their atomic volumes. If we take a crystal containing N M_2 atoms and replace CN of them by M_1 atoms, the volume of the crystal becomes $N\Omega_2 + CN\Delta V$ where ΔV is the volume expansion due to one M_1 atom. Thus the mean volume per atom at a (small) atomic con-

[39] C. Zener, *Phys. Rev.* **74**, 639 (1948).

centration C of solute atoms is, on our elastic model,

$$\Omega(C) = \Omega_2 + C(V_i - V_h)$$

provided $\gamma = \gamma'$ (identical elastic constants for solvent and solute). If M_1 and M_2 have the same crystal structure, it seems reasonable to put

$$\Omega_1 = kV_i, \qquad \Omega_2 = kV_h. \tag{8.23}$$

Then

$$\Omega(C) = C\Omega_1 + (1 - C)\Omega_2 + (k - 1)(\Omega_1 - \Omega_2)C. \tag{8.24}$$

The question of determining k really lies outside the scope of the continuum theory. The choice $k = 1$ leads to the law of additivity of atomic volumes

$$\Omega(C) = C\Omega_1 + (1 - C)\Omega_2$$

or, on the linear approximation, equally well to the law of additivity of atomic radii (Vegard's law)

$$r(C) = Cr_1 + (1 - C)r_2. \tag{8.25}$$

To the same approximation, the fractional rate of change of lattice constant $(dr/dC)/r$ has the constant value

$$\epsilon = (r_1 - r_2)/r_1 \simeq (r_1 - r_2)/r_2$$

right across the composition diagram.

There seems to be no compelling reason to take $k = 1$. We might be tempted, for example, to take the radius of the hole or inclusion equal to the nearest neighbor distance in the appropriate metal. For face-centered cubic this would give $k = (3\sqrt{2})/\pi$ and upset the agreement with (8.25). We shall take the approximate validity of Vegard's law as a justification for putting $k = 1$ in the discussion of the energy of alloys.

When the solute and solvent have different elastic constants, we have by (8.21)

$$\Omega(C) = \Omega_2 + \gamma C(V_i - V_h)/\gamma'.$$

With $k = 1$ this gives

$$r(C) = Cr_1 + (1 - C)r_2 + \beta C$$

where

$$\beta = \frac{4\mu_2}{3\gamma'}\left(\frac{1}{K_2} - \frac{1}{K_1}\right)(r_1 - r_2).$$

Thus the actual value of $r(C)$ should lie above or below the value predicted by Vegard's law according to whether β is positive or negative.[40,41]

[40] B. J. Pines, *J. Phys. U.S.S.R.* **3**, 308 (1940).

[41] J. Friedel, *Phil. Mag.* [7] **46**, 514 (1955).

Friedel[41] has shown that this is qualitatively correct and has discussed the quantitative agreement.

Consider next the elastic energy of the alloy. Each successive solute atom added contributes E_s (8.22) and an interaction energy with the image field of all its predecessors. The image hydrostatic pressure is $-K\Delta V^I$ times the number of defects per unit volume. Since the image pressure builds up linearly with composition, the mean image interaction per solute atom is $\frac{1}{2}K\Delta V\Delta V^I$. If we put $k = 1$ in (8.23), the energy per atom of alloy is easily found to be

$$E(C) = E_s C \left\{1 - \frac{\gamma(\gamma - 1)}{\gamma'(\gamma' - 1)} C\right\}. \tag{8.26}$$

The free energy per atom is

$$F(C) = E(C) - TS_{\text{mix}}$$

where S_{mix} is the configurational entropy of mixing. The entropy $-\partial F/\partial T$ is made up of S_{mix} and an additional term

$$\Delta S = -\partial E(C)/\partial T$$

where ΔS may be estimated by assuming that E depends on T only through the variation with temperature of the elastic constants in (8.26).[42,42a] Friedel[42] finds good agreement between the theoretical and experimental values of E and ΔS for AuNi alloys.

If the solvent and solute are nearly alike elastically, we may put $\gamma = \gamma'$ in (8.26). Moreover, E_s will be the same for the insertion of an M_1 atom into an M_2 matrix or conversely. Then the formula

$$E(C) = \frac{6\mu\Omega}{\gamma} \epsilon^2 C(1 - C) \tag{8.27}$$

is valid for both $C \ll 1$ and $(1 - C) \ll 1$, and we may perhaps take it as a reasonable interpolation for intermediate compositions. Equation (8.27) has the simple parabolic dependence on composition predicted by the chemical theory of alloys. The constant involved depends only on the elastic constants, the atomic volume and the misfit constant ϵ, equal to the fractional rate of change of lattice parameter with composition.

From (8.27) we can give a formal derivation of Hume-Rothery's rule that if $|\epsilon|$ exceeds 15%, solubility is severely limited. According to the chemical theory of alloys,[43] there is a dome-shaped two-phase region on the temperature-composition diagram with a maximum for $C = \frac{1}{2}$ at

[42] J. Friedel, *Advances in Phys.* **3**, 446 (1954).

[42a] E. S. Machlin, *Trans. Am. Inst. Mining Met. Engrs.* **200**, 592 (1954).

[43] A. H. Cottrell, "Theoretical Structural Metallurgy." Edward Arnold, London, 1954.

a temperature T such that kT is half the coefficient of $C(1 - C)$ in (8.27) (k is Boltzmann's constant). If there is to be no miscibility gap, T must be less than the melting-point T_m of the alloy. This gives

$$|\epsilon| < \left(\frac{kT_m}{\mu\Omega}\frac{\gamma}{3}\right)^{\frac{1}{2}}.$$

Reasonable values for the constants give about 15% for the limiting misfit.[42] More elegantly we may use Leibfried's[44] theory of melting; it gives directly $kT_m/\mu\Omega = 0.042$. Or again, this quantity may be written as $RT_m/\mu V_M$ where R is the gas constant and V_M the volume per mole. In this form we may relate Hume-Rothery's rule to two other empirical rules. Richard's rule[45] states that the entropy of melting is nearly R, so that $kT_m/\mu\Omega$ may be equated to the latent heat of melting per unit volume divided by the shear modulus. Bragg[46] has noted that this is nearly 0.034 for many metals. With $\gamma = 1.5$ these two values for $kT_m/\mu\Omega$ give 14.5 and 13% for $|\epsilon|$, respectively.

d. Point Defects in Anisotropic Media

Two of the point defects discussed in Section 8a do not interact with one another except indirectly via their image fields. This behavior depends

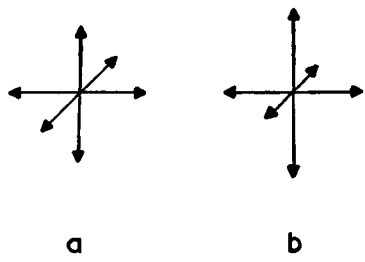

FIG. 8. Crossed double forces.

on the satisfaction of two rather special conditions: (i) the interaction energy is proportional to the dilatation produced at one defect by the other; (ii) the dilatation produced by either defect (omitting image terms) is zero.

Condition (i) can be upset by choosing a less symmetrical defect. In the sphere-in-hole model we may replace the misfitting sphere by an ellipsoid, or, more manageably, we can replace the equal double forces of

[44] G. Leibfried, *Z. Physik* **127**, 344 (1949).

[45] L. S. Darken and R. W. Gurry, "Physical Chemistry of Metals." McGraw-Hill, New York, 1953.

[46] W. L. Bragg, "Symposium on Internal Stresses," p. 221. Institute of Metals, London, 1947.

Fig. 8a by unequal double forces (Fig. 8b). With the horizontal doublets of equal magnitude, Fig. 8b is a model for an interstitial carbon atom in iron.[39] For this case we may write in place of (8.4)

$$f_i = -a_{ij} \frac{\partial}{\partial x_j} \delta(\mathbf{r}).$$

A repetition of the argument leading from (8.8) to (8.9) now gives

$$E_{\text{int}} = -a_{ij} u_{i,j}{}^T = -a_{ij} e_{ij}{}^T. \tag{8.28}$$

The last step follows from the fact that the force density f_i must produce no twisting moment. This requires that a_{ij} be symmetric. The interaction no longer depends on the dilatation but on a more general linear combination of the strain or stress components of the field T with which the defect is interacting.

Again, if we drop the limitation to an isotropic medium, condition (ii) is no longer satisfied even if we take the symmetrical force system of Fig. 8a.

We consider in more detail a cubic material containing a point defect with a cubically symmetric elastic field. The equilibrium equations are

$$c_{44}\nabla^2 u_1 + (c_{12} + c_{44}) \frac{\partial e}{\partial x_1} + d \frac{\partial^2 u_1}{\partial x_1{}^2} + f_1 = 0 \tag{8.29}$$

and two similar equations. The c_{ij} are the elastic constants c_{ijkl} in the usual abbreviated notation.[7] The quantity

$$d = c_{11} - c_{12} - 2c_{44}$$

vanishes for isotropy. To define the field of the defect we may require the displacement to fall off with distance and to have cubic symmetry, or equivalently we may solve (8.29) with f_i given by (8.4). If we take the latter point of view, we see at once that the interaction energy with a stress system T is given by (8.9), the transition from (8.8) to (8.9) being equally valid for the cubic case. That the coefficient ΔV in (8.8) is still the total volume change produced by the defect follows from (3.24), which is also true in the cubic case. (The bulk modulus is $K = c_{11} + 2c_{12}$.)

We could find the field of the defect merely by differentiation if we knew the displacement arising from a point force in a cubic medium. Unfortunately the elastic field caused by a point-force in any medium other than an isotropic or hexagonal one cannot be given explicitly,[47,48] a fact which considerably hinders the solution of any but trivial three-

[47] I. M. Lifshitz and L. N. Rosenzweig, *Zhur. Eksptl. i Teort. Fiz.* **17**, 783 (1947).
[48] E. Kröner, *Z. Physik* **136**, 402 (1953).

dimensional elastic problems in an anisotropic medium. We have to be content, therefore, with an approximate solution.

Write $c_{ij} = c_{ij}^0 + c_{ij}'$ where c_{ij}^0 satisfies the condition for isotropy, $c_{11}^0 - c_{12}^0 - 2c_{44}^0 = 0$. If we treat the c_{ij}' as small, we may solve (8.29), (8.8) by successive approximation. To the second order the dilatation is found to be[49]

$$e^\infty(\mathbf{r}) = \frac{\Delta VK}{c_{11}^0}\left\{\delta(\mathbf{r}) + \frac{15}{8\pi}\frac{d}{c_{11}^0}\frac{x_1^4 + x_2^4 + x_3^4 - \frac{3}{5}r^4}{r^7}\right\} \tag{8.30}$$

The value of c_{11}^0 depends on how we split off an isotropic component from the c_{ij}. Lifshitz and Rosenzweig[47] limit themselves to "weak anisotropy" and in effect take $c_{11}^0 = c_{11}$. Leibfried's[50] method of averaging gives

$$c_{11}^0 = \tfrac{3}{5}(c_{11} + 2c_{12} + 4c_{44}).$$

For many materials there seems to be no way of arranging that the c_{ij}' shall be convincingly smaller than the c_{ij}^0. It should be a fair approximation to replace c_{11}^0 in (8.30) by $\lambda + 2\mu$, where λ, μ are the Lamé constants for the bulk material in polycrystalline form.

The value of ΔV^∞ is found by integrating (8.30) over all space: it is thus the coefficient of $\delta(\mathbf{r})$. (The second term is zero when averaged over all directions.) The relation between ΔV, ΔV^∞, and ΔV^I is easily shown to be the same as in (8.6) with $\gamma = K/c_{11}^0$, that is, the value calculated from the averaged isotropic constants.

The interaction energy between two such defects for which $\Delta V = \Delta V_1$, $\Delta V = \Delta V_2$ is from (8.30) and (8.9)

$$E_{\text{int}} = -\frac{15d}{8\pi\gamma^2}\Delta V_1 \Delta V_2 \frac{\Gamma}{r^3}$$

with

$$\Gamma = l^4 + m^4 + n^4 - \tfrac{3}{5}$$

where r is the distance between them and (l,m,n) are the direction cosines of the line joining them. As a function of angle, Γ has a maximum in the 100 direction, a minimum in the 111 direction, and a saddle-point in the 110 direction. Thus whatever the signs of ΔV_1, ΔV_2, d may be, there is a direction for which the interaction is attractive.

By an extension of the argument of Section 8a it may be shown that a uniform distribution of these defects gives a uniform macroscopic dilatation. It will no longer be exactly true that there is a uniform dilatation between the defects, because of the second term in (8.30). Since this term averages to zero over angles, however, the results obtained for the

[49] J. D. Eshelby, *Acta Metallurgica* **3**, 487 (1955).
[50] G. Leibfried, *Z. Physik* **135**, 23 (1953).

energy of an alloy should not be affected unless the solute atoms take up ordered positions relative to one another.

e. Point Defects as Inhomogeneities

When calculating the "strength" of a point defect in Section 8c in terms of the sphere-in-hole model, we considered the general case in which the sphere had different elastic constants from its surroundings. On this model the defect is both a source of internal stress and an elastic inhomogeneity in the sense of Section 6. So far we have neglected its interaction as an inhomogeneity. On the linear theory this can be treated separately from its effect as a source of stress, so that we consider a perfectly fitting sphere with elastic constants λ', μ' embedded in a medium with constants λ, μ. Let surface forces produce a uniform strain e_{ij}^T in the homogeneous medium. When the sphere is introduced, the change of total energy is

$$E_{\text{int}} = \tfrac{1}{2}\int\{(\lambda' - \lambda)e^T e' + 2(\mu' - \mu')e_{ij}^T e_{ij}'\}dv$$

according to (6.4). The integral is taken only over the sphere (since the elastic constants do not change outside it), and e_{ij}' is the strain in the inclusion. It can be shown[49] that e_{ij}' is uniform. It is a linear function of the e_{ij}^T, and by symmetry it must be an isotropic function, say

$$e_{ij}' = Ae^T\delta_{ij} + 2Be_{ij}^T \tag{8.31}$$

so that

$$E_{\text{int}} = -\tfrac{1}{2}\Omega\{\Lambda(e^T)^2 + 2\mathrm{M}e_{ij}^T e_{ij}^T\} \tag{8.32}$$

where Ω is a volume which, in applications, may conveniently be the volume per atom; Λ and M have the dimensions of elastic constants and can be calculated. Their ratio is a definite function of λ, μ, λ', μ', but it would be taking the model too seriously to suppose that this relation will be satisfied if, for example, we apply (8.32) to the interaction of a vacant lattice site with a stress field. It is better to regard them as independent constants which may, in principle, be found from the macroscopic elastic constants of a material containing a large number of defects. In fact, according to (6.3), with constant external loading, the normal elastic energy density $\frac{1}{2}\lambda(e^T)^2 + \mu e_{ij}^T e_{ij}^T$ of the medium is increased by $-nE_{\text{int}}$ when n defects per unit volume are introduced. The apparent elastic constants are thus

$$\lambda_{\text{app}} = \lambda + C\Lambda, \qquad \mu_{\text{app}} = \mu + C\mathrm{M}$$

if C is the atomic concentration of defects.

We have supposed that e_{ij}^T is uniform, but we may take (8.32) to apply also to a nonuniform field, provided it varies little over a distance of the order of the size of the inclusion. Thus the force exerted on the

inhomogeneity by a stress field T is

$$F_l = \Omega\{\Lambda e^T \delta_{ij} + 2M e_{ij}^T\} e_{ij,l}^T. \tag{8.33}$$

Although we have derived this for the particular case where e_{ij}^T is produced by externally applied forces, it must hold also when e_{ij}^T is an internal stress, for the expression (6.6), from which in effect we derived (8.33), is the same as the general expression (7.4) which covers all cases.

Equation (8.32) is just the same as (8.28) with a_{ij} a linear function of e_{ij}^T. Calculation shows that, whereas the perturbation $e_{ij}' - e_{ij}^T$ produced by the presence of the inhomogeneous sphere has a uniform value given by (8.31) inside the sphere, it has the form of the stress field produced by the forces of Fig. 8b outside the sphere. Thus we may say that the applied field "induces" a complex point defect in the inhomogeneity and then exerts a force on it.

For two point defects 1 and 2 a distance r apart, we have from (8.32), (8.2), (8.6)

$$E_{\text{int}} = -6\Omega(M_1 \Delta V_2^2 + M_2 \Delta V_1^2)/r^6$$

in an obvious notation, and, by differentiation, a radially directed force

$$F = -36\Omega(M_1 \Delta V_2^2 + M_2 \Delta V_1^2)/r^7. \tag{8.34}$$

Had we found the force by evaluating (6.6) over a surface surrounding defect 1, we might have expected to get only the first term in (8.33). However, a detailed calculation shows that the second term appears as the image force on 1 due to the inhomogeneous sphere 2, so that (8.34) is correct.

9. Dislocations

a. Interaction Energy

To carry out a formal calculation of the interaction energy of the stress field S of a dislocation loop with another stress field T without using explicit expressions for the field of the dislocation, it seems to be necessary to make the three following assumptions:

(i) The displacement changes by a constant vector $\mathbf{b}$ on traversing any circuit c embracing the dislocation line:

$$\int_c u_{i,j}^S dx_j = b_i.$$

(ii) If $\mathbf{r}$ is the position vector from any fixed point on the dislocation line then

$$\lim_{r \to 0} r u_i^S(\mathbf{r}) = 0.$$

(iii) The integral

$$\int p_{ij}^{S} dS_j$$

vanishes even when taken over the surface bounding a volume which is traversed by the dislocation line.

The essential character of the dislocation is expressed by (i). Assumption (ii) excludes other line singularities, e.g. a line of dilatation[13] coinciding with the dislocation line, whereas (iii) excludes the possibility of distributions of body force along the dislocation line. Assumption (ii) ensures that the integral in (iii) will converge even though the stresses become infinite where the dislocation cuts the surface.

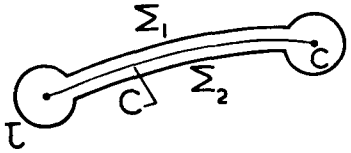

FIG. 9. To illustrate Section 9a.

Let C be any cap bounded by the dislocation line. We use (5.1) and take for Σ a surface, closely enveloping C, made up of surfaces Σ_1 and Σ_2 parallel to C and joined by a tube τ whose axis is the dislocation line (Fig. 9). As the radius of τ approaches zero, the second term in (5.1) vanishes because of (ii), since p_{ij}^{T} is supposed to be continuous in the neighborhood of the tube. If we divide the tube into many small segments, we see that the first term in (5.1) also vanishes as the tube contracts, in virtue of (iii) and the continuity of u_i^{T}. We are left with the contributions of Σ_1 and Σ_2. The contributions from the first term of (5.1) cancel and the remaining term gives

$$E_{\text{int}}(S,T) = \int_{\Sigma_1+\Sigma_2} (-p_{ij}^{T} u_i^{S}) dS_j = b_i \int p_{ij}^{T} dS_j \tag{9.1}$$

since u_i^{S} has a discontinuity b_i across C.

Let the shape of the loop be altered by giving a short segment of it having length l and direction $\mathbf{s}$ a small displacement $\boldsymbol{\xi}$. This adds to C a new surface element and $l\mathbf{s} \times \boldsymbol{\xi}$ is the product of its area and normal vector. The change in (9.1) is

$$\delta E_{\text{int}}(S,T) = l b_i p_{ij}^{T} \epsilon_{jkl} s_k \xi_l.$$

We may thus regard

$$F_l = \epsilon_{kjl} b_i p_{ij}^{T} s_k \tag{9.2}$$

as the force per unit length on the dislocation.[51,52]

[51] M. O. Peach and J. S. Koehler, *Phys. Rev.* **80**, 436 (1950).
[52] F. R. N. Nabarro, *Phil. Mag.* [7] **42**, 213 (1951).

For an infinite edge or screw dislocation along the x_3 axis, (9.2) gives the well-known results

$$F_1 = bp_{12}{}^T, \qquad F_2 = -bp_{11}{}^T \text{ (edge)} \tag{9.3}$$

$$F_1 = bp_{23}{}^T, \qquad F_2 = -bp_{13}{}^T \text{ (screw)}. \tag{9.4}$$

Koehler's[53] pioneer calculation gave an incorrect numerical factor for F_1 in (9.3) which, of course, causes no trouble if we are only interested in equilibrium with $F_1 = 0$. His method was equivalent to evaluating (7.5) with the term $p_{ij}u_{i,l}$ omitted. The result then depends on the shape of Σ. Read and Shockley's[54] method is equivalent to evaluating the same expression with the term $W\delta_{ij}$ omitted. The result again depends on the choice of Σ, but for their choice (a pair of parallel planes above and below the slip plane) gives the correct result. Leibfried[55] first clearly stated that the interaction term in the internal energy between an internal and an external stress system is zero. His results appeared to show that (5.1) gave correctly the force exerted on a dislocation by surface tractions or another dislocation, but not by a point defect. This difficulty has been resolved.[5,6]

Detailed discussion of the interaction between various configurations of dislocations may be found in references 9 and 10. Blin[56] has given an expression for the interaction energy between two dislocation loops in the form of a line integral.

Nabarro[57] constructed a solution of the Peierls-Nabarro equation representing two edge dislocations and a uniform external stress and verified that the latter was just what was required by (9.3) to give zero total force on either dislocation. Since this is one of the few cases where direct contact can be made between the elastic theory and an approximate atomic theory it seems worthwhile to sketch the solution of the corresponding problem for screw dislocations, where the analysis is quite simple.

The displacement around a screw dislocation in an infinite isotropic medium is everywhere parallel to the dislocation line (which we choose as z axis) and of magnitude

$$w = \frac{b}{2\pi}\tan^{-1}\frac{y}{x} = \frac{b\theta}{2\pi} \tag{9.5}$$

in Cartesian or polar coordinates. The Peierls-Nabarro condition requires that the stress and displacement at the atom plane adjacent to the slip

[53] J. S. Koehler, *Phys. Rev.* **60**, 397 (1941).
[54] W. T. Read and W. Shockley, *Phys. Rev.* **78**, 275 (1950).
[55] G. Leibfried, *Z. Physik* **126**, 781 (1949).
[56] J. Blin, *Acta Metallurgica* **3**, 199 (1955).
[57] F. R. N. Nabarro, *Proc. Phys. Soc. (London)* **59**, 256 (1947).

plane shall satisfy the relation

$$p_{zy} = -\frac{\mu b}{2\pi a} \sin \frac{4\pi w}{b}, \tag{9.6}$$

where a is the spacing of atom planes parallel to the slip plane.

It is well known that the purely elastic solution (9.5) itself satisfies (9.6). In fact we have

$$p_{zy} = \mu \frac{\partial w}{\partial y} = -\frac{\mu b}{2\pi} \frac{\cos \theta}{r} = -\frac{\mu b}{4\pi y} \sin 2\theta$$

which satisfies (9.6) with $y = \frac{1}{2}a$.

According to (9.4), two screw dislocations separated by a distance $2l$ exert a force $\mu b^2/4\pi l$ on one another. They should be kept apart, therefore, by an applied stress $-\mu b/4\pi l$. Let the dislocation be situated at the vertices $A(l,0)$, $B(-l,0)$ of the triangle ABC, $C(x,y)$ being any arbitrary point. From the properties of the triangle, the displacement and stress at C arising from the two dislocations and the applied stress are easily seen to be

$$w(x,y) = \frac{b}{2\pi} C - \frac{b}{4\pi l} y + w_0 \tag{9.7}$$

$$p_{zy}(x,y) = \frac{\mu b}{4\pi y} (\sin 2A + \sin 2B) - \frac{\mu b}{4\pi l} \tag{9.8}$$

where w_0 is an arbitrary constant. We shall show that this purely elastic solution satisfies (9.6) with only trivial modifications. To do this we evidently need a relation between the sines of $2A$, $2B$, $2C$ for a fixed value of y. Join the vertices of ABC to the center of its circumscribed circle to form three isosceles triangles whose equal sides are, in each case, radii $R = l \csc C$ of the circle and which embrace angles $2A$, $2B$, $2C$. Their areas must add up to ly, the area of ABC. This gives at once

$$\sin 2A + \sin 2B + \sin 2C = 2yl/R^2 = (y/l)(1 - \cos 2C)$$

or

$$y^{-1}(\sin 2A + \sin 2B) - l^{-1} = -[(y^{-2} + l^{-2})^{\frac{1}{2}}] \sin 2\{C + \tan^{-1}(y/l)\}.$$

When $y = \frac{1}{2}a/\{1 - (a/2l)^2\}^{\frac{1}{2}} \equiv y_0$, the factor [ ] is $2/a$, so that (9.3) and (9.4) satisfy (9.6) on the plane $y = y_0$ (instead of on the required plane $y = \frac{1}{2}a$), provided we give to w_0 the value $-G\{\tan^{-1}(y_0/l) + y_0/l\}$ in the upper half-plane and, to preserve the antisymmetry, an equal and opposite value in the lower half-plane. Thus the Peierls solution is derived from the elastic solution merely by removing the slab between $y = \pm y_0$, narrowing the gap to a, and giving a certain constant shift to the upper and lower half-planes. Thus, within the limits of the Peierls-Nabarro approximation,

we have found a state of affairs in which each atom is in equilibrium under the action of the same applied stress as is required by the elastic theory to maintain the dislocations in equilibrium on the continuum approximation.

b. Image Effects

The discussion of the interaction of dislocations with free surfaces usually involves rather lengthy calculations. We take up first the problem of a screw dislocation in a cylinder. The calculation is simple, but the result is rather unexpected. It turns out, in fact, that the image force need

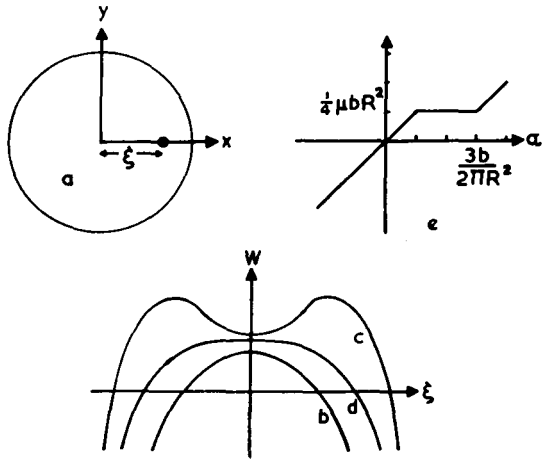

FIG. 10. Behavior of a screw dislocation in a cylinder.

not always tend to make a source of internal stress move towards the surface.

As may easily be verified, the displacement about a screw dislocation at the point $x = \xi$, $y = 0$ (Fig. 10a) in an isotropic infinite cylinder whose surface $x^2 + y^2 = R^2$ is free of stress has the form

$$w = \frac{b}{2\pi} \tan^{-1} \frac{y}{x - \xi} - \frac{b}{2\pi} \tan^{-1} \frac{y}{x - R^2/\xi} \tag{9.9}$$

if we stipulate a state of antiplane strain. Equation (9.9) is made up of an expression like (9.5), centered at $(\xi,0)$, and a similar expression of opposite sign centered at $(R^2/\xi,0)$. The "image displacement" in this case is just that produced by an image dislocation at the image point in the sense of electrostatics. The image force is directed radially outwards and is inversely proportional to the dislocation-image distance. It is convenient to write

$$F_x = -\partial W/\partial \xi \tag{9.10}$$

with

$$W = (\mu b^2/4\pi) \ln (R^2 - \xi^2). \tag{9.11}$$

Equation (9.11) is sketched in Fig. 10b; evidently the dislocation is in unstable equilibrium when $\xi = 0$ and will tend to leave the cylinder if disturbed.

A calculation like this, which assumes an infinite rod and a state of antiplane strain, is, however, unrealistic. On any cross section of the cylinder there are tractions which have zero resultant but give a twisting moment about the axis of the cylinder whose magnitude can easily be shown to be[58]

$$M = \tfrac{1}{2}\mu b(R^2 - \xi^2). \tag{9.12}$$

Thus for a finite rod cut from the infinite cylinder, the displacement will only retain the form (9.9) if suitable tractions are distributed over the ends,[59] and (9.10) is really the sum of the image force and the force due to these tractions. To find the true image force in a cylinder free of all surface tractions we must get rid of these end couples. Their removal gives a twist per unit length

$$\alpha(\xi) = M/\tfrac{1}{2}\mu\pi R^4 = (b/\pi R^2)(1 - \xi^2/R^2) \tag{9.13}$$

to the rod, together with certain end corrections which we may neglect if the length of the cylinder is many times its diameter. The production of twist by a screw dislocation in a cylinder (or rather the converse) may easily be verified by slitting a length of thick-walled rubber tubing along a radial plane. Twisting the tube produces an obvious screw dislocation, which can be made permanent by coating the cut with rubber solution.

The total elastic field is found by superimposing (9.9) and the field arising from the twist (9.13). From it the true image force may be calculated. It is easily found that (9.11) must be replaced by

$$W = (\mu b^2/4\pi)[\ln (R^2 - \xi^2) - (R^2 - \xi^2)^2/R^4]. \tag{9.14}$$

As ξ increases, the elastic energy for the case in which twist is prevented decreases and the part of this energy which is released by allowing twist to take place also decreases, initially rather rapidly. The upshot is that W first increases and then decreases (Fig. 10c). The dislocation is now bound to the center of the rod by the image forces. Only if it is somehow displaced about half (more precisely 0.54) the distance to the surface, do the image forces tend to pull it out of the rod.

[58] J. D. Eshelby, *J. Appl. Phys.* **24**, 176 (1953).
[59] E. H. Mann, *Proc. Roy. Soc.* **A199**, 376 (1949).

These results may have some application in the study of metallic "whiskers." Present theories[60,61,62] suggest that whiskers which grow at the tip may depend for their growth on an axial screw dislocation, while those which grow at the root may be free of dislocations. Figure 10c assures us that an axial screw dislocation, if present, will be stable against quite large displacements from the axis. Equation (9.13) suggests that there should be an easily observable rotation of the crystal lattice as we move along the whisker. For example with $\xi = 0$, $b = 3.10^{-8}$ cm, $R = 10^{-4}$ cm, the twist is about 50 degrees per centimeter.

It is a simple matter to find out how much the whisker must be bent or twisted in order to dislodge the dislocation. For example, an external couple M' produces a shear stress proportional to the distance from the axis, and hence a force on the dislocation proportional to ξ. This can be taken into account by adding a term $M'b\xi^2/\pi R^4$ to (9.14). For small M' this blunts the maxima in Fig. 10c and moves them nearer the center. For

$$M' = \tfrac{1}{2}\mu b R^2 \tag{9.15}$$

the maxima coalesce at the origin (Fig. 10d). For greater values of M' the center becomes an unstable position and the dislocation should be ejected from the rod. What has just been said applies when the sign of M' is such as to produce a twist tending to undo the twist arising from the dislocation itself. (We see from (9.12) and (9.15) that M' need annul only half the twist caused by the dislocation.) A couple of the opposite sign would merely deepen the well in Fig. 10c and bind the dislocation more tightly to the axis. The torsional stress-strain curve for a whisker containing a screw dislocation should thus ideally have the form of Fig. 10e. The horizontal portion represents the disappearance of the twist (9.13) when ξ suddenly changes from 0 to R as the dislocation leaves the whisker. The behavior of the dislocation under other types of external loading may also be discussed.*

The problem of a screw dislocation along the axis of a finite cylinder, with end effects included, has been solved.[63] For a long cylinder (rod) the unimportance of the end effects is confirmed, whilst for a very short cylinder (disk) the image field is, so to speak, all end effect. The stress

* The writer is indebted to Professor F. X. Eder for pointing out an error in the version of Fig. 10e in reference 58. He also points out that a factor 2 is missing from the right-hand side of Eq. (4) of the same reference: this leads to errors of 2 or $\frac{1}{2}$ in some subsequent formulas.

[60] F. C. Frank, *Phil. Mag.* [7] **44**, 854 (1953).

[61] J. D. Eshelby, *Phys. Rev.* **91**, 755 (1953).

[62] G. W. Sears, *Acta Metallurgica* **3**, 361 (1955).

[63] J. D. Eshelby and A. N. Stroh, *Phil. Mag.* [7] **42**, 1401 (1951).

components p_{zy} and p_{zx} become nearly zero at distances from the dislocation greater than the thickness of the disk. Consequently two screw dislocations in a plate interact with a short-range force, in contrast to the inverse first power law interaction in an infinite medium.

Koehler[53] has considered the problem of an edge dislocation parallel to the axis of a circular cylinder. Let Fig. 10a now refer to an edge dislocation with its Burgers vector along the x axis. His results show that

$$F_x = \frac{\mu b^2}{2\pi(1-\sigma)} \frac{1}{R^2/\xi - \xi} \tag{9.16}$$

This is just the force arising from an edge dislocation at the image point, although the image field is in fact more complex.

Koehler actually solved the problem of a dislocation in an infinite cylinder in a state of plane strain. As in the case of the screw dislocation, there will be nonzero tractions on the ends of a finite rod cut from the cylinder, and we might suppose that their removal would modify F_x. They have, however, no resultant or moment, and so, according to St. Venant's principle, removing them gives rise only to small end effects. Apart from these, the elastic state of an edge dislocation in a long cylinder coincides with the state derived on the assumption of plane strain, and (9.16) gives correctly the image force per unit length. There is nothing analogous to the odd behavior of the screw dislocation; an edge dislocation in a rod will always tend to leave it. Evidently a mixed dislocation will be attracted to or repelled from the axis of a whisker according to the relative strength of its screw and edge components.

Head[64,65] has given an extensive discussion of the interaction of dislocations with plane boundaries. The boundary may be a free or clamped surface, a surface where tangential but not normal displacement is allowed (slipping surface), or the boundary between regions of differing elastic constants.

c. Dislocations in Motion

At one time it appeared that the dynamical behavior of dislocations might play an important role in the theory of plasticity. Roughly we may say that a moving dislocation exhibits dynamical behavior when the kinetic energy of the disturbance caused by its passage is comparable with its elastic strain energy. It now seems likely that frictional forces on a dislocation prevent this condition being realized in practice.

[64] A. K. Head, *Phil. Mag.* [7] **44**, 92 (1953).
[65] A. K. Head, *Proc. Phys. Soc.* (*London*) **B66**, 793 (1953).

A number of writers have discussed dislocations in uniform motion.[66–71] The case of a screw dislocation in an isotropic medium is particularly simple. The displacement w in a state of antiplane strain satisfies

$$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} = 0 \tag{9.17}$$

when w is independent of time and

$$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} - \frac{1}{c^2}\frac{\partial^2 w}{\partial t^2} = 0, \qquad c = (\mu/\rho)^{\frac{1}{2}}, \qquad \rho = \text{density}$$

when it is not. For an elastic field moving uniformly parallel to the x axis with velocity v, the displacement $w = \varphi(x - vt,y)$ satisfies

$$\frac{\partial^2 w}{\partial x^2} + \frac{1}{\beta^2}\frac{\partial^2 w}{\partial y^2} = 0 \qquad \beta = (1 - v^2/c^2)^{\frac{1}{2}}. \tag{9.18}$$

Thus if

$$w = w(x,y) \tag{9.19}$$

satisfies (9.17), then

$$w = w\left(\frac{x - vt}{\beta}, y\right) \tag{9.20}$$

satisfies (9.18). If we take for (9.19) the expression (9.5), the corresponding relation (9.20) still has the property characteristic of a screw dislocation, namely that w increases by b on encircling the point $x = vt$. The field of the moving dislocation is derived from the field of the static dislocation by giving it a "Lorentz contraction." The contracted field continues to satisfy the Peierls condition (9.6). Leibfried and Dietze[69] considered a screw dislocation moving in the midplane of a plate with free surfaces. They established the "relativistic" relation

$$E^v = E_{\text{kin}}{}^v + E_{\text{el}}{}^v + E_{\text{pot}}{}^v = E^0/\beta \tag{9.21}$$

for the total energy at velocity v, made up of contributions from the kinetic and elastic energy of the continuum and the potential energy of the atomic forces maintaining the law (9.6) at the slip plane.

These results may be generalized. If a static dislocation satisfies any generalization of the law (9.6), say $p_{zy}(x, \pm\frac{1}{2}a) = f[w(x,\frac{1}{2}a) - w(x,-\frac{1}{2}a)]$, its contracted moving version satisfies the same relation. Equation (9.21)

[66] F. C. Frank, *Rept. Conf. on Strength of Solids Univ. Bristol* p. 48, 1947.
[67] F. C. Frank, *Proc. Phys. Soc. (London)* **A62,** 131 (1949).
[68] J. D. Eshelby, *Proc. Phys. Soc. (London)* **A62,** 307 (1949).
[69] G. Leibfried and H. D. Dietze, *Z. Physik* **126,** 790 (1949).
[70] R. Bullough and B. A. Bilby, *Proc. Phys. Soc. (London)* **B67,** 615 (1954).
[71] A. W. Sáenz, *J. Rat. Mech. Analysis* **2,** 83 (1953).

continues to hold for this more general law, even if the slip plane does not lie at the center of the plate, and if the surfaces of the plate are either free ($\partial w/\partial y = 0$) or clamped ($w = 0$). The proofs are simple and do not require a knowledge of the explicit form of $w(x,y)$. Let the point $(x = X,y)$ in the static solution $w = w(x,y)$ and the point $(x = \beta X,y)$ in the moving solution $w = w(x/\beta,y)$ be called corresponding. (We take t to be zero.) Then at corresponding points the following pairs of quantities are evidently equal:

	(i)	(ii)	(iii)	(iv)	(v)	(vi)
static	w	$\dfrac{\partial w}{\partial y}$	$\dfrac{\partial w}{\partial x}$	$(\text{grad } w)^2$	dy	dx
moving	w	$\dfrac{\partial w}{\partial y}$	$\dfrac{1}{\beta}\dfrac{\partial w}{\partial x}$	$(\text{grad } w)^2 - \dfrac{\dot{w}^2}{c^2}$	dy	$\dfrac{dx}{\beta}$.

The line elements in (v), (vi) are supposed to be bounded by corresponding points. Column (iv) expresses the "relativistic" invariance of the Lagrangian density, and follows from (ii), (iii), since $\dot{w} = -v\partial w/\partial x$.

Columns (i), (ii) show that the two solutions satisfy either of the boundary conditions $w = 0$ or $\partial w/\partial y = 0$ together at the surfaces of the plate and that along the slip plane p_{zy} is the same function of w in the two cases; thus, if a certain law of force holds the static field together, it will hold its Lorentz-contracted version together. The potential energy per unit length of the slip plane depends only on the difference in w across the slip plane and so from (i) and (vi) $E_{\text{pot}}{}^v = \beta E_{\text{pot}}{}^0$. The total energy is thus

$$E^v = \tfrac{1}{2}\int\{\mu(\text{grad } w)^2 + \rho\dot{w}^2\}dxdy + \beta E_{\text{pot}}{}^0$$

where the integral extends over the elastic region. The integral can be rearranged with an eye to making use of column (iv), and we easily find

$$E^v = \frac{E^0}{\beta} + \frac{v^2}{c^2\beta}\left[E_{\text{pot}}{}^0 + \frac{1}{2}\int\left\{\left(\frac{\partial w}{\partial x}\right)^2 - \left(\frac{\partial w}{\partial y}\right)^2\right\}dxdy\right]$$

where the integral is evaluated for the static case. By integration by parts and use of (9.17), the integral can be converted to

$$\int_{-\infty}^{\infty} xp_{zy}\frac{dw}{dx}\,dx\Bigg|_{y=-\frac{1}{2}a}^{y=\frac{1}{2}a}.$$

But by an argument of Foreman and Nabarro (reference 9, p. 360: put $\sigma = 0$ for antiplane strain), this is just $-E_{\text{pot}}{}^0$, which establishes (9.21). If a approaches zero, $E_{\text{pot}}{}^0$ becomes negligible compared with $E_{\text{el}}{}^0$ and we recover a formal result of Frank[67] for the purely elastic case.

The behavior of an edge dislocation in an isotropic medium or of any

dislocation in an anisotropic medium is "relativistic with complications,"[67] owing to the existence of several velocities of sound.

We turn now to the properties of dislocations in nonuniform motion. Nabarro[72] has given a general method for calculating the elastic field of a dislocation loop which is changing its shape in an arbitrary way. The result takes a relatively simple form for the two-dimensional problem of a screw dislocation whose center moves in an arbitrary manner.[6,73] If the position of its center at time τ is $x = \xi(\tau)$, $y = \eta(\tau)$, the displacement is

$$w(x,y,t) = \frac{b}{2\pi} \int_{-\infty}^{\tau_0} \frac{c(t-\tau)\{(y-\eta)\dot{\xi} - (x-\xi)\dot{\eta}\}}{(x-\xi)^2 + (y-\eta)^2} \frac{d\tau}{s}$$

where $s^2 = c^2(t-\tau)^2 - (x-\xi)^2 - (y-\eta)^2$ and τ_0 is the root of $s^2 = 0$ which is less than t. Such an arbitrary motion will require an external stress system varying suitably in space and time to maintain it. For simple cases this field can be calculated by imposing suitable conditions at the center of the dislocation. For example, we may require that the Peierls-Nabarro condition be satisfied there,[74,73] or we may, in effect, require that the force which the dislocation exerts on itself balance the force due to the external field.[73] At any moment the field at a point on the dislocation is made up of the applied field and contributions from all other points of the dislocation. Because of the finite time of propagation of elastic disturbances, the present motion depends on the previous history of the motion extending back over a time of the order of the maximum dimension of the dislocation loop divided by the velocity of sound. As a result, the equation of motion of the dislocation takes the form of an integral equation giving the external field required to maintain the prescribed motion. The more interesting problems of finding the motion in a prescribed applied elastic field requires the inversion of this integral equation. It can be carried out approximately in simple cases.[73] Roughly speaking, the rectilinear motion of an infinite screw dislocation is the same as that of a Newtonian particle of mass $(\rho b^2/4\pi) \ln (R/a)$ acted on by a force $F = bp_{zy}$, where p_{zy} is the applied stress; R is a distance of the order of the dimensions of the disturbed region surrounding the dislocation. For motion which starts from rest at $t = 0$ and in which the distance of the dislocation from the starting point increases monotonically, $R \sim ct$. Thus, for example, a dislocation which is started by an impulsive force and then runs freely will slow down as its effective mass increases. For oscillatory motion with frequency ω, $R \sim c/\omega$.

In discussing a screw dislocation, we can make use of an electro-

[72] F. R. N. Nabarro, *Phil. Mag.* [7] **42**, 1224 (1951).
[73] J. D. Eshelby, *Phys. Rev.* **90**, 248 (1953).
[74] F. R. N. Nabarro, *Proc. Roy. Soc.* **A209**, 278 (1951).

magnetic analogy.[74,73] If the dislocation is parallel to the z axis, the only nonzero elastic quantities are the z component w of the displacement and the stresses p_{zx}, p_{zy}. Consider an electromagnetic field in which

$$E_z = H_x = H_y = 0$$

and all quantities are independent of z. Make the identification

$$\partial w/\partial t = H_z/\rho^{\frac{1}{2}}, \qquad p_{zx} = -E_y/\mu^{\frac{1}{2}}, \qquad p_{zy} = E_x/\mu^{\frac{1}{2}}.$$

Here μ and ρ are the shear modulus and density. We identify the velocity of shear waves $c = (\mu/\rho)^{\frac{1}{2}}$ with the velocity of light and use Heaviside units for the electromagnetic field. The electromagnetic energy and Poynting vector translate into the sum of the elastic and kinetic energy densities and the elastic energy-flux vector. The analog of a dislocation

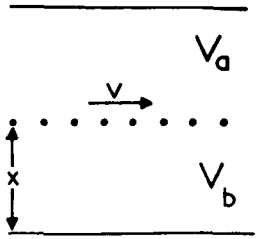

FIG. 11. Lorentz force on a procession of dislocations.

with Burgers vector b is a line charge of $b/\mu^{\frac{1}{2}}$ units per unit length. The force on a stationary charge translates correctly into the force on a stationary dislocation. The Lorentz force on a moving charge translates into a force perpendicular to the direction of motion of the dislocation of magnitude

$$F = \rho b v V \tag{9.22}$$

where v is the speed of the dislocation and V is the velocity of the medium along the z axis "at the center of the dislocation" (to avoid the singularity at the dislocation, we may take V to be the average of $\dot{w}$ over a small circle centered on the dislocation). Nabarro[74] has elucidated the physical meaning of the Lorentz force. The following is a crude illustration.

Let a closely spaced procession of n screw dislocations per unit length move with velocity v in a plate of unit thickness (Fig. 11). Their motion makes the blocks above and below the slip plane slide over each other in a direction perpendicular to the paper with relative velocity

$$V_a - V_b = bnv. \tag{9.23}$$

The effective velocity of the medium at the slip plane is $V = \frac{1}{2}(V_a + V_b)$;

we can give this any value, while still maintaining the relation (9.23). The kinetic energy per unit length and depth of the plate is

$$T = \tfrac{1}{2}\rho V_a^2(1 - x) + \tfrac{1}{2}\rho V_b^2 x = \tfrac{1}{2}\rho(V - \tfrac{1}{2}bnv)^2 + \rho bnvVx.$$

If we raise the height of the procession by δx, maintaining v and V constant, some external source must do work $\delta T = \rho bvnV\delta x$ and we may say that there is a force $F = \rho bvVn$ on the n dislocations (or a force (9.22) on each) resisting vertical motion.

Replace the screw dislocations by a procession of edge dislocations. The blocks now move with velocities V_a, V_b parallel to the slip direction: otherwise the argument is word for word the same as before and we obtain a Lorentz force (9.22) on an *edge* dislocation. Now V is the velocity of the medium in the slip-direction and F is still perpendicular to the slip plane. This Lorentz force on a procession of edge or screw dislocations agrees with what one gets by integrating the energy-momentum tensor (7.7) over a loop embracing unit length of the procession.

An aerofoil moving relative to a fluid generates a dislocation in it. To see this, suppose that the aerofoil is at rest with the fluid streaming past it. Consider a particle upstream straddling the critical streamline which divides at the nose of the aerofoil. The particle is split into two parts which traverse the upper and lower surfaces of the aerofoil and leave the trailing edge at different times, so that downstream they both lie on the critical streamline, but are separated by a certain distance, the "Burgers vector." This Burgers vector can be shown to be equal to the ratio of circulation and stream velocity, and so the lift is equal to the Lorentz force (9.22). The lift is a "real" force: if we remove the aerofoil, leaving a free vortex with the same circulation, the force takes on the "fictitious" character of the force on a dislocation.

By a very general argument,[75] it may be shown that an electron moving with velocity v through an isotropic flux of electromagnetic waves experiences a retarding force

$$F = -\alpha\sigma Wv/c \tag{9.24}$$

where W is the energy density of the electromagnetic field, σ is the Thompson scattering cross section, and $\alpha = \frac{4}{3}$. If we take σ to be a prescribed constant, we can apply the same argument to a line charge moving in a flux of electromagnetic waves isotropic in the xy plane, and, hence, to the related dislocation problem. We should obtain (9.24) again, where now F is the retarding force per unit length of line charge or dislocation, σ is the scattering area of unit length, and α is changed from $\frac{4}{3}$ to $\frac{3}{2}$ by the

[75] L. Landau and E. Lifshitz, "The Classical Theory of Fields." Addison-Wesley, 1951.

transition from three to two dimensions. The same expression should be valid for a screw dislocation in a three-dimensional flux of sound waves if we reduce the value of α to allow for the fact that the "antiplane" sound waves contribute only a part of the total energy density W. Leibfried[44] has considered the corresponding problem for an edge dislocation. He obtains (9.24) with $\alpha = \frac{1}{10}$. By taking σ to be of the order of b and identifying W with the energy of thermal vibrations, he finds a retarding force which is sufficient to keep v a small fraction of c for any reasonable applied stress.

Nabarro[74] has given a critical discussion of Leibfried's theory. The scattering cross section of a screw dislocation for an elastic wave need not be assumed, but can be found from the electromagnetic analogy. Unlike the cross section for an electron it is not independent of the wave length of the scattered wave, but very nearly proportional to it. The arguments leading to (9.24) thus need modification. The result is found to be that F vanishes at least to order v/c. The electromagnetic analogy assumes that Hooke's law is valid even for infinite strains and neglects the atomic structure. In fact the disturbed region at the center of the dislocation may well act as a scatterer with a cross section of the order of b for waves near the top of the Debye spectrum, but smaller for long waves. This would lead to a force of the form (9.24) with an α presumably less than Leibfried's value. According to Granato and Lücke,[76] damping experiments enable the limits $0.015 < \alpha < 0.12$ to be set for dislocations in germanium.

d. Continuous Distributions of Dislocations

Having replaced the dislocations of a crystal lattice by their continuum analogs, it may be convenient to go a stage further and regard a body containing a large number of dislocations as being filled with a continuous distribution of dislocations. Following Nye[77] we may define a tensor α_{ij} whose ij element gives the sum of the x_i components of the Burgers vectors of all the dislocations threading unit area perpendicular to the x_j axis. The total Burgers vector of the dislocations threading a circuit c will be

$$b_i = \int_C \alpha_{ij} dS_j \tag{9.25}$$

where C is a cap bounded by c. So far α_{ij} merely provides a convenient description of the distribution of dislocations; we need to relate it to the deformation of the lattice and the state of internal stress. Since the

[76] A. Granato and K. Lücke, Technical Report, Contract No: DA-36-039 SC-52623 Part II. Brown University, 1955.

[77] J. F. Nye, *Acta Metallurgica* **1**, 153 (1953).

internal stress is, in principle, adequately described by the incompatibility tensor, we should be able to express S_{ij} in terms of α_{ij}. Kröner[78] has made the necessary connection. On the other hand, the Riemannian geometry associated with S_{ij} is not adequate for description of a continuous distribution of dislocations. Kondo[79] and Bilby and co-workers[80] have given an elegant interpretation in terms of non-Riemannian geometry. We give a rather over-simplified sketch of this work, basing it directly on the idea of the Burgers circuit.

Let the comparison crystal be simple cubic with a unit cell defined by the vectors $\epsilon\mathbf{i}_1$, $\epsilon\mathbf{i}_2$, $\epsilon\mathbf{i}_3$ in the notation of Section 3 (ϵ need not be infinitesimal). The possibility of carrying out associated circuits in the real and comparison crystals implies that for every vector step $\epsilon\mathbf{i}_i$ we take in the comparison crystal we can pick out a step, say $\epsilon\mathbf{e}_i(P)$, at the corresponding point P in the real crystal. We may express $\mathbf{e}_i(P)$ in terms of the $\mathbf{i}_i$:

$$\mathbf{e}_i(P) = D_{ij}(P)\mathbf{i}_j \tag{9.26}$$

and conversely

$$\mathbf{i}_i = E_{ij}(P)\mathbf{e}_j(P) \qquad \text{with} \qquad D_{ij}E_{jk} = \delta_{ik}. \tag{9.27}$$

When there is a descrete distribution of dislocations, the Burgers circuit is drawn in "good" crystal which by definition is a region where the identification (9.26) can be made by inspection. If we pass to the case of a continuous distribution of dislocations, there is no "good" crystal, nor indeed any crystal lattice. Then (9.26) becomes a direct specification of the particular vector triplet $\mathbf{e}_j$ at a point of one continuum (representing the real crystal) which corresponds with the triplet $\mathbf{i}_j$ at the corresponding point of a second continuum (representing the comparison crystal). For ease of description, we shall adopt the hybrid point of view that the $\epsilon\mathbf{e}_j$ are lattice vectors of the real crystal, but that ϵ is small enough in comparison with the dimensions of the Burgers circuit for sums of lattice steps to be replaced by integrals.

Draw a closed circuit c in the real crystal. The element of path joining x_i to $x_i + dx_i$ is the vector $\mathbf{i}_i dx_i$ and the sum

$$\int_c \mathbf{i}_i dx_i$$

is zero. We can exhibit this explicitly as a sum of lattice steps in the real crystal by expressing $\mathbf{i}_i$ in terms of $\mathbf{e}_i$:

$$\int_c E_{ij}(P)\mathbf{e}_j(P)dx_i.$$

[78] E. Kröner, *Z. Physik* **142**, 463 (1955).
[79] K. Kondo, *Proc. 2nd Japan Natl. Congr. Appl. Mech. 1952*, p. 41 (1953).
[80] B. A. Bilby, R. Bullough, and E. Smith, *Proc. Roy. Soc.* **A231**, 263 (1955).

The sum of the corresponding steps in the comparison lattice is found by replacing $\mathbf{e}_j$ by its associated vector $\mathbf{i}_j$ in the comparison lattice. Thus the Burgers vector of the circuit is

$$\mathbf{b} = \int_c E_{ij}(P)\mathbf{i}_j dx_i.$$

By Stokes's theorem, this becomes the surface integral

$$\mathbf{b} = \mathbf{i}_j \int_C \epsilon_{ikl} E_{ij,l} dS_k$$

taken over a cap C bounded by c. Comparison with (9.25) gives

$$\alpha_{jk} = \epsilon_{ikl} E_{ij,l}.$$

The divergence $\alpha_{jk,k}$ vanishes, so that the choice of the cap C is arbitrary. This is the continuum analog of the rule that a dislocation cannot end in the material. The Burgers vector associated with a surface element dS_k is

$$d\mathbf{b} = \alpha_{jk}\mathbf{i}_j dS_k.$$

The *local* Burgers vector is, by definition, the vector in the real lattice which corresponds to the Burgers vector in the comparison lattice. It is found by replacing $\mathbf{i}_j$ by $\mathbf{e}_j = D_{jp}\mathbf{i}_p$:

$$d\mathbf{b}' = \alpha_{jk} D_{jl}\mathbf{i}_l dS_k.$$

If we choose to take the surface element in the form of an antisymmetric tensor dS_{mn}, where $dS_k = -\frac{1}{2}\epsilon_{kmn} dS_{mn}$ the components of $d\mathbf{b}'$ are easily found to be

$$db_p' = T_{mn}{}^p dS_{mn}$$

where

$$T_{mn}{}^p = \tfrac{1}{2} D_{jp}\{E_{mj,n} - E_{nj,m}\}. \tag{9.28}$$

For simplicity we now suppose that $\mathbf{e}_i$ and $\mathbf{i}_i$ differ only infinitesimally from one another and write

$$D_{ij} = \delta_{ji} + U_{ji}$$

in analogy with (3.1). Then $E_{ij} = \delta_{ji} - U_{ji}$ and[80a]

$$\alpha_{ij} = -\epsilon_{mjp} U_{im,p}. \tag{9.29}$$

We may still define a rotation in terms of the $\mathbf{e}_i$ and $\mathbf{i}_i$ by means of (3.13). This gives

$$\tilde{\omega}_{ij} = \tfrac{1}{2}(U_{ij} - U_{ji}) \qquad \text{or} \qquad \tilde{\omega}_k = -\epsilon_{kij} U_{ij}.$$

If we regard $\epsilon\mathbf{e}_1$, $\epsilon\mathbf{e}_2$, $\epsilon\mathbf{e}_3$ as the edges of a distorted unit cell in the real

[80a] B. A. Bilby, *Rept. Conf. Defects Crystalline Solids, Univ. Bristol*, p. 124, 1955.

crystal, it is reasonable to call

$$e_{ij} = \tfrac{1}{2}(\mathbf{e}_i \cdot \mathbf{e}_j - \delta_{ij}) = \tfrac{1}{2}(U_{ij} + U_{ji}) \tag{9.30}$$

the strain components. This is the point of view of Kröner,[78] who supposes there exists in a crystal with a continuous distribution of dislocations a "nonsysmmetric state of strain" given by U_{ij} (replacing the $u_{i,j}$ of the compatible case), from which one can derive a symmetrical strain and a rotation which are no longer connected by (3.14). We have, rather,

$$\kappa_{ji} \equiv \tilde{\omega}_{j,i} = \alpha_{ij} - \tfrac{1}{2}\alpha_{mm}\delta_{ij} - \epsilon_{jmp}e_{im,p}. \tag{9.31}$$

(Write $U_{im} = e_{im} + \tilde{\omega}_{im}$ in (9.29), express $\tilde{\omega}_{im}$ as a vector, and note that $\alpha_{mm} = -2\tilde{\omega}_{mm}$.) The incompatibility tensor corresponding to the strain (9.30) is easily found by operating on (9.31) with $\epsilon_{ikq}\partial/\partial x_q$; we find

$$S_{kj} = \epsilon_{ikq}(\alpha_{ij} - \tfrac{1}{2}\alpha_{mm}\delta_{ij})_{,q}.$$

Kröner[78] gave the explicitly symmetric form

$$S_{kj} = \tfrac{1}{2}\epsilon_{ikq}\alpha_{ij,q} + \tfrac{1}{2}\epsilon_{ijq}\alpha_{ik,q}.$$

The two expressions can be shown to be identical because of the relation $\alpha_{ik,k} = 0$. When α_{ij} is known, S_{ij} can be found, and hence the stresses are determined, if we assume with Kröner that they are derived from (9.30) by Hooke's law. Evidently if there is a uniform distribution of dislocations ($\alpha_{ij,k} = 0$), there is no stress.

The quantity (9.31) gives the rate of rotation of the triplet $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ as we follow it about the lattice, just as in the compatible case. It is Nye's[77] curvature tensor. Nye gave (9.31) for cases where the term in e_{mi} could be neglected. Kröner[78] gave the complete form, but with a slight difference in interpretation. When $\alpha_{ij} = 0$, and consequently $S_{ij} = 0$, (9.31) reduces to the ordinary compatible relation (3.14) giving the gradient of the rotation. Thus, in general, (9.31) gives the lattice rotation arising from dislocations and any compatible strain caused by body and surface forces. Kröner assumes, on the other hand, that the strain may be divided into a compatible and an incompatible part, and that the last term in (9.31) refers to only the latter. Thus κ_{ji} vanishes in his formulation if $\alpha_{ij} = 0$ and is a measure of the rotations due to the dislocations alone.

It is clear that $\alpha_{ij} - \tfrac{1}{2}\alpha_{mm}\delta_{ij}$ is a measure of the failure to satisfy the condition (3.14) for compatibility between strain and rotation, just as S_{ij} is a measure of the failure to satisfy the more rigorous strain compatibility conditions. We may give the following physical interpretation. Mark out a thin straight rod in the material and cut it out. It becomes a rod with curvature and torsion specified by $\kappa_{ji}' = \epsilon_{mjp}e_{mi,p}$ owing to

relaxation of internal stress. If we annihilate the dislocations contained in it, it undergoes a further curvature and torsion specified by

$$\kappa_{ji}'' = -(\alpha_{ij} - \tfrac{1}{2}\alpha_{mm}\delta_{ij}).$$

The connection with non-Riemannian geometry comes about as follows. (We no longer assume that D_{ij} differs only slightly from δ_{ij}.) In an obvious sense, the vectors $\mathbf{e}_1(P)$ and $\mathbf{e}_1(Q)$ at points P, Q are "equivalent." More generally, we can say that $\mathbf{A}(P) = a_i(P)\mathbf{e}_i(P)$ and

$$\mathbf{A}(Q) = a_i(Q)\mathbf{e}_i(Q)$$

are equivalent if $a_1(P) = a_1(Q)$, $a_2(P) = a_2(Q)$, $a_3(P) = a_3(Q)$. Evidently $\mathbf{A}(P)$ and $\mathbf{A}(Q)$ are generated by the transformation (9.26) from equal vectors in the comparison crystal. Let $\mathbf{A}$ have rectangular coordinates A_i; then

$$\mathbf{A} = A_i\mathbf{i}_i = a_i\mathbf{e}_i = a_iD_{ij}\mathbf{i}_j$$

and $A_k = a_iD_{ik}$ or, multiplying by E_{kj} and using (9.27), $a_i = A_kE_{kj}$. The condition $a_i(P) = a_i(Q)$ is thus

$$A_k(P)E_{kj}(P) = A_k(Q)E_{kj}(Q).$$

If P, Q are neighboring points x_i, $x_i + dx_i$ and we put

$$A_i(Q) - A_i(P) = dA_i$$

this gives

$$dA_kE_{kj} = -A_kE_{kj,l}dx_l$$

or by (9.27)

$$dA_m = -L_{kl}{}^mA_kdx_l \tag{9.32}$$

where

$$L_{kl}{}^m = D_{jm}E_{kj,l}.$$

In the language of differential geometry, a relation like (9.32) prescribing which vectors at neighboring points of a coordinate network (manifold) are to be considered equivalent is known as a *linear connection* with coefficients $L_{kl}{}^m$. In a Riemannian geometry, $L_{kl}{}^m$ is symmetric in k and l. (In the geometry of Section 4, $L_{kl}{}^m = e_{lm,k} + e_{mk,l} - e_{kl,m}$ to the first order.) The geometry associated with the dislocated lattice is more complex since $L_{kl}{}^m$ is not symmetric. In fact, its antisymmetric part (torsion tensor) $\frac{1}{2}(L_{kl}{}^m - L_{lk}{}^m)$ is just the local Burgers vector density in the form (9.28).

10. Surface and Volume Defects

We saw in Section 6 that when the elastic constants of a body are changed from one function of position to another under constant external

loading, half the work done by the external forces goes to increase the internal elastic energy. Since the calculation rests on a comparison of the equilibrium states before and after the change, it cannot tell us what happens to the missing half of the energy. It may be dissipated or it may reappear, for example, as kinetic or surface energy. Apart from its application to point defects (Section 8e), this result has a bearing on the behavior of grosser inhomogeneities of the lattice, in particular of cracks and of boundaries across which the orientation of the crystal changes.

A crack may be regarded as a narrow zone where the elastic constants are zero; the extension of a crack qualifies as a change in the distribution of elastic constants of the type we are considering. In the Griffith criterion for the spread of a crack, the energy made available in a small extension of the crack must be equal to the resulting increase of surface energy. According to (6.3), this means that at constant load the increase of surface energy must be equal to the *increase* of elastic energy. On the other hand, suppose that the body is strained by giving parts of its surface fixed displacements and leaving the rest free of traction. Then δE_{ext} is zero in any change and the criterion for spread of the crack is that the increase of surface energy shall be equal to the *decrease* of elastic energy.[81,82]

There is a force on a grain boundary or twin boundary in virtue of the fact that it represents an array of dislocations.[10] There is also a less obvious contribution arising from the fact that it is effectively a junction between regions with different elastic constants, even though the material is homogeneous. As we cross the boundary, the orientation of the crystal axes changes and so does the array of elastic coefficients c_{ijkl}. In this wider sense, the material is elastically inhomogeneous.

The force which a stress-field exerts on an element of the boundary, regarded as an array of dislocations, can be found by applying (9.2) to the dislocations it contains. In simple cases it can be found directly. Figure 12a illustrates schematically the experiment of Parker and Washburn[83] on the movement of small-angle grain boundaries. A beam is loaded at one end and contains a tilt boundary AB of angle ω. If the boundary moves a distance dx to the left, the load descends a distance ωdx and loses potential energy $W\omega dx$. Thus the force on the boundary has magnitude $W\omega$ and is directed to the left. If the load were upward, the force would be directed to the right.

Contrast Fig. 12a with the rather artificial situation shown in Fig. 12b. Here AB marks not a grain boundary but the junction between regions

[81] A. A. Griffith, *Phil. Trans. Roy. Soc.* **A221,** 163 (1920).

[82] E. Orowan, *Welding J.* **34,** 157s, 1955.

[83] E. R. Parker and J. Washburn, *Trans Am. Inst. Mining Met. Engrs.* **194,** 1076 (1952).

with different elastic constants. Suppose that the Young's modulus E' on the right is less than the Young's modulus E on the left. Per unit length, the beam is more flexible on the right than on the left. If the junction is moved to the left the beam as a whole becomes more flexible and the load descends, losing potential energy. If the load were directed upward instead of downward, moving the boundary to the left would make the tip of the beam move further upward, so that the potential energy of the load would again decrease. Thus there is a force on the

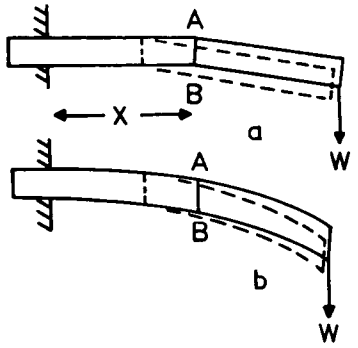

FIG. 12. To illustrate Section 10.

boundary in Fig. 12b which (unlike the force on the boundary in Fig. 12a) does not reverse when the load is reversed. According to (6.3), its magnitude is

$$F = -\frac{d}{dx}(E_{\text{el}} + E_{\text{ext}}) = -\frac{1}{2}\frac{d}{dx}E_{\text{ext}}. \tag{10.1}$$

Elementary beam theory gives the deflection of the load as a function of x and leads to

$$F = \frac{M^2}{2I}\left(\frac{1}{E} - \frac{1}{E'}\right)$$

where M is the bending moment at x, and I is the moment of inertia of the cross section. (Strictly the boundary conditions necessary for (6.3) to hold are not exactly satisfied at the clamped end, but this makes no difference within the limits of elementary beam theory.)

Again, suppose that instead of the load W there is an external couple M twisting the beam about its axis. The twist per unit length in the two sections is $M/D\mu$ or $M/D\mu'$, where D is the torsional rigidity when $\mu = 1$. The total twist at the load end is thus

$$\theta = \frac{M}{D}\left(\frac{x}{\mu} + \frac{L-x}{\mu'}\right).$$

Here E_{ext} is $-M\theta$ + const. Thus (10.1) gives for the effective force on the junction

$$F = \frac{M}{2D}\left(\frac{1}{\mu} - \frac{1}{\mu'}\right). \tag{10.2}$$

These results may be applied to the more realistic case where the array of elastic coefficients c_{ijkl} differs on opposite sides of a grain boundary by taking E, E', μ, μ' to be effective moduli for the bending or twisting of anisotropic beams cut with slightly different orientations from the same crystal.

Generally, then, an element of a grain or twin boundary will experience two forces, namely F^D because it is an array of dislocations (or equivalently, because its movement alters the form of the crystal) and F^R because it is the junction of two regions in which the crystal axes are rotated with respect to one another. Apart from questions of relative magnitude, there is the qualitative distinction that when the applied stresses are reversed F^D reverses but F^R does not.

Usually we may expect F^R to be swamped by F^D. However, in Thomas and Wooster's[84] phenomenon of *piezocrescence* F^R comes into its own. If a quartz crystal transforms into its Dauphiné (or electrical) twin, its external form is unaltered, but its internal crystal structure is rotated 180° about the pseudo-hexad axis. Thus, if a region inside a crystal changes to its Dauphiné twin, it will constitute a region of elastic inhomogeneity unaccompanied by internal stress.

Thomas and Wooster carried out what in effect is the analog for F^R of the Washburn-Parker experiment for F^D. They found that a Dauphiné boundary in a quartz rod twisted by an applied couple moved (at high enough temperatures) in a direction determined by the sign of $(\mu^{-1} - \mu'^{-1})$ in (10.2) but independent of the sign of the applied couple. $(\mu^{-1} - \mu'^{-1})$ may be positive or negative according to the orientation of the crystal axes in the rod.

They have also given what in effect is a calculation of the force per unit area on an inhomogeneity boundary in an arbitrary stress field. Following them, we neglect both the possible discontinuity in the stress components across the boundary and the fact that moving the boundary will itself upset the applied stress distribution. Then (6.5) may be rewritten as

$$\delta E_{el} = \tfrac{1}{2}\int (s_{ijkm}' - s_{ijkm}) p_{ij} p_{km} dv$$

omitting the prime on p_{km}. If a surface element of the boundary is displaced a distance $\delta\xi$ in the x_l direction, it sweeps out a volume $dv = dS\delta\xi n_l$

[84] L. A. Thomas and W. A. Wooster, *Proc. Roy. Soc.* **A208** (1951).

where n_l is the normal to dS. Then δE_{el} is $dv\Delta s_{ijkm}p_{ij}p_{km}$, where Δs_{ijkm} is the value of s_{ijkm} on the side of the positive normal minus its value on the negative side. The force on the boundary per unit area is thus a normal pressure

$$F_l{}^R = \frac{\delta E_{el}}{dS\delta\xi} = \Delta s_{ijkm}p_{ij}p_{km}n_l. \tag{10.3}$$

The coefficient of n_l in (10.3) has the form of an energy density derived from fictitious elastic constants Δs_{ijkm}. Unlike a true energy density, it may be positive at some points and negative at others. In equilibrium the twin boundary must coincide with the surface separating positive from negative regions, for there $F_l{}^R = 0$.

Thomas and Wooster verified this experimentally for a quartz plate in a complex state of stress. In their theory they correctly maximized the elastic energy, invoking Le Chatelier's principle. Stepanov[85] in similar work minimized the energy. This gives the shape of the boundary correctly but interchanges the twinned and untwinned regions.

It is interesting to compare the magnitudes of F^D and F^R for a grain or twin boundary in a metal. Let ω be the misorientation, p a typical stress component, and s a typical component of s_{ijkl}. The fractional change of s on crossing the boundary is of order ω. Then $F^D \sim \omega p$ and from (10.3) $F^R \sim \omega p^2 s \sim \omega p^2/\mu$ where μ is some elastic modulus. Hence F^R/F^D is of the order of the usually small quantity p/μ.

[85] A. V. Stepanov, *Zhur. Eksptl. i Teort. Fiz.* **20**, 438 (1950).