Constitutive Equations for Elastic-Plastic Flow in Cubic Crystals

T. Y. THOMAS

1. Introduction. It was shown in a recent article [1] that the elastic-strain relations for cubic crystals can be written in the form

$$(1) \quad \sigma_{ij} = \lambda e_{kk} \delta_{ij} + 2\mu e_{ij} + \alpha e_{km} \nu_a^k \nu_a^m \nu_{ai} \nu_{aj}$$

in a dynamically admissible rectangular coordinate system, where the λ , μ and α are material constants or *elastic moduli* and the ν 's are the components of the three mutually orthogonal unit vectors ν_a which give the orientation of the crystal. Also the δ_{ij} in (1) are Kronecker deltas; the σ_{ij} are the components of the stress tensor and are functions $\sigma_{ij}(x, t)$ of the coordinates x^k and the time t ; and finally the quantities e_{ij} are the components of the usual elastic-strain tensor, *i.e.*

$$(2) \quad e_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}),$$

where the comma denotes partial differentiation, with respect to the coordinates, of the functions $u_i(x, t)$ which give the components of the elastic displacement.

Now consider a dynamical situation in which plastic as well as elastic deformations occur within the medium. Denote by x_0^i the coordinates of the points P of the unstrained medium, referred to a rectangular system, and by x^i the coordinates of the points Q into which the points P are displaced by the combined elastic and plastic deformation. At any time t the displacement $P \rightarrow Q$ can be represented by equations of the form

$$(3) \quad x^i = A^i(x_0, t).$$

We assume that the functions A^i are continuous and differentiable and that the equations (3) have a unique inverse

$$(4) \quad x_0^i = B^i(x, t),$$

where the B^i are likewise continuous and differentiable functions. Hence the total velocity v of the displaced points Q has components v_i given by

$$(5) \quad v_i = \frac{\partial A^i(x_0, t)}{\partial t} = v_i(x, t),$$

when account is taken of the inverse relation (4). To ascertain the contribution of the purely plastic deformation to the velocity v of the points Q , we assume that this deformation can also be represented by equations of the type (3) and (4), namely

$$(6) \quad y^i = E^i(x_0, t); \quad x_0^i = F^i(y, t),$$

where the functions E^i and F^i are continuously differentiable functions of their arguments. Then if $\tilde{w}_i$ are the components of the plastic contribution to the velocity of the point Q , i.e. the *plastic velocity* of Q , we have

$$(7) \quad \tilde{w}_i = \frac{\partial E^i(x_0, t)}{\partial t} = \tilde{w}_i(x, t),$$

as we see when use is made of the second set of equations (6). Moreover

$$(8) \quad y^i = E^i(B(x, t), t) = G^i(x, t),$$

from (6) and (4). Hence the purely elastic displacement associated with the point Q will have components u_i given by

$$(9) \quad u_i = x^i - y^i = x^i - G^i(x, t) = u_i(x, t).$$

The following assumption will now be made. *In any dynamically admissible rectangular system the elastic displacements $u_i(x, t)$ defined by (9) will satisfy the stress-strain equations (1) in which the quantities e_{ij} are given by (2) and the stress components σ_{ij} are functions of the coordinates x^i and the time t .*

Denoting by w_i the components of the elastic contribution to the velocity, i.e., the *elastic velocity*, of the moving point Q , it follows from (3), (6) and (9) that

$$w_i = \frac{\partial A^i(x_0, t)}{\partial t} - \frac{\partial E^i(x_0, t)}{\partial t} = v_i(x, t) - \tilde{w}_i(x, t),$$

in which we have also made use of the equations (5) and (7). The components w_i of the elastic velocity are therefore functions $w_i(x, t)$ of the coordinates x^i and the time t such that

$$(10) \quad v_i = w_i + \tilde{w}_i,$$

i.e., the total velocity of any point Q in the medium is the sum of its elastic and plastic velocities.

To obtain another relation which will have application in the following discussion, let us differentiate the functions u_i partially with respect to the time t when we regard the u 's as given by

$$u_i = x^i - y^i = A^i(x_0, t) - E^i(x_0, t).$$

But this gives the components w_i of the elastic velocity as we have just observed. Now when we apply this same operation to the elastic displacements u_i regarded as functions $u_i(x, t)$ we obtain

$$(11) \quad \frac{\partial u_i}{\partial t} + u_{i,k} \frac{\partial A^k}{\partial t} = \frac{\partial u_i}{\partial t} + u_{i,k} v^k$$

on account of (3) and (5). Equating the components w_i to the right members of the equations (11), we have

$$(12) \quad w_i = \frac{\partial u_i}{\partial t} + u_{i,k} v^k.$$

Deviations from the structure of the cubic crystal which are produced by the elastic and plastic displacements must be so small that we are justified in employing the stress-strain relations (1) in accordance with the above assumption. In this connection we shall assume the following *approximation conditions* to be satisfied. *The elastic displacements $u_i(x, t)$ and the components $w_i(x, t)$ of the elastic velocity, their coordinate and time derivatives, and also the coordinate derivatives of the components $\tilde{w}_i(x, t)$ of the plastic velocity are small quantities whose products can be neglected in any dynamically admissible coordinate system.* Certain of the restrictions placed on the magnitudes of the elastic quantities by these conditions will not be needed in this article; however, they are usually considered to be valid in the ordinary theory of elasticity and they have been included for this reason. It is observed that the above conditions will allow the occurrence of comparatively large plastic velocities $\tilde{w}$ and plastic displacements. But such plastic displacements will be essentially of a translational nature due to the restriction on the magnitude of the derivatives $\tilde{w}_{i,j}$ and they will therefore not destroy the characteristic structure of the crystal.

2. Covariant time differentiation. It is generally recognized that constitutive equations of the type under consideration must be invariant with respect to transformations of the group G relating the coordinates of arbitrarily moving rectangular coordinate systems [2]. Now any transformation $x \rightarrow \bar{x}$ of the group G can be represented by writing

$$(13) \quad \bar{x}^i = a_j^i(t)x^j + b^i(t); \quad a_j^i a_k^j = \delta_{ik},$$

in which it will be assumed that the b 's are arbitrary differentiable functions of the time t and the a 's are differentiable functions of t subject to the orthogonality conditions given by the second set of these equations. Let us think of the equations (13) as giving specifically the coordinates $\bar{x}^i$ in the $\bar{x}$ system of the above displaced point Q whose coordinates are x^i in the x system. Similarly we have the transformation relations

$$(14) \quad \bar{y}^i = a_j^i(t)y^j + b^i(t)$$

for the above coordinates y^i introduced in Sect. 1. Subtracting corresponding members of the two sets of equations (13) and (14) we now have

$$(15) \quad \bar{x}^i - \bar{y}^i = a_j^i(t)(x^j - y^j), \quad \text{or} \quad \bar{u}^i(\bar{x}, t) = a_j^i(t)u^j(x, t)$$

as the relations between the components $u^i(x, t)$ and $\bar{u}^i(\bar{x}, t)$ of the elastic

displacement in the x and $\bar{x}$ systems. Hence the quantities $u^i(x, t)$ are the components of a vector under transformations of the group G . Writing u_i instead of u^i since there is no distinction between covariant and contravariant indices in rectangular coordinate systems, it follows immediately by differentiation of the equations (15) that the quantities $u_{i,j}$ are also the components of a tensor under transformations of the group G and a similar remark can be made regarding the components e_{ij} of the elastic strain which are given by the equations (2). The Kronecker deltas δ_{ij} or δ^{ij} are obviously the components of a tensor under the group G ; also the stress components σ_{ij} and the ν 's in (1) can be regarded as the components of a tensor and three vectors respectively under such transformations. Since λ , μ and α are scalars the following result has now been proved. *The stress-strain relations (1) are invariant in form under the group of transformations G relating the coordinates of arbitrarily moving rectangular systems.*

In view of the invariance of the stress-strain relations (1) as stated in the above italicized result, the operation of covariant time differentiation [3] can be applied to obtain

$$(16) \quad \frac{\mathfrak{D}\sigma_{ij}}{\mathfrak{D}t} = \lambda \frac{\mathfrak{D}e_{kk}}{\mathfrak{D}t} \delta_{ij} + 2\mu \frac{\mathfrak{D}e_{ij}}{\mathfrak{D}t} + \alpha \frac{\mathfrak{D}e_{km}}{\mathfrak{D}t} \nu_a^k \nu_a^m \nu_{ai} \nu_{aj} \\ + \alpha e_{km} \left(\frac{\mathfrak{D}\nu_a^k}{\mathfrak{D}t} \nu_a^m \nu_{ai} \nu_{aj} + \nu_a^k \frac{\mathfrak{D}\nu_a^m}{\mathfrak{D}t} \nu_{ai} \nu_{aj} + \nu_a^k \nu_a^m \frac{\mathfrak{D}\nu_{ai}}{\mathfrak{D}t} \nu_{aj} + \nu_a^k \nu_a^m \nu_{ai} \frac{\mathfrak{D}\nu_{aj}}{\mathfrak{D}t} \right).$$

In these equations the quantities $\mathfrak{D}\sigma_{ij}/\mathfrak{D}t$, $\mathfrak{D}e_{ij}/\mathfrak{D}t$ and $\mathfrak{D}\nu_a^i/\mathfrak{D}t$ or $\mathfrak{D}\nu_{ai}/\mathfrak{D}t$ are the components of the covariant time derivatives of the stress tensor, the elastic strain tensor, and the orientation vectors, respectively, and they are given specifically by the following formulas

$$(17) \quad \frac{\mathfrak{D}\sigma_{ij}}{\mathfrak{D}t} = \frac{d\sigma_{ij}}{dt} + \sigma_{ik}\phi_{ki} + \sigma_{ki}\phi_{ki} ,$$

$$(18) \quad \frac{\mathfrak{D}e_{ij}}{\mathfrak{D}t} = \frac{de_{ij}}{dt} + e_{ik}\phi_{ki} + e_{ki}\phi_{ki} ,$$

$$(19) \quad \frac{\mathfrak{D}\nu_a^i}{\mathfrak{D}t} = \frac{\mathfrak{D}\nu_{ai}}{\mathfrak{D}t} = \frac{d\nu_{ai}}{dt} + \nu_{ak}\phi_{ki} .$$

The first sets of terms in the right members of the above equations (17), (18) and (19) are ordinary total time derivatives based on the velocity v which results from the combined elastic and plastic flow (see Sect. 1) and the quantities ϕ_{ij} are given by the equations

$$\phi_{ij} = \frac{1}{2}(v_{i,j} - v_{j,i}).$$

Since the covariant time derivatives defined by (17), (18) and (19) are tensors or vectors under transformations of the group G , the equations (16) will be invariant in form under transformations of this group.

The dynamically admissible coordinate systems for this problem are, of course, contained among the systems related by transformations of the group G ; furthermore the components of the orientation vectors ν_a are constant by assumption in any admissible system [1]. Relative to an admissible coordinate system the equations (19) therefore become

$$(20) \quad \frac{\mathfrak{D}\nu_a^i}{\mathfrak{D}t} = \frac{\mathfrak{D}\nu_{ai}}{\mathfrak{D}t} = \nu_{ak}\phi_{ki} ,$$

and the equations (18) immediately reduce to

$$(21) \quad \frac{\mathfrak{D}e_{ij}}{\mathfrak{D}t} = \frac{de_{ij}}{dt} ,$$

as a consequence of the italicized approximation conditions in Sect. 1. But

$$(22) \quad \frac{de_{ij}}{dt} = \frac{1}{2} \left[\left(\frac{\partial^2 u_i}{\partial t \partial x^j} + u_{i,jk} v^k \right) + \left(\frac{\partial^2 u_j}{\partial t \partial x^i} + u_{j,ik} v^k \right) \right]$$

by total time differentiation of (2) since the u_i are functions $u_i(x, t)$ of the coordinates x^i and the time t . Also it follows by coordinate differentiation of (12) that

$$(23) \quad w_{i,j} = \frac{\partial^2 u_i}{\partial t \partial x^j} + u_{i,jk} v^k$$

to within a set of terms which can be neglected on account of the approximation conditions. Making the substitution (23) in (22) we now find that the equations (21) become

$$(24) \quad \frac{\mathfrak{D}e_{ij}}{\mathfrak{D}t} = \eta_{ij} ; \quad \eta_{ij} = \frac{1}{2}(w_{i,j} + w_{j,i}) ,$$

where the quantities η_{ij} are defined by the second set of these equations. Finally when we substitute (24) into (16) and again make use of the approximation conditions, we readily see that the equations (16) can be replaced by

$$(25) \quad \frac{\mathfrak{D}\sigma_{ij}}{\mathfrak{D}t} = \lambda \eta_{kk} \delta_{ij} + 2\mu \eta_{ij} + \alpha \eta_{km} \nu_a^k \nu_a^m \nu_{ai} \nu_{aj}$$

in any dynamically admissible rectangular coordinate system.

The quantities η_{ij} which appear in (25) are the components of the *rate of elastic strain*; we shall not be concerned with the behavior of the components η_{ij} under coordinate transformations since these quantities will not enter explicitly in the final form of the constitutive equations. Introducing the deviators σ^* and η^* whose components are defined by

$$\sigma_{ij}^* = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij} ; \quad \eta_{ij}^* = \eta_{ij} - \frac{1}{3} \eta_{kk} \delta_{ij}$$

respectively, the equations (25) can be written in the equivalent form

$$(26) \quad \frac{\mathfrak{D}\sigma_{kk}}{\mathfrak{D}t} = \frac{d\sigma_{kk}}{dt} = (3\lambda + 2\mu + \alpha)\eta_{kk} ,$$

$$(27) \quad \frac{\mathfrak{D}\sigma_{ij}^*}{\mathfrak{D}t} = 2\mu\eta_{ij}^* + \alpha\eta_{km}^*\nu_a^k\nu_a^m\nu_{ai}\nu_{aj} ,$$

as can easily be shown. The above equations (26) and (27) will have an important application in the following discussion.

3. Purely plastic flow. It was assumed in the foregoing discussion that the elastic displacements $u_i(x, t)$ defined by the equations (9) satisfy the elastic stress-strain relations (1) for cubic crystals. Correspondingly we shall now assume that the purely plastic flow which is determined by the plastic velocity $\mathfrak{w}$ defined by (7), satisfies conditions in any dynamically admissible rectangular coordinate system similar to those which characterize the flow in a perfectly plastic solid. These conditions are

A₁. The plastic flow is incompressible,

A₂. The components of the deviator of the stress tensor are proportional to the components of the deviator of the rate of plastic strain,

A₃. The coefficient in the proportionality relating the components of the deviators of the stress and the rate of plastic strain is a positive function of the components of the deviator of the rate of plastic strain,

A₄. There does not exist a (1, 1) correspondence between the components of the deviators of the stress and the rate of plastic strain.

On the basis of the above assumptions $A_1, \dots, A_4$ it can be shown that [4]

$$(28) \quad \sigma_{ij}^* = \frac{M(\sqrt[3]{\tilde{\eta}_{ab}\tilde{\eta}_{bc}\tilde{\eta}_{ac}}/\sqrt{\tilde{\eta}_{ab}\tilde{\eta}_{ab}})}{\sqrt{\tilde{\eta}_{ab}\tilde{\eta}_{ab}}} \tilde{\eta}_{ij} ,$$

and

$$(29) \quad \sigma_{ij}^*\sigma_{ij}^* = \left[M\left(\frac{\sqrt[3]{\sigma_{ab}^*\sigma_{bc}^*\sigma_{ac}^*}}{\sqrt{\sigma_{ab}^*\sigma_{ab}^*}}\right) \right]^2$$

in any dynamically admissible rectangular coordinate system, where M is an arbitrary positive function of the ratio of the two radicals which constitutes its argument, and

$$(30) \quad \eta_{ij} = \frac{1}{2}(\mathfrak{w}_{i,i} + \mathfrak{w}_{j,i}).$$

The quantities $\tilde{\eta}_{ij}$ are the components of the *rate of plastic strain* $\tilde{\eta}$ and they are equal to the corresponding components $\tilde{\eta}_{ij}^*$ of the deviator of $\tilde{\eta}$ since the quantity $\tilde{\eta}_{kk}$ or $\mathfrak{w}_{k,k}$ vanishes as a consequence of assumption A_1 . We cannot conclude that the $\tilde{\eta}_{ij}$ transform as the components of a tensor under transformations of the group G ; but the actual equations of transformation of the components $\tilde{\eta}_{ij}$ will not be needed since these quantities will not enter directly into the constitutive equations which we shall derive in the next section.

4. The constitutive equations. Our problem is now to construct a system of constitutive equations which will involve only directly observable quantities, *e.g.* the stress σ and the total velocity v . It will be shown in this section that such constitutive equations follow readily from the above results; the equations so obtained will be an extension to cubic crystals of the well known Prandtl-Reuss equations for elastic-plastic flow in isotropic media.

We see from (10) and the second set of equations (24) that

$$v_{k,k} = w_{k,k} + \tilde{w}_{k,k} = w_{k,k} = \eta_{kk}$$

when account is taken of the fact that $\tilde{w}_{k,k}$ vanishes. Hence (26) can be written

$$(31) \quad \frac{d\sigma_{kk}}{dt} = (3\lambda + 2\mu + \alpha)v_{k,k}.$$

Next observe that

$$(32) \quad \epsilon_{ij}^* = \eta_{ij}^* + \tilde{\eta}_{ij}^* = \eta_{ij}^* + \tilde{\eta}_{ij},$$

as a consequence of (10) where η_{ij}^* and $\tilde{\eta}_{ij}^*$ are the components of the deviators of the rates of elastic and plastic strain and the ϵ_{ij}^* are the components of the deviator of the rate of total strain ϵ ; the components of ϵ are given by

$$\epsilon_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i}).$$

The relations (32) can also be expressed as

$$(33) \quad \epsilon_{ij}^* = \eta_{ij}^* + \psi\sigma_{ij}^*,$$

where ψ is the reciprocal of the positive proportionality factor in the right members of (28). When we eliminate the quantities η_{ij}^* from (27) by means of the substitution (33) we now have

$$(34) \quad \frac{\mathcal{D}\sigma_{ij}^*}{\mathcal{D}t} = 2\mu(\epsilon_{ij}^* - \psi\sigma_{ij}^*) + \alpha(\epsilon_{km}^* - \psi\sigma_{km}^*)\nu_a^k\nu_a^m\nu_{ai}\nu_{aj}.$$

It can be proved that the quantities ϵ_{ij} are the components of a tensor under the group G of coordinate transformations [3]; this implies the tensor character of the components ϵ_{ij}^* under the group G . To determine an appropriate expression for the function ψ we may differentiate the relation (29) covariantly with respect to the time t and then eliminate the quantities $\mathcal{D}\sigma_{ij}^*/\mathcal{D}t$ which thereby arise by means of the equations (34); this procedure is possible since (29) is invariant under transformations belonging to the group G . Solving the resulting equation for ψ we thus find that ψ can be expressed as a function of the components of the deviators σ^* and ϵ^* and the components of the orientation vectors ν_a . As so expressed the function ψ will be a positive scalar invariant, under transformations of the group G , of the basic tensors σ^* and ϵ^* and the three vectors ν_a which give the orientation of the crystal. *The equations (31) and (34) in which ψ is the above mentioned scalar invariant are the desired constitutive equations for the elastic-plastic flow in the cubic crystal.* It is clear from

the above discussion that the constitutive equations (31) and (34) are invariant in form under transformations relating the coordinates of arbitrarily moving rectangular coordinate systems.

5. The yield condition. The relation (29) in which M is a *material function* is the *yield condition* and it imposes a restriction on the deviator σ^* of the stress tensor for the occurrence of plastic flow. When the function M is assumed to be a *material constant*, the yield condition (29) becomes the well known quadratic or von Mises yield condition

$$(35) \quad \sigma_{ij}^* \sigma_{ij}^* = 2k^2; \quad k = \text{const.}$$

Calculating the function ψ as explained in Sect. 4 for the case of the yield condition (35), we readily find that

$$\psi = \frac{2\mu\sigma_{ij}^* \epsilon_{ij}^* + \alpha(\sigma_{ij}^* \nu_a^i \nu_a^j)(\epsilon_{km}^* \nu_a^k \nu_a^m)}{4\mu k^2 + \alpha(\sigma_{ij}^* \nu_a^i \nu_a^j)(\sigma_{km}^* \nu_a^k \nu_a^m)}.$$

Other selections of the function M can be made which will lead to a more accurate description of the physical situation than the simple condition (35). For example, if we take M to be a linear function of its argument, *i.e.*

$$M = a - b \left(\frac{\sqrt[3]{\sigma_{ab}^* \sigma_{bc}^* \sigma_{ac}^*}}{\sqrt{\sigma_{ab}^* \sigma_{ab}^*}} \right),$$

where a and b are positive material constants, the yield condition can be written

$$(36) \quad \sqrt{\sigma_{ij}^* \sigma_{ij}^*} = a - b \left(\frac{\sqrt[3]{\sigma_{ab}^* \sigma_{bc}^* \sigma_{ac}^*}}{\sqrt{\sigma_{ab}^* \sigma_{ab}^*}} \right).$$

By using a yield condition of the type (36) and making an appropriate choice of the constants a and b , one can account for the fact that a numerically greater compressive than tensile load is required to produce plastic flow and fracture in a solid.

REFERENCES

- [1] T. Y. THOMAS, On the stress-strain relations for cubic crystals, *Proc. Nat. Acad. Sci.*, 55 (1966) 235-239.
- [2] W. PRAGER, *Introduction to Mechanics of Continua*, Ginn and Co., New York, 1961, p. 155.
- [3] T. Y. THOMAS, Kinematically preferred coordinate systems, *Proc. Nat. Acad. Sci.*, 41 (1955) 762-770; also *Plastic Flow and Fracture in Solids*, Mathematics in Science and Engineering, Vol. 2, Academic Press, New York, 1961, pp. 83-95.
- [4] T. Y. THOMAS, *Plastic Flow and Fracture in Solids*, *loc. cit.*, reference [3], p. 70.

Mathematical Physics Branch
Solid State Division
U. S. Naval Research Laboratory
Washington, D. C.