

Equation (A1.15) would appear to be the basis of the pre-exponential factor in the phenomenological form of the shear strain rate equation (eqn. 1.5) found by Hart, Li and their co-workers (see Chapter 5).

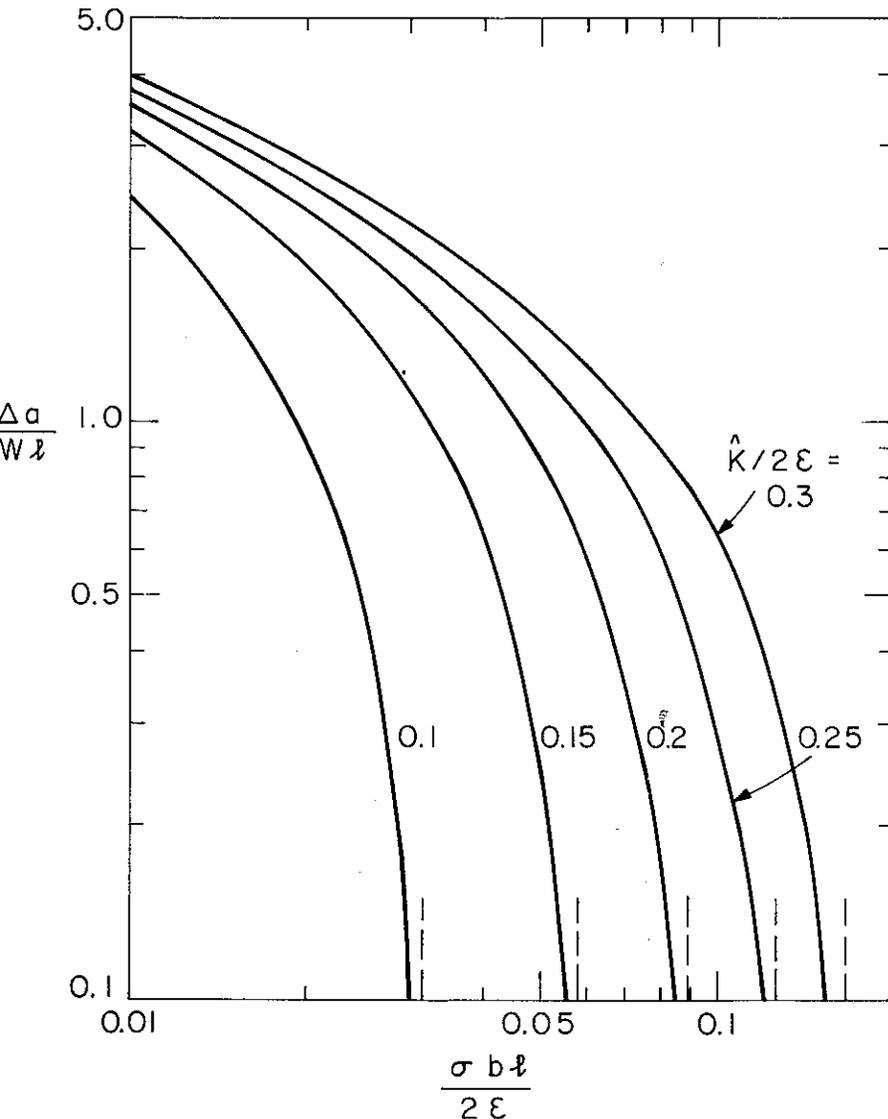


Fig. A1.1 The stress dependence of the activation area for a dislocation segment overcoming a simple discrete obstacle.

ABSTRACT. This chapter presents the foundations in continuum mechanics and irreversible thermodynamics for constitutive relations governing plasticity. Special emphasis is given to the connection of macroscopic formulations to deformation mechanisms as operative on the microscale. Indeed, much of the chapter is organized around an internal variable framework by which inelastic structural rearrangements of a representative material sample can be related to its macroscopic deformation. This is illustrated most extensively for deformation by slip, but other mechanisms such as diffusion and phase changes are discussed as well. An extended synopsis is given in the summary section.

J. R. Rice, "Continuum Mechanics and Thermodynamics of Plasticity in Relation to Microscale Deformation Mechanisms", Chapter 2 of Constitutive Equations in Plasticity (ed. A. S. Argon), M.I.T. Press, 1975, pp. 23-79.

2. CONTINUUM MECHANICS AND THERMODYNAMICS OF PLASTICITY IN RELATION TO MICROSCALE DEFORMATION MECHANISMS

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2.1 INTRODUCTION

The aim of this chapter is to discuss macroscopic constitutive relations in metal plasticity, with special reference to the form and framework for these relations as set by underlying microscale mechanisms of deformation. Subsequent chapters (e.g., those by Kocks and Ashby) will study the detailed kinetic laws of separate deformation mechanisms. Here, after a review of what can be said on constitutive laws from a purely macroscopic or continuum standpoint, a general thermodynamic formalism is developed by which structural rearrangements of material elements on the microscale, by slip, diffusion, and the like, can be related to corresponding increments of macroscopic plastic strain. This framework is already sufficient for ascertaining certain broad structural features of macroscopic constitutive laws, for example a plastic "normality" structure which follows from only the most essential features of a broad class of microscale relations for the kinetics of processes of

structural rearrangement. Specifically, this entails that the rate of some scalar rearrangement process be stress state dependent only through the thermodynamic force conjugate to the extent of that rearrangement.

The general framework set forth for the micro-macro transition leaves unresolved the detailed steps by which one averages, for example, over all the possible slip systems within a given grain and over all grains in a polycrystalline material sample to arrive finally at specific functional forms for constitutive relations. There are, however, approximate means for doing this, involving models of the "self consistent" type for polycrystals, and work in that area is reviewed. Other chapters (e.g., by Zarka and Chin) provide detailed studies of such averaging procedures.

Such models result in predictions of behavior which do reflect, at least approximately, some of the very real, complex features of plastic response when general states of combined stress and non-proportional stressing paths are examined.

Still, the polycrystal models involve great complexity of analysis with moderately large computer programs and large storage requirements to evaluate stress-strain relations for even relatively simple processes of macroscopically homogeneous deformation. Hence they do not seem to be feasible as input to, say, large scale finite element analyses of inhomogeneously stressed structural or machine elements.

Thus, in addition to the desire for physical and mathematical rigor in formulating constitutive laws from microscale processes, there is a compelling desire for simplicity of description in terms of a comparatively small number of averaged microstructural parameters or, equivalently, in terms of parameters that are defined from relatively simple functionals of prior deformation history. This brings one back to the context of continuum descriptions but in the effort, microscale information can be gainfully utilized if only in a suggestive rather than a rigorously derived manner. Indeed, the chapter closes with some suggestions of the forms that might be employed for such relations. The same approach is, of course, discussed in several other chapters of the book (e.g., those by Ilshner, Gittus, and Weeks and Poepfel).

The discussion in Sections 2.2 to 2.7 is intended for arbitrary amounts of strain, although it is frequently specialized, where noted, to small strains or, more commonly, to small elastic distortions from a finitely deformed plastic state. This finite deformation context, or at least the latter variant with small elastic distortions, is essential to any full discussion not just because many practical problems involve large plastic strains. Even in circumstances of small strain, by comparison to unity,

the distinctions that arise in a rigorous finite strain analysis between different measures of stress and stress rate become important, e.g. in the case of a time-independent material, whenever the rates of increase of stresses with strains have magnitudes that are comparable to those of the stresses themselves. Indeed, it seems objectionable in a general thermo-mechanical theory to contemplate other than arbitrarily large plastic distortions, for the current shapes of many metallic objects are obtained by the finite strains of, say, rolling or forging or extrusion from some prior shape in the solid state.

2.2 CONTINUUM REPRESENTATIONS OF INELASTIC CONSTITUTIVE LAWS

We admit the concept of a macroscopic stress tensor T in a continuum and suppose that alterations of stress at a point of the continuum are determined solely by the history, experienced at that point in processes emanating from a standard reference state, of the temperature θ and deformation gradient F . The latter is defined by $F = \partial x / \partial X$ or, on a cartesian frame, $F_{ij} = \partial x_i / \partial X_j$ where X_1, X_2, X_3 and x_1, x_2, x_3 are coordinates of material points before and after deformation, respectively, referred to fixed background axes. Hence it is elementary to write that the stress tensor T at time t is expressible by a relation of the form

$$T(t) = \mathcal{F}[F(s), \theta(s); 0 \leq s \leq t] \quad (2.1)$$

where the notation indicates that T is a functional of all prior values of F and θ , including the current values. Here T is the Cauchy (or "true") stress. We shall later introduce stress tensors σ with work conjugate properties relative to rotation invariant strain measures.

Now, F may be written as RU where U , with $U_{ij} = U_{ji}$, denotes a pure deformation and R denotes a rigid rotation, hence satisfying $R^T = R^{-1}$ and $\det(R) = 1$ where R^{-1} is the matrix inverse and R^T the transpose of R . If the deformation history $F(s)$ is altered by an additional rotation history $R'(s)$ in eqn. (2.1), it is evident that the resulting stress at time t is changed only insofar as it is further rotated by $R'(t)$. Hence, with $R'(s) = R^{-1}(s)$, eqn. (2.1) becomes

$$R^T(t)T(t)R(t) = \mathcal{F}[U(s), \theta(s); 0 \leq s \leq t] \quad (2.2)$$

so that the stress tensor, when rotated backward by the inverse to R , depends only on the history of pure deformation (and temperature) at the material point.

There are many possible definitions of a strain tensor. Except where noted otherwise, we shall consistently use ϵ to denote some rotation invariant, or objective, strain tensor, by which is meant that ϵ has the same principle axes as U and that the three principle values ϵ_α and U_α , $\alpha = I$ to III , of each are related by a monotonic scalar function $h(\dots)$, such that

$$\epsilon_\alpha = h(U_\alpha) \quad , \quad \alpha = I, II, III \quad , \quad (2.3)$$

where $h(1) = 0$, $h'(1) = 1$.

The latter conditions assure that ϵ agrees with the infinitesimal strain tensor for small stretches and rotations; each different monotonic function h , vanishing at unity with unit slope, defines a different finite strain measure.

To each strain measure there corresponds a symmetric work conjugate stress tensor σ . This is defined so that, if material elements are instantaneously given virtual velocities \dot{x} to which there correspond strain rates $\dot{\epsilon}$, then

$$\sigma_{ij} \dot{\epsilon}_{ij} = \text{rate of stress working per unit volume of reference state} = \det(F) T_{ij} \dot{\partial x}_j / \partial x_i \quad (2.4)$$

By using $\dot{\partial x} / \partial x = \dot{F} F^{-1}$, $F = RU$, and noting that T is symmetric, this becomes

$$\sigma_{ij} \dot{\epsilon}_{ij} = \det(U) U_{ij}^{-1} (R^T T R)_{jk} \dot{U}_{ki} \quad (2.5)$$

Further, since ϵ is expressible, at least in principle, as a function of U and conversely $U = U(\epsilon)$, where a symmetrical dependence on ϵ and ϵ^T is adopted, this defines σ as

$$\sigma_{mn} = \det(U) U_{ij}^{-1} (R^T T R)_{jk} \partial U_{ki} / \partial \epsilon_{mn} \quad (2.6)$$

Since only $R^T T R$ and functions of U are involved, we can evidently write eqn. (2.2) as

$$\sigma(t) = \mathcal{G}[\epsilon(s), \theta(s); 0 \leq s \leq t] \quad (2.7)$$

This is a memory functional representation of a constitutive law. Later we shall specialize it to elastic-plastic materials, which can exhibit a purely elastic response to alterations of ϵ and θ when these take place rapidly or, in the time-independent material idealization, are appropriately directed. This means that $\sigma(t)$ is a direct function of $\epsilon(t)$ and $\theta(t)$, of a form that can be regarded as having a memory functional dependence on those portions of history at which other than elastic response occurred. Alternatively, the dependence on history can be replaced by a dependence on what it has produced, namely, the current pattern of structural arrangement, on the microscale, of material elements. The latter suggests an internal variable representation in the constitutive law. Such forms have been introduced for viscoelastic deformation by Eckart (1948), Meixner (1953), and Biot (1954), and have been studied in some generality by Coleman and Gurtin (1967). In these studies the internal variables are taken to be macroscopic parameters, but the appropriate variables and their rate laws are often not readily identifiable. By contrast, the internal variable formulation in Sections 2.5 to 2.8 takes the variables to characterize specific, local structural rearrangements at sites throughout a representative sample of material, the emphasis being on a rigorous formulation of the rate laws of the sample at that level, with the required averaging to form the macroscopic constitutive relations being taken up separately.

2.3 SOME STRESS AND STRAIN TENSORS AND STRESS RATES

The simplest material strain tensor to calculate for general deformations is the Green strain, and its conjugate is the symmetric Piola-Kirchhoff stress (e.g., Truesdell & Toupin, 1960). These are given by

$$\epsilon = \frac{1}{2} (U^2 - I) = \frac{1}{2} (F^T F - I)$$

$$\sigma = \det(U) U^{-1} (R^T T R) U^{-1} = \det(F) F^{-1} T F^{-1T} \quad (2.8)$$

However, in metal plasticity we are almost always concerned with small elastic distortions from a nearby, unloaded state, even though that state itself may be finitely removed from some prior reference configuration. Hence it is convenient to have a stress measure which can be interpreted, apart from the effect of small elastic distortions, as a force per unit area of that unloaded

state. The stress measure $R^T \sigma R$ would be ideal to that purpose, although it is not a conjugate stress. We may think of this as a rotation-invariant "true" stress, having components that are always properly referenced to material elements for use in constitutive relations. There is a conjugate stress measure which has many of the properties of this rotation-invariant true stress, equaling or differing negligibly from the volume ratio, $\det(U)$, times it in some important circumstances. This is the σ associated with logarithmic strain, the latter being defined on principal axes as the logarithm of the corresponding stretch ratios,

$$\epsilon_\alpha = \log U_\alpha, \quad \alpha = I, II, III, \quad (2.9)$$

and for any axes orientation, $\epsilon = \log U$ and $U = \exp \epsilon$ where $\log U$ and $\exp \epsilon$ are understood as infinite matrix power series in $U - I$ and ϵ , respectively. Thus, following an analysis by Hill (1968), one may show from eqn. (2.6) that σ has the following properties:

(i) $\sigma = \det(U) R^T \sigma R$ precisely when principal axes of deformation and rotation-invariant true stress coincide,

(ii) The normal components of σ along the principal directions of deformation coincide always with the corresponding normal components of $\det(U) R^T \sigma R$, and

(iii) σ differs from $\det(U) R^T \sigma R$ by terms that are of quadratic order in ϵ .

In particular, when the cartesian background frame is aligned with the principal directions of ϵ , one computes that

$$\sigma_{ij} = \det(U) (R^T \sigma R)_{ij} \left[1 - \frac{1}{6} (\epsilon_{ii} - \epsilon_{jj})^2 + \dots \right]. \quad (2.10)$$

(no sum here on repeated indices)

Even at the finite strain state $\epsilon_{11} = .25$, $\epsilon_{22} = -.25$, with all other $\epsilon_{ij} = 0$, the maximum difference between components of σ and of $\det(U) R^T \sigma R$ is approximately 4%, and occurs for σ_{12} . Further, since plastic flow is nearly volume preserving, the volume ratio $\det(U)$ differs from unity only by terms of

the size of elastic distortions. Hence, $\sigma \approx R^T \sigma R$ to moderately large strains. A more consequential result of (iii) above and of eqn. (2.10) is that

$$\frac{d\sigma}{dt} = \frac{d}{dt} [\det(U) R^T \sigma R] \quad (2.11)$$

precisely when the reference state for strain measurement is chosen to coincide, instantaneously, with the current state, apart from an arbitrary rotation R (i.e., when $U = I$ and, hence, $\epsilon = 0$ instantaneously). Further, for $\epsilon \neq 0$, eqn. (2.10) assures that the difference between the two rates in eqn. (2.11) is of order σ times ϵ times $d\epsilon/dt$ and this would, for example, typically be negligible in comparison to $d\sigma/dt$ if ϵ was a strain of elastic order. This is an unusual feature. In general, the difference between two stress rates is of order σ times $d\epsilon/dt$ (Hill, 1968), and hence is not negligible in comparison to $d\sigma/dt$ if the latter were, for example, computed well into the plastic range, where the slope of a stress-strain diagram has a magnitude comparable to that of the stress itself. This is readily demonstrated by writing the analogous formula to eqn. (2.11) in terms of the Green strain and symmetric Piola-Kirchhoff stress of eqn. (2.8). When the reference state is likewise chosen to correspond instantaneously with the current state, except for an arbitrary rotation R ,

$$\frac{d\sigma}{dt} + \frac{d\epsilon}{dt} \sigma + \sigma \frac{d\epsilon}{dt} = \frac{d}{dt} [\det(U) R^T \sigma R], \quad (2.12)$$

although in the current state itself, $\det(U) = 1$ and $\sigma = R^T \sigma R$, just as for the stress σ conjugate to logarithmic strain.

As Hill (1968) has shown, the derivative on the right sides of eqns. (2.11,12) coincides with the Jaumann or co-rotational derivative of Kirchhoff stress [= $\det(U) T$] when the reference state corresponds instantaneously with the current state. If it corresponds except for an arbitrary rotation R , this result is generalized to

$$\frac{d}{dt} [\det(U) R^T \sigma R] = R^T \left\{ \frac{D}{Dt} [\det(U) T] \right\} R, \quad (2.13)$$

where $\frac{D}{Dt}$ denotes the Jaumann rate, defined as the ordinary time rate of components of the tensor involved, when these are referred to a coordinate frame that is instantaneously coincident with the background frame but spinning relative to it with an angular velocity given by the antisymmetric part of $\dot{F} F^{-1}$ ($= \partial \dot{x} / \partial x$)

The utility of these results is as follows. For the type of elastic-plastic constitutive law introduced subsequently, it is possible to associate an instantaneously unloaded state, having deformation gradient F^P , with any state encountered in a process. The rotation R^P is not uniquely determined, and must be specified by, say, making F^P a pure deformation or by fixing certain material or, as appropriate, lattice or fiber directions relative to the background frame, or by some other means conducive to simplicity of constitutive description of the deformation from F^P to F . In most cases of practical interest the deformation $F^P \rightarrow F$ involves (elastic) strains that are minute fractions of unity, but possibly large rotations.

The procedure, then, is to write constitutive relations relative to some fixed reference state that is appropriately chosen for the instant at hand, so as to coincide instantaneously with the unloaded state (i.e. $F^P = I$ instantaneously). These relations will, in general, be most simply expressed in terms of the rotation-invariant true stress R^{TTR} , where R is now the rotation from the instantaneous reference state to the current state. But, with the assumption of small elastic dimension

changes, both R^{TTR} and its rate coincide, from what has been said, with those of the stress σ conjugate to logarithmic strain. Thus one may identify R^{TTR} as a proper conjugate stress σ for the constitutive rate relations of the following sections and, further, directly calculate its time derivative in terms of the Jaumann rate in eqn. (2.13). The strain rate $d\varepsilon/dt$ can then be identified, for small elastic dimension changes, as R^{TDR} where D is the instantaneous rate of deformation tensor (i.e. the symmetric part of $\dot{F}F^{-1}$) and R is again the rotation from the instantaneous reference state to the current state.

Further, within the small elastic strain assumption, it is permissible to replace R by F , or by $F(F^P)^{-1}$ when both F and F^P are measured from some distant reference state, in the expression for $d\varepsilon/dt$ and on the right in eqn. (2.13). One may also set $\det(U) = 1$ in eqn. (2.13) with impunity. The practical

result of all this is that one need finally involve only F^P , F , D and D in the constitutive rate law; there is no need to directly calculate R and U . Similar simplifications of constitutive representations at finite deformation have been discussed by Willis (1969).

2.4 ELASTIC-PLASTIC MATERIALS AND THERMODYNAMIC CONSIDERATIONS

To further specialize eqn. (2.7) it is assumed that the materials under consideration may, under appropriate conditions, exhibit a purely elastic response to stress or temperature alterations at any stage of their deformation history. This response is regarded as due to lattice stretching, in the absence of any structural rearrangements of constituent elements of the material by plastic processes such as slip, twinning, diffusion, or the like. It is taken to be fully reversible. Such elastic response is actually elicited only in the limit of fast alterations of σ and θ in the case of time-dependent materials, for which instantaneous σ , θ alterations cause an alteration only in the plastic contribution to strain rate, but not to strain itself. This is often called "instantaneous elasticity". Within the time-independent idealization of plasticity, when the concept of a yield surface in stress space bounding an elastic range is introduced, such elastic response is elicited from a point of elastic-plastic deformation only when the σ , θ alterations are directed into the current elastic range. Of course, it does not matter that any finite range of purely elastic response exists, from the standpoint of a micro-mechanical model of the material, in that one can always define the purely elastic response as the deformation that would have resulted in a given case had the lattice stretching not been accompanied by plastic processes of structural rearrangement.

The further discussion in this section follows the work of Hill and Rice (1973) in showing how the existence, on thermodynamic grounds, of a work potential for the elastic response sets a concise structure for elastic-plastic constitutive laws in conjugate variables. We let H denote, symbolically, the current plastic state of the material, in the sense that variations of σ and θ at fixed H necessarily induce a purely elastic response. From the standpoint of the discussion leading to eqn. (2.7), H may be viewed as denoting some functional taken over those portions of the prior deformation history during which inelastic response occurred. Alternatively, from the standpoint of a mechanical micro-model of the material, H denotes, symbolically, the current pattern of microstructural arrangement of constituent elements of the material.

With either viewpoint, we may evidently specialize eqn. (2.7) to

$$\sigma = \sigma(\varepsilon, \theta, H) , \quad (2.14)$$

where the notation means that at fixed H , the current stress is

a direct function, with form dependent on the plastic state, of the current strain ϵ and temperature θ . Alterations of state at fixed H are evidently reversible and hence must be in accord with the existence of thermodynamic potentials. Letting η denote entropy and u the internal energy, both per unit volume of the adopted reference state,

$$\sigma_{ij} d\epsilon_{ij} + \theta d\eta = du \quad \text{at fixed } H \quad (2.15)$$

It proves more convenient to employ the Helmholtz free energy,

$$\phi = u - \theta\eta = \phi(\epsilon, \theta, H), \quad (2.16)$$

and its dual on ϵ , to be introduced shortly, so that

$$\sigma_{ij} d\epsilon_{ij} - \eta d\theta = d\phi(\epsilon, \theta, H) \quad \text{for fixed } H \quad (2.17)$$

Hence the stress-strain relations (2.14) have the structure

$$\sigma_{ij} = \partial\phi(\epsilon, \theta, H)/\partial\epsilon_{ij}, \quad (2.18)$$

when ϕ is symmetrized in the components of ϵ . Also, $\eta = -\partial\phi/\partial\theta$. It is important to realize that eqn. (2.18) applies throughout some program of inelastic deformation, the potential ϕ being taken at each instant as that appropriate to purely elastic response at the plastic state H prevailing at that instant. Equation (2.18) has been obtained alternatively from the Coleman-Noll thermodynamic formalism (Coleman and Noll, 1963; Coleman, 1964) for materials exhibiting instantaneous elasticity (Bowen and Wang, 1966), and this would include many representations of time-dependent plasticity. It was also derived by adapting the same formalism to the time-independent idealization by Green and Naghdi (1965). Indeed, in at least the present case, for which constitutive relations of the type eqn. (2.14) apply, the Coleman-Noll formalism and the classical thermodynamic approach adopted in this chapter lead to identical results (Kestin and Rice, 1970; Rivlin, 1970).

The dual potential to ϕ is

$$\psi = \sigma_{ij} \epsilon_{ij} - \phi = \psi(\sigma, \theta, H), \quad (2.19)$$

and in terms of it, when ψ is symmetrized in components of σ ,

$$\epsilon_{ij} = \partial\psi(\sigma, \theta, H)/\partial\sigma_{ij}. \quad (2.20)$$

Provided that eqn. (2.19) can be defined, either directly or by some process of analytic continuation, for the current H when $\sigma = 0$ and $\theta = \theta_0$ (the reference temperature) the strain that remains can be called the plastic strain associated with the plastic state H . That is, if $\epsilon = \epsilon(\sigma, \theta, H)$, then

$$\epsilon^P = \epsilon(0, \theta_0, H). \quad (2.21)$$

When dealing with increments of constitutive functions of σ , or ϵ , θ , and H , the prefix d^P will denote the "plastic" part of the change in that function, defined as the change in the function when H is changed to $H+dH$ but σ or ϵ , respectively, and θ are given the same values. In particular

$$d^P\phi = \phi(\epsilon, \theta, H+dH) - \phi(\epsilon, \theta, H), \quad (2.22)$$

$$d^P\psi = \psi(\sigma, \theta, H+dH) - \psi(\sigma, \theta, H), \quad (2.23)$$

where, for example, $d^P\psi$ is to be regarded as a function of σ , θ , H and whatever differential parameters comprise dH .

Further, one may show that $d^P\psi$ and $-d^P\phi$ are numerically equal when evaluated at corresponding values of σ and ϵ . The plastic part of a strain increment is

$$d^P\epsilon = \epsilon(\sigma, \theta, H+dH) - \epsilon(\sigma, \theta, H), \quad (2.24)$$

and since ϵ at each of the two plastic states is given by eqn. (2.20), by differentiating eqn. (2.23) one has for $d^P\epsilon$ (and analogously for $d^P\sigma$)

$$d^P\epsilon_{ij} = \partial(d^P\psi)/\partial\sigma_{ij}, \quad d^P\sigma_{ij} = \partial(d^P\phi)/\partial\epsilon_{ij}. \quad (2.25)$$

Thus the plastic variations in the potentials are themselves potentials for the plastic variations in stress and strain. A full strain increment includes the parts due to variations in σ and θ as well as H :

$$d\epsilon_{ij} = M_{ijkl} d\sigma_{kl} + \alpha_{ij} d\theta + d^P\epsilon_{ij}, \quad (2.26)$$

where the instantaneous compliances $M = \partial^2 \psi / \partial \sigma \partial \sigma$ (so that M is symmetric on interchange of ij and kl) and thermal expansivities $\alpha = \partial^2 \psi / \partial \sigma \partial \theta$.

It is simplest to see the relation of $d^P \epsilon$ to $d\epsilon^P$ by assuming that M is independent of σ (as appropriate for small lattice stretches) and considering isothermal deformation at θ_0 . Then

$$\epsilon = M\sigma + \epsilon^P \quad \text{whereas} \quad d\epsilon = Md\sigma + d^P \epsilon. \quad (2.27)$$

Thus

$$d^P \epsilon - d\epsilon^P = (d^P M)\sigma, \quad (2.28)$$

and the two agree precisely only when the moduli are unaltered by changes in H . This is certainly an exceptional circumstance for moduli based on conjugate variables, even if moduli based on a "true" stress measure, say R^{TR} , are essentially unaltered by deformation. On the other hand, it seems plausible that $d^P M$ is of the same order as $Md\epsilon^P$, which means that the right side of eqn. (2.28) is of the order $M\sigma$ times $d\epsilon^P$. But $M\sigma$ is the strain due to elastic lattice stretching and, so long as this is a minute fraction of unity, we have $d^P \epsilon = d\epsilon^P$ to a suitable approximation.

Implicit to the framework is the assumption that thermodynamic potentials have meaning during processes of inelastic deformation. This can be given justification within the internal variable framework of Sections 2.5 to 2.7, where processes necessary to reversibly separate, shift, and rejoin lattice planes, or to reversibly accomplish other microstructural rearrangements can be considered in principle for purposes of finding the change in potentials owing to changes in H . Otherwise, the existence of the potentials is simply postulated (as in the Coleman-Noll formalism) although the resulting equations of the theory do not allow their complete operational determination, even in principle. For example, a function varying arbitrarily with H , but not depending on ϵ or σ and θ , could be added with impunity to ϕ or ψ , since only their derivatives on ϵ or σ are involved in, say, eqns. (2.18), (2.20), and (2.25).

For general irreversible processes (i.e., those in which H changes), let Q be the heat supply to a material element, per

unit of reference volume, so that the first law reads

$$\sigma_{ij} d\epsilon_{ij} / dt + Q = du / dt \quad (2.29)$$

It will suffice to assume that all of Q results by radiant heating at spatially uniform temperatures over an element, so that the heat flux times $\partial\theta/\partial x$ does not complicate the entropy production inequality. This is permissible because $\partial\theta/\partial x$ is assumed to not enter the constitutive relations (2.7,14,18). Hence

$$d\eta / dt \geq Q / \theta. \quad (2.30)$$

By substituting the inequality into eqn. (2.29) and recovering ϕ from eqn. (2.16), this becomes

$$\sigma_{ij} d\epsilon_{ij} / dt - \eta d\theta / dt \geq d\phi / dt. \quad (2.31)$$

But $d\phi$ may be split into $d^P \phi$ plus another part which, by eqn. (2.17), cancels the left side, to leave as the second law requirement,

$$\frac{d^P \phi}{dt} \equiv \frac{\phi(\epsilon, \theta, H+dH) - \phi(\epsilon, \theta, H)}{dt} \leq 0, \quad (2.32)$$

where dH is the variation in plastic state occurring during time dt . This attains a very clear meaning when written subsequently in terms of internal variables.

We shall later see that various microscale mechanisms for plastic deformation lead to macroscopic constitutive laws that are in accord with the following "normality" structure. Specifically, for time-dependent plastic flow, this entails that a scalar function $\Omega = \Omega(\sigma, \theta, H)$ exist at each H so that the plastic portion of the instantaneous strain rate is

$$d^P \epsilon_{ij} / dt = \frac{\partial \Omega(\sigma, \theta, H)}{\partial \sigma_{ij}} \quad (2.33)$$

Further, in the time-independent idealization, for which an H dependent yield surface

$$F(\sigma, \theta, H) = 0 \quad (2.34)$$

can be assumed to exist in stress-temperature space, the plastic

portion of the strain increment is given by

$$d^P \epsilon_{ij} = d\Lambda \frac{\partial F(\sigma, \theta, H)}{\partial \sigma_{ij}} \quad (2.35)$$

when the yield surface is smooth at the considered point. The scalar $d\Lambda$ is homogeneous of degree one in $d\sigma$, $d\theta$ and of a sign such that $d^P \epsilon$ aligns with the outer normal in σ space, at the current θ , from the elastic to elastic-plastic domain. Alternatively, if the yield surface is not smooth at the current stress state, but has instead limiting segments $F_\alpha = 0$, $\alpha = 1, 2, \dots, m$, then

$$d^P \epsilon_{ij} = \sum_{\alpha} d\Lambda_{\alpha} \frac{\partial F_{\alpha}(\sigma, \theta, H)}{\partial \sigma_{ij}} \quad (2.36)$$

so that $d^P \epsilon$ lies within the cone of limiting outer normals. Hill and Rice (1973) were able to prove, on the basis of the existence of the potentials ϕ, ψ and $d^P \phi, d^P \psi$ as in eqns. (2.18, 20, 25), that:

- (i) If the above normality structure applies for any one choice of conjugate stress and strain measures and choice of reference state, then it necessarily applies for every choice of conjugate variables and reference state; and
- (ii) If a composite material is made up of subelements that can be modelled as continua in which the above normality structure applies to the local stress-strain relations, then the same normality structure is necessarily transmitted to the overall stress-strain relations of the composite, when these are phrased in work-conjugate variables.

The last remark is of particular importance for polycrystalline aggregates, to the extent that these can be modelled as simple composites of single crystal continua. It is then well known that when elastic distortions of the crystal are small, and Schmid's law or its time-dependent generalization applies to describe the plastic response of the crystal, that the normality structure is identically satisfied for the stress-strain relations of each crystal. Hence it is necessarily satisfied by the macroscopic stress-strain relations for an aggregate of such crystals. This is a case for which the general framework developed here reveals a key structural feature of a constitutive

law, even though very little can be said on the detailed form of the constitutive law for the polycrystal. There is an extensive literature on the approximate calculation of polycrystal properties from those of single crystals; this is discussed in Section 2.8. The works of Havner (1973), Hill and Rice (1972), and Rice (1971) may be consulted for rigorous formulations of crystal constitutive laws in a finite strain context.

Two separate quasi-thermodynamic postulates (Drucker, 1951, 1960; Il'yushin, 1961) have been proposed in the time-independent plasticity literature, and lead to the normality structure of eqns. (2.35,36). That by Il'yushin postulates that non-negative net work is done in enforcing an isothermal cycle of straining that begins and ends at the same arbitrary state. This is a separate postulate rather than a consequence of the second law because restoration of ϵ and θ does not fully restore the state - H has changed. Drucker's postulate deals with a material element under an arbitrary prestress and postulates that the net work done by an external agency in a cycle of adding and removing some additional set of loadings is non-negative. The postulate is not independent of the adopted stress measure and hence cannot be unambiguously interpreted in general. However, if limited to cycles involving only an infinitesimal accumulation of plastic straining, it is invariant to stress measure and leads to the normality structure of eqns. (2.35,36) in conjugate variables.

2.5 GENERAL FRAMEWORK FOR TRANSITION FROM MICROSCALE PROCESSES TO MACROSCOPIC STRAIN

This section presents a general framework by which microstructural deformation mechanisms are related to macroscopic plastic straining. The formalism is wide enough to include crystalline slip, which will be the mechanism of primary concern here, and also phase transformations, twinning, diffusional transport, etc. For maximum generality, a collection of "internal variables" are introduced to describe the local, microstructural rearrangements of a material sample by such mechanisms. The approach followed is due to Rice (1971); it is related to, and provides a unified setting for similar general studies by Havner (1969), Hill (1967), Kestin and Rice (1970), Lin (1968), Mandel (1966), Rice (1970), and Zarka (1972).

Consider a representative macroscopic sample of material, having volume V in an unloaded reference state. This is subjected to boundary loadings causing macroscopically homogeneous deformation; σ_{ij} and ϵ_{ij} are the conjugate macroscopic stresses and

strains thus induced, and these are supposed to satisfy

$$V \sigma_{ij} d\epsilon_{ij} = \text{work increment of boundary loadings} \quad (2.37)$$

Here, for simplicity, results are given as appropriate to isothermal behavior; θ is not explicitly listed as a variable in constitutive functions except when it proves fruitful to indicate the manner of generalization to the non-isothermal regime. The latter regime is fully discussed in the work by Rice (1971). Given that we now focus on a definite macroscopic sample of material, σ and ϵ have exact specifications in terms of averages of local surface stress and displacement fields over the boundary of the body. These can be converted to volume averages involving the local, inhomogeneous stress and strain fields. A full discussion is given by Hill (1967) and, in conjugate variables for finite strain, by Rice (1971) and Hill (1972).

The material sample may deform by: (i) elastic stretching of lattice bonds, and (ii) local microstructural rearrangements of its constituent elements by slip, etc. Following the notation of the last section, we let H denote symbolically the current pattern of microstructural rearrangement; this pattern is due to the prior history of inelastic deformation experienced by the sample, and H may equally be thought of as representing this history. The free energy ϕ of the sample depends on ϵ and H . When isothermal processes at fixed H are considered, we have, as in eqns. (2.16,17)

$$V \sigma_{ij} d\epsilon_{ij} = [d\phi]_{H \text{ constant}}, \text{ and } \sigma_{ij} = \frac{1}{V} \frac{\partial \phi(\epsilon, H)}{\partial \epsilon_{ij}} \quad (2.38)$$

Alternatively, if we introduce the dual potential

$$\psi = V \sigma_{ij} \epsilon_{ij} - \phi, \text{ then } \epsilon_{ij} = \frac{1}{V} \frac{\partial \psi(\sigma, H)}{\partial \sigma_{ij}} \quad (2.39)$$

Evidently, we can identify $\phi/V = \phi$, $\psi/V = \psi$ and use the formulae of the last section.

Consider two neighboring patterns of microstructural rearrangement denoted by $H, H+dH$. We suppose that a set of incremental internal variables $d\xi_1, d\xi_2, \dots, d\xi_n$ characterize

the specific local rearrangements, which are represented collectively by dH , at sites throughout the sample. The required number of such variables increases in proportion to the size of the sample. Indeed, we shall see that an essentially infinite number of continuous variables defined piecewise throughout the

sample is required for, say, a description of crystalline slip within this framework (Rice, 1971), but the structure of the theory is made evident more simply in terms of the discrete $d\xi$'s and there is no loss of generality. In analogy with the definition of the thermodynamic "force" on a dislocation line or crack front, we define a set of forces $f_\alpha = f_\alpha(\epsilon, H)$ conjugate to the variables by

$$\Sigma f_\alpha(\epsilon, H) d\xi_\alpha = - [\phi(\epsilon, H+dH) - \phi(\epsilon, H)] \equiv - d^P \phi. \quad (2.40)$$

The analogous expression in terms of the dual potential is

$$\Sigma f_\alpha(\sigma, H) d\xi_\alpha = [\psi(\sigma, H+dH) - \psi(\sigma, H)] \equiv d^P \psi. \quad (2.41)$$

The intent of these relations is to define the f 's from a continuum model at the microscale level. Specifically, atomic scale fluctuations with position of the energy of a configuration are regarded as being averaged out, although the size of these fluctuations could well be important to determining the kinetic relations satisfied by the rates of the rearrangements, as e.g. in thermal activation models. In this regard, the f 's differ from the force defined by Kocks (Chapter 3), who includes these short range fluctuations as well. In the case of a dislocation moving in a perfect lattice, the present f 's would include the effects of the applied and other long range stress fields acting on the slip plane, but would not include the periodic Peierls stress due to the lattice itself, whereas Kocks' force definition would include both. The next section identifies various internal variables and their conjugate forces.

On rewriting eqns. (2.24,25) for the plastic part of a strain increment, namely

$$d^P \epsilon_{ij} = \epsilon_{ij}(\sigma, H+dH) - \epsilon_{ij}(\sigma, H) = \frac{\partial}{\partial \sigma_{ij}} \left(\frac{1}{V} d^P \psi \right), \quad (2.42)$$

and then expressing $d^P \psi$ in terms of the conjugate forces by eqn. (2.41), we obtain the following fundamental relation between a plastic increment of macroscopic strain and the corresponding extents $d\xi$ of microstructural rearrangements:

$$d^P \epsilon_{ij} = \frac{1}{V} \Sigma \frac{\partial f_\alpha(\sigma, H)}{\partial \sigma_{ij}} d\xi_\alpha. \quad (2.43)$$

The summation extends over all the individual sites in the sample where rearrangements take place and, in view of the factor $1/V$, provides a volume average over the sample. The relation plays a key role in establishing a normality structure to constitutive laws that is valid for a wide range of kinetic mechanisms for the rearrangements. When the elastic stretching of the lattice is small and suitably linearized in its stress dependence over the range of interest,

$$\epsilon_{ij} = \epsilon_{ij}^P(H) + M_{ijkl}(H)\sigma_{kl} \quad (2.44)$$

Ψ may then be determined by integrating eqn. (2.39)₂ on σ , noting from eqn. (2.39)₁ that $\Psi = -\phi$ when $\sigma = 0$; the "locked-in" free energy at $\sigma = 0$ will be denoted $\phi^0 = \phi^0(H)$. Thus

$$\Psi = -\phi^0(H) + V\sigma_{ij}\epsilon_{ij}^P(H) + \frac{1}{2}V\sigma_{ij}M_{ijkl}(H)\sigma_{kl} \quad (2.45)$$

and by inserting this into the definition given by eqn. (2.41),

$$\begin{aligned} \sum f_{\alpha}(\sigma, H)d\xi_{\alpha} &= -d\phi^0(H) + V\sigma_{ij}d\epsilon_{ij}^P(H) \\ &+ \frac{1}{2}V\sigma_{ij}\sigma_{kl}dM_{ijkl}(H) \end{aligned} \quad (2.46)$$

Since this must hold for arbitrary $d\xi$'s, with corresponding dH 's on the right side, it is seen that in general the f 's are quadratic functions of stress. However, as discussed in connection with eqns. (2.27,28), elastic moduli when phrased in terms of, say, the stress measure R^T_{TR} and strain increment measure $U^{-1}dU + dU U^{-1}$ are very little affected by processes such as dislocation motion. This means that dM based on some conjugate measure will be of the order $Md\epsilon^P$, and hence that the third term in eqn. (2.46) is of the order $M\sigma$ times the second. This means that it is negligible and hence each f is linear in stress, taking the form

$$f_{\alpha}(\sigma, H) = f_{\alpha}^0(H) + \sigma_{ij}f_{\alpha, ij}^1(H) \quad (2.47)$$

It is seen that f_{α}^0 is associated with the "locked-in" free

energy whereas, to the order of the approximation,

$$d^P\epsilon = d\epsilon^P = \frac{1}{V} \sum f_{\alpha, ij}^1(H)d\xi_{\alpha} \quad (2.48)$$

The situation is otherwise when the mechanism of inelastic deformation is due to a phase change or, as a simple limiting case, due to the stable growth of elastic-brittle Griffith microcracks. If the material sample contains no initial stresses, then its shape will be fully recovered on unloading and $\epsilon^P = 0$. In this case all of $d^P\epsilon$ arises from the σdM term of eqn. (2.28), where dM is the change in compliance due to the crack growth. Hence in this case the forces f , conjugate to increments $d\xi$ of crack extension, contain no linear term but only the quadratic term in eqn. (2.46).

For non-isothermal behavior, θ is simply entered as another canonical variable in ϕ and Ψ , as in Section 2.4, and in the f 's; eqn. (2.43) remains valid with $f_{\alpha} = f_{\alpha}(\sigma, \theta, H)$. Also eqn. (2.44) and, under the conditions cited, eqns. (2.47,48) remain valid if re-interpreted so that all H -dependent terms now depend on θ and H . In particular, ϵ^P is then re-interpreted as the strain when $\sigma = 0$ but θ and H remain at their current values, which differs from eqn. (2.21) unless $\theta = \theta_0$.

Now, eqn. (2.46) defined the f 's in terms of macroscopic stresses and the associated plastic changes in macroscopic quantities such as ϕ^0 , ϵ^P and M . However, for each type of mechanism, f can be expressed in terms of the local field of stress and lattice strain prevailing near the site of the associated rearrangement. Some examples follow.

2.6 EXAMPLES OF INCREMENTAL INTERNAL VARIABLES AND CONJUGATE FORCES

2.6.1 Crystalline slip

Suppose that the transition between H and $H+dH$ can be described as due to incremental glide motions of the dislocations in a metal, where the dislocations are regarded as line defects and dn is a continuous variable along each dislocation loop, denoting

the local advance of the line normal to itself in its slip plane. Then in eqns. (2.40,41)

$$\sum f_{\alpha} d\xi_{\alpha} \rightarrow \int_L [q \, dn] dL, \quad (2.49)$$

where q is the force per unit length of dislocation line and L denotes an integration along all lines in the material sample. With this representation eqn. (2.43) becomes

$$d^p \epsilon_{ij} = \frac{1}{V} \int_L \left[\frac{\partial q(\sigma, H)}{\partial \sigma_{ij}} \, dn \right] dL. \quad (2.50)$$

Here the notation means that q is a function of the macroscopic stress and of the entire current pattern of dislocations within the sample. It is known that within the linear elastic model the force on a dislocation contains a term τb , where τ is the local shear stress in the slip direction at a point along the dislocation line, acting in addition to the self stress of that segment of the line itself; b is the Burgers vector. Thus

$$q = q_0(H) + \bar{\tau} b \quad (2.51)$$

where $\bar{\tau}$ is a homogeneous linear function of σ , giving the shear stress at the dislocation site in the slip direction as would be induced elastically by applying macroscopic stresses σ to the material sample while the dislocations are held in position (i.e., at fixed H). The term q_0 represents contributions from the self stress and from all other sources of internal stress within the material sample. Note that in addition to containing geometric orientation factors, $\bar{\tau}$ also varies from point to point within the sample because the elastic application of σ induces a highly non-uniform stress field on the scale of, say, the grains and inclusions making up the material sample. Thus we obtain, in correspondence to eqn. (2.48) of the general formalism, an expression given by Rice (1970),

$$d^p \epsilon_{ij} = \frac{1}{V} \int_L \left[\frac{\partial \bar{\tau}}{\partial \sigma_{ij}} \, b \, dn \right] dL. \quad (2.52)$$

The terms dn and dL of eqns. (2.49,50) must be measured in units of, say, lattice spacing at finite lattice strain, to re-

main invariant under elastic distortion (Rice, 1971).

More generally, we shall average out the individual dislocations, specifying instead the local amounts of shear $d\gamma^{(1)}, d\gamma^{(2)}, \dots$ on the operative slip systems of the crystalline subelement encompassing any considered point of the material sample. If eqn. (2.52) were applied to a single crystal under macroscopically homogeneous deformation we would have

$$d\gamma^{(k)} = \frac{1}{V} \int_L^{(k)} [b^{(k)} \, dn] dL = \rho^{(k)} b^{(k)} \langle dn \rangle^{(k)} \quad (2.53)$$

where now the integral extends only over the dislocations on system (k) , and we express the result in terms of dislocation density $\rho = L/V$, b , and average advance $\langle dn \rangle$ on that system. The same interpretation is adopted locally within the heterogeneous material sample in that, e.g., we consider the ρ 's and γ 's to be defined locally throughout each grain of a polycrystal. Thus in eqns. (2.40,41)

$$\sum f_{\alpha} d\xi_{\alpha} \rightarrow \int_V [\sum \tau^{(k)} \, d\gamma^{(k)}] dV, \quad (2.54)$$

where this defines thermodynamic "stresses" conjugate to the $d\gamma$'s, and from eqn. (2.43)

$$d^p \epsilon_{ij} = \frac{1}{V} \int_V \left[\sum \frac{\partial \tau^{(k)}(\sigma, H)}{\partial \sigma_{ij}} \, d\gamma^{(k)} \right] dV. \quad (2.55)$$

Here, from eqns. (2.51-53), it is evident that the τ 's will have the form

$$\tau^{(k)} = \tau_0^{(k)}(H) + \bar{\tau}^{(k)} \quad (2.56)$$

where, again when the lattice elasticity can be treated as linear, $\bar{\tau}^{(k)}$ is the homogeneous linear function of σ giving the shear stress that would be elastically induced on the slip plane in the slip direction by σ . The term $\tau_0^{(k)}$ includes the shear stress induced by misfits and other sources of residual stress, and also a part accounting for energy that is "locked-in" at the discrete dislocation level.

An alternate, direct mechanical identification of the thermo-

dynamically defined τ 's is made by calculating the total reversible work, or change in Φ , done in the following steps, which are carried out under fixed overall deformation of the sample. These are assumed to take place under circumstances of small elastic stretches with moduli, referred to crystallographic axes, being unaffected by plastic shears.

(i) Cut free an element δV , applying to it and the walls of the cavity thus created surface tractions appropriate to the local stress field s_{ij} at that point; no work is involved.

(ii) Remove s_{ij} from δV ; the work of elastic unloading is done.

(iii) Move the dislocations as appropriate to accomplish the considered increment $d\gamma$ of plastic shear; $\delta V d^P\phi_0$ is the energy change, where $\phi_0(H)$ is the density of locked-in energy at the discrete dislocation level.

(iv) Elastically reload the body to the shape it had in (i); this regains the work of (ii) except that there is a deficit $-s_s d\gamma$ times δV (where s_s is the resolved shear component of s_{ij}) which arises because the required elastic reloading strain is less by the shear $d\gamma$, plus a term of order $(d\gamma)^2$ which arises because s_{ij} is now altered by some amount ds_{ij} .

(v) Put the element back into the cavity, removing the unwanted layer of body force arising from ds_{ij} of (iv); this causes displacements of its own order and hence the net work of this step is of order $(d\gamma)^2$

Thus, the net change in Φ , which must equal $-(\tau d\gamma)\delta V$ from eqns. (2.40,54), is, by summing the contributions of steps (iii), (ii) and (iv)

$$d^P\Phi = -\tau d\gamma \delta V = d^P\phi_0 \delta V - s_s d\gamma \delta V. \quad (2.57)$$

If we divide s_s into a part due to residual stresses, say s_s^{res} , plus the part $\bar{\tau}$ that is induced elastically by σ this becomes

$$\tau = -d^P\phi_0(H)/d\gamma + s_s^{\text{res}} + \bar{\tau}, \quad (2.58)$$

in conformity with the discussion following eqn. (2.56). Rice (1971) and Hill and Rice (1972) have discussed the identification of τ when no simplifying assumptions are made as to the size of lattice stretches or the effect of slip on moduli.

Often eqn. (2.54) will be insufficient to completely represent the H change in Φ ; e.g., during annealing, dislocations may annihilate one another without creating $d\gamma$'s. Put another way, increments in dislocation density ρ on the various slip systems cannot, especially at elevated temperature, be considered universally related to the corresponding $d\gamma$'s. Thus eqns. (2.54,55) may be generalized to

$$\Sigma f_\alpha d\xi_\alpha + \int_V [\Sigma \tau^{(k)} d\gamma^{(k)} + A^{(k)} d\rho^{(k)}] dV \quad (2.59)$$

$$d^P\epsilon_{ij} = \frac{1}{V} \int_V [\Sigma \frac{\partial \tau^{(k)}}{\partial \sigma_{ij}} d\gamma^{(k)} + \frac{\partial A^{(k)}}{\partial \sigma_{ij}} d\rho^{(k)}] dV, \quad (2.60)$$

where $A^{(k)}$ are affinities conjugate to the dislocation densities on the various slip systems. A simpler generalization would involve just one ρ , the sum of those for all systems.

But alterations in ρ when the γ 's are fixed can create no strain, unless there is an effect of ρ on elastic moduli [and even then the resulting effect is second order in σ by eqn. (2.46)]. Thus from eqn. (2.60) $\partial A^{(k)}/\partial \sigma = 0$ and $A^{(k)} = A^{(k)}(H)$. The simplest assumption is that the locked-in energy ϕ_0 depends only on the ρ 's, and not on the γ 's. Then, through the type of argument leading to eqns. (2.57,58), one has

$$A^{(k)} = -\partial \phi_0 / \partial \rho^{(k)}, \quad \tau^{(k)} = s_s^{\text{res}} + \bar{\tau}. \quad (2.61)$$

2.6.2 Diffusion

For simplicity, consider a single, foreign diffusing substance which can move through the lattice of the crystallites in the

sample and along its internal surfaces A , where A includes grain interfaces, boundaries of cavities, etc. Let the structural rearrangement of the material sample be characterized by the increase dn in concentration of the substance per unit volume of V and dN per unit area of interface A . Then the local chemical potential μ of the substance, at points throughout the sample, is defined by writing the change in Helmholtz free energy at fixed temperature and overall strain of the sample as

$$d^P\phi = \int_V [\mu dn]dV + \int_A [\mu dN]dA - \int_S [\mu dN]dS \quad (2.62)$$

for arbitrary alterations dn , dN in composition. In the last integral over the external surface S of the material sample, dN represents the amount of substance that has exited. Hence one can make the identity

$$\sum f_\alpha d\xi_\alpha \rightarrow - \int_V [\mu dn]dV - \int_A [\mu dN]dA + \int_S [\mu dN]dS \quad (2.63)$$

However, as is well known, quantities such as dn/dt and dN/dt cannot be written in rate equations of a local kind. Hence the $d\xi$'s are identified with increments of diffusive flux. These characterize structural rearrangements by the local amount dq_i ($i=1,2,3$) of material crossing unit area in the x_i direction within V , and the amount dQ_i ($i=1,2$) crossing unit length in the z_i direction on A , where z_1, z_2 is an orthogonal cartesian coordinate system locally tangent to A . Further, for mass balance

$$dn = - \partial(dq_i)/\partial x_i \quad \text{in } V \quad (2.64)$$

and, in the simple form when A is locally flat,

$$dN = -\partial(dQ_i)/\partial z_i + (v_i dq_i)^+ + (v_i dq_i)^- \quad \text{on } A, \quad (2.65)$$

where the last two terms represent fluxes from the two sides of A , v being the local outward normal to the portion of V supplying the dq (the divergence term is more complicated when A is curved). Thus, applying the divergence theorem in eqn. (2.62), taking $dN = v_i dq_i$ on S , assuming that incoming and

outgoing fluxes dQ balance at all intersections of internal surfaces, and assuming that μ is continuous and piecewise differentiable, there results

$$\sum f_\alpha d\xi_\alpha \rightarrow \int_V [-(\partial\mu/\partial x_i)dq_i]dV + \int_A [-(\partial\mu/\partial z_i)dQ_i]dA, \quad (2.66)$$

and this final result is valid for locally curved A as well.

The dependence of μ on the local stress field within the sample can be ascertained directly from eqn. (2.62). Suppose that addition of an amount dN of the substance to a grain boundary thickens it by an amount $k dN$ where $k=k(H)$, which means that k depends on the current arrangement of the material sample and concentration level at the place where dN is added. Then the work done by inserting the matter in presence of the local stress field contains the term $-s_n k dN$ where s_n is the normal stress acting on the interface. Hence

$$\mu = \mu_b(H) - s_n k \quad (2.67)$$

Similarly, if the addition of dn to an element of volume causes the shape change strain $\beta_{ij} dn$ then, by arguments analogous to that for the continuum slip model,

$$\mu = \mu_v(H) - s_{ij} \beta_{ij} \quad (2.68)$$

when elastic lattice distortions are small and moduli negligibly affected, where s_{ij} is the local stress field at the site within the material sample. As for τ , s_n and s_{ij} can be split into portions \bar{s}_n and \bar{s}_{ij} which are the parts elastically induced by the macroscopic stress, and therefore homogeneous linear functions of σ with position-dependent coefficients, in general, plus portions due to residual and misfit stresses. Thus the force terms $-\partial\mu/\partial x_i$ and $-\partial\mu/\partial z_i$ of eqn. (2.66) can be thought of as functions of σ and H , linear in the former for the present circumstances, and the relation analogous to eqn. (2.43) can be written. In the special case when the above linear forms are used,

$$d^P\epsilon_{ij} = \frac{1}{V} \int_V \left[\frac{\partial}{\partial x_\ell} (\beta_{qr} \frac{\partial \bar{s}_{qr}}{\partial \sigma_{ij}}) dq_\ell \right] dV + \frac{1}{V} \int_A \left[\frac{\partial}{\partial z_\ell} (k \frac{\partial \bar{s}_n}{\partial \sigma_{ij}}) dQ_\ell \right] dA \quad (2.69)$$

Here, in the differentiation on σ , \bar{s}_n and \bar{s}_{ij} are regarded as functions of σ and H , whereas the differentiations on x and z are, of course, total spatial derivatives in the usual sense. It is reasonably straightforward to generalize this discussion to multi-species diffusion, including self diffusion, and hence to provide a framework for inelastic deformation by diffusional creep.

2.6.3 Phase changes

Here we consider diffusionless phase changes, examples being martensitic transformations and twinning, in which a form α of a solid is converted to form β at an interface. Let A be the locus of all internal $\alpha - \beta$ interfaces in the material sample. The structural rearrangement in this case is characterized by the amount dz of normal advance of the interface into the α phase, where dz is a function of position on A . The thermodynamic force per unit area of the interface is denoted by p , so that eqns. (2.40,41) become

$$\Sigma f_{\alpha} d\xi_{\alpha} \rightarrow \int_A [pdz]dA . \quad (2.70)$$

Thus eqn. (2.43) gives

$$d^P \epsilon_{ij} = \frac{1}{V} \int_A \left[\frac{\partial p(\sigma, H)}{\partial \sigma_{ij}} dz \right] dA . \quad (2.71)$$

Eshelby (1970) has given the explicit formula which relates p to the local field at the interface. This can be obtained by (i) cutting out the volume of α involved in the advance dz over an element of A and applying tractions in accord with the local stress field acting there, (ii) unloading, (iii) transforming the α to β , (iv) applying stresses to regain the initial shape, (v) reinserting and removing the unwanted layer of surface force. Eshelby's result is

$$p = (\phi)_{\alpha} - (\phi)_{\beta} - T_i \left[\left(\frac{\partial u_i}{\partial n} \right)_{\alpha} - \left(\frac{\partial u_i}{\partial n} \right)_{\beta} \right] , \quad (2.72)$$

where the ϕ 's are local free energy densities on the two sides of the interface, T_i is the surface traction vector, and the

terms $\partial u_i / \partial n$ are the normal spatial derivatives of the displacement vector on the two sides. Of course, the base levels for the ϕ 's are not arbitrary since β obtains from α or vice-versa.

When the transformation corresponds to the growth of a void by cutting away material at a traction free surface, this reduces to the formula derived by Rice and Drucker (1966) with the ϕ difference being the strain energy density at the void surface. If the interface is considered to have a surface free energy γ , Eshelby's formula must be given an additional term of the form $-\gamma(\kappa_1 + \kappa_2)$, where the κ 's are principal curvatures of the interface.

2.6.4 Griffith cracks

The formalism can also be applied to a material sample containing some distribution of Griffith cracks and this forms a final example. Indeed, in rock and some other brittle materials microcrack growth is an important mechanism of inelastic deformation. Let the locus of all crack fronts be denoted by L and let $d\ell$ be a function of position along L describing the amount of local advance of the cracks, and hence constituting the structural rearrangements. The advances considered here will be such that the surfaces of cracking have continuously turning tangent planes, without abrupt forking or branching. If F denotes the thermodynamic crack extension force per unit length along L , then eqns. (2.40,41) become

$$\Sigma f_{\alpha} d\xi_{\alpha} \rightarrow \int_L [F d\ell] dL . \quad (2.73)$$

The model conventionally adopted, following Griffith, computes the change in free energy $d^P \Phi$ in quasistatic crack advance as the sum of the change in that part of Φ representing elastic deformation (i.e., in the "strain energy") plus that in the part of Φ representing surface energy. Thus

$$F = G - 2\gamma \quad (2.74)$$

where G is the elastic energy release rate as introduced by Irwin (1957) and γ is the surface free energy. Thus, when the local crack tip energy release rate is expressed in terms of the macroscopic stress σ on the sample, there results from eqn. (2.43)

$$d^p \epsilon = \frac{1}{V} \int_L \left[\frac{\partial G(\sigma, H)}{\partial \sigma_{ij}} d\ell \right] dL. \quad (2.75)$$

In the absence of residual stress, ϵ^p will always be zero and hence, in terms of eqns. (2.27,28) all of $d^p \epsilon$ reflects changes in overall elastic compliances under stress.

The local representation for G , within the linear elastic treatment of lattice stretching, can be given as a homogeneous quadratic function of the crack tip stress intensity factors, denoting the strength of the characteristic $r^{-1/2}$ stress singularity. Indeed, while a somewhat different notation is usually employed, these are here defined for the most general anisotropic material so that the stress vector T_i at distance r ahead of the crack, on the plane of prospective growth, is given by

$$T_i = k_i r^{-1/2} + \dots, \quad i=1,2,3 \quad (2.76)$$

the dots representing non-singular terms, whereas the crack opening $u_i^+ - u_i^-$ at a small distance r behind the tip is

$$u_i^+ - u_i^- = C_{ij} k_j r^{1/2} + \dots \quad (2.77)$$

Here C_{ij} are certain coefficients dependent on the local elastic compliances, and the stress intensity factors k_i , $i=1,2,3$, are linearly dependent on the applied stress σ . Thus, following Irwin's (1957) method of calculation of the work of unloading the crack surfaces,

$$G = \lim_{\Delta \ell \rightarrow 0} \frac{1}{\Delta \ell} \frac{1}{2} \int_0^{\Delta \ell} [k_i r^{-1/2} + \dots] [C_{ij} k_j (\Delta \ell - r)^{1/2} + \dots] dr = \frac{\pi}{4} C_{ij} k_i k_j \quad (2.78)$$

One may write

$$k_i = k_i^{\text{res}} + \bar{k}_i \quad (2.79)$$

where k^{res} is induced by residual stresses and where \bar{k} is a homogeneous linear function of σ , denoting the stress intensity factor induced by elastic application of σ . Also, writing $d^p \epsilon = d\epsilon^p + dM\sigma$ from eqn. (2.28), one finds from eqns. (2.75,78,79) that the increments of plastic strain and of overall elastic compliances due to crack advance are:

$$d\epsilon_{ij}^p = \frac{1}{V} \int_L \left[\frac{\pi}{2} C_{qr} k_q^{\text{res}} \frac{\partial \bar{k}_r}{\partial \sigma_{ij}} d\ell \right] dL$$

$$dM_{ijkl} = \frac{1}{V} \int_L \left[\frac{\pi}{2} C_{qr} \frac{\partial \bar{k}_q}{\partial \sigma_{ij}} \frac{\partial \bar{k}_r}{\partial \sigma_{kl}} d\ell \right] dL \quad (2.80)$$

The latter formula is closely connected with Irwin's (1960) relation between the stress intensity factor and load-point compliance changes for a cracked body. It also provides a general solution for the effect of cracking on overall elastic moduli, as has been considered in some particular cases by Walsh (1965). Equation (2.78) for G is generalized to non-linear elastic behavior as the crack tip J Integral (Rice, 1968; see also Cherepanov, 1967) which takes the same form as Eshelby's (1956,1970) general formula for the force on a point or line defect in an elastic field.

2.7 KINETIC RELATIONS AND PLASTIC NORMALITY

The last two sections have outlined the general method by which macroscopic strains are related to structural rearrangements on the microscale, and some specific $d\xi$'s with their conjugate f 's have been identified. The framework is completed in principle by a specification of kinetic relations for the rates $d\xi/dt$ of structural rearrangement.

Of course, the assumption throughout is that such f 's as we have introduced (force on dislocation or interface, chemical potential, etc.) retain meaning at states far removed from global thermodynamic equilibrium for the material sample.

Specifically, the relations that define the f 's and relate the $d\xi$'s to $d^p \epsilon$ are strictly valid when one considers the transition from one to another constrained equilibrium state, having structural arrangements H and $H+dH$ respectively. But the structural arrangements are unconstrained during actual

processes and it is assumed that eqn. (2.43) and its various specializations of the last section can be applied then as well, provided always that the f 's are identified as those of the imagined state of constrained equilibrium corresponding to the current H . The same assumption is tacitly adopted in much of dislocation theory and physical metallurgy, but bears statement before proceeding to kinetic aspects.

The kinetic equations are restricted by the second law as in eqn. (2.32). Indeed, writing $d^P\phi$ as in eqn. (2.40), this becomes

$$\sum f_{\alpha} d\xi_{\alpha}/dt \geq 0 \quad (2.81)$$

In the special cases for which f_{α} is linear in σ as in eqn. (2.47) we can note that $\sum f_{\alpha}^0 d\xi_{\alpha} = -d\phi^0(H)$ and use eqn.

(2.48) to convert this to

$$\sigma_{ij} d\epsilon_{ij}^P/dt \geq d\phi^0/dt \quad (2.82)$$

for isothermal processes, where ϕ^0 is the locked-in energy. Hence the macroscopic plastic work rate need not be positive, but can be negative when "locked-in" energy is being taken from the sample. This is evidently the case for a Bauschinger effect which commences during unloading in a tensile test, while the stress is still acting in tension. It is also the case for time-dependent strain recovery after reduction of the load on a specimen to a small but still tensile value.

In several instances it has been seen that the structural rearrangements can be resolved into individual, scalar processes characterized by some set (effectively infinite) of scalar variables $d\xi_{\alpha}$. For these cases it is natural to think of the rate $d\xi_{\alpha}/dt$ at which a particular rearrangement takes place as being primarily dependent on its associated thermodynamic force f_{α} , for a given θ and current pattern H of structural arrangement. That is, when some instantaneous rate $d\xi_{\alpha}/dt$ is thought of as a function of σ, θ , and H , the dependence on σ occurs primarily through dependence of the rate on the associated scalar force $f_{\alpha} = f_{\alpha}(\sigma, \theta, H)$. To this approximation, kinetic rate laws have the form

$$d\xi_{\alpha}/dt = r_{\alpha}(f_{\alpha}, \theta, H) \quad (2.83)$$

with each rate being stress dependent only via its conjugate thermodynamic force. The second law requirement will be satisfied so long as the rate function r_{α} has always the same sign as does f_{α} . The form is suggested by thermal activation models, in which case f_{α} represents the effect of applied stresses on biasing the pre and post-barrier energy levels. However, as a secondary effect, local stress terms not included in f could alter the size of the barrier itself, at least to the extent that lattice dimensions are affected, so that eqn. (2.83) should be thought of only as an approximation and not as a physical law.

Kinetic relations of the Schmid type that are usually taken to describe crystalline slip are, in fact, in accord with this class of rate law. Specifically, these relations entail that the rate of slip $d\gamma^{(k)}/dt$ [or average dislocation velocity $\langle dn/dt \rangle^{(k)}$] on a given slip system is dependent on the local stress state only via the resolved shear stress $s_s^{(k)}$ on that system. As seen in eqns. (2.56, 58, 61), the net resolved shear stress differs from the thermodynamic shear stress only by a term dependent on H (and θ in a non-isothermal analysis) so that the type of kinetic law just described for crystalline slip has the form

$$d\gamma^{(k)}/dt = \Gamma^{(k)}(\tau^{(k)}, \theta, H) \quad (2.84)$$

and is thus a special case of the general class of eqn. (2.83). This form includes, of course, such effects as direct and latent hardening against further slip, via the dependence on H . Again, some approximation is entailed. The large isotropic compression of a crystalline lattice by high pressure would alter the resolved shear stress for a given shear force only insofar as the area is changed, but sufficiently large pressures are likely to alter eqn. (2.84) in a more complicated way. Of greater interest, however, is the possibility, pointed out in private communication by F. Kocks, that when dislocations split into partials, not only is the resolved shear stress on the slip system important but so also are the resolved shears on different planes which tend to either coalesce or widen the partials. In such cases the stresses which "set-up" the deformation are not synonymous with those that drive the dislocation.

For vector processes of structural rearrangement as in diffusion, it is in general not possible to associate a given com-

ponent dq_i/dt of the matter flux only with its force $-\partial\mu/\partial x_i$. Nevertheless, it is usually taken as sufficient to assume, in the absence of, say, large lattice strain effects on the intrinsic height of energy barriers, that the flux vector for some diffusing species at a point depends only on the various forces $-\partial\mu/\partial x$ as defined for all the diffusing species at that point. Hence, within the general framework, considerable interest attaches to the case for which an individual rate $d\xi_\alpha/dt$ depends, at a given θ and H , on some set of forces f , conjugate to that rate and to others present locally. The special case in which these are taken to be instantaneously linear,

$$d\xi_\alpha/dt = \sum L_{\alpha\beta}(\theta, H) f_\beta, \quad (2.85)$$

with Onsager reciprocity $L_{\alpha\beta} = L_{\beta\alpha}$ is, in fact, just a particular case of eqn. (2.83). This is because, as Kestin and Rice (1970) have remarked, re-definition of the f 's and $d\xi$'s by linear combinations, in accord with the rotation to principal axes of L in f space, reduces eqn. (2.85) to a diagonal form, in which each instantaneous rate is stress-state dependent only via its conjugate force.

It is of interest that rate laws of the class of eqn. (2.83), for which conjugate forces govern rates, lead to a remarkable normality structure for macroscopic constitutive laws (Kestin and Rice, 1970; Rice, 1970, 1971), independently of the detailed form of the rate equations. Indeed, the balance of this section is devoted to an exploration of the topic. The structure under consideration is such that a macroscopic scalar flow potential $\Omega = \Omega(\sigma, \theta, H)$ exists at each instant of the deformation such that the instantaneous plastic portion of the macroscopic strain rate is given by

$$d^P \epsilon_{ij}/dt = \frac{\partial \Omega(\sigma, \theta, H)}{\partial \sigma_{ij}}. \quad (2.86)$$

It is easiest to derive the equation by directly writing the microscale representation for Ω :

$$\Omega(\sigma, \theta, H) = \frac{1}{V} \sum \int_0^{f_\alpha(\sigma, \theta, H)} r_\alpha(f_\alpha, \theta, H) df_\alpha, \quad (2.87)$$

where the integration is done at fixed θ and H , and with this eqn. (2.86) may be proven as a direct application of eqn. (2.43):

$$\frac{\partial \Omega}{\partial \sigma_{ij}} = \frac{1}{V} \sum \frac{\partial f_\alpha}{\partial \sigma_{ij}} r_\alpha = \frac{1}{V} \sum \frac{\partial f_\alpha}{\partial \sigma_{ij}} d\xi_\alpha/dt = d^P \epsilon_{ij}/dt.$$

If we specialize these results to the crystalline slip model, with the rate law of eqn. (2.84),

$$\Omega(\sigma, \theta, H) = \frac{1}{V} \int_V \sum \left\{ \int_0^{\tau^{(k)}(\sigma, \theta, H)} \Gamma^{(k)}(\tau^{(k)}, \theta, H) d\tau^{(k)} \right\} dV, \quad (2.88)$$

and now eqn. (2.86) may be proven directly from the corresponding special version (2.55) of eqn. (2.43). This shows also that the macroscopic flow potential is just the volume average of local flow potentials for each slip system of each individual crystallite of the material sample.

Consider the significance of the flow potential from a purely macroscopic standpoint: Now instead of requiring six separate constitutive relations for the stress and history dependence of the instantaneous plastic strain rate components, we require only one for the scalar Ω , from which the others are generated. Further, this has a geometric interpretation in a stress space having coordinate axes which are the components of σ . At each epoch in the history of deformation, a family of surfaces of the form $\Omega = \text{constant}$ exists in this space, and have the property that the instantaneous plastic strain rate has a direction 'normal' to the Ω surface through the current stress point, and a magnitude equal to the gradient between neighboring Ω surfaces. Provided that the local rates are steadily increasing functions of the conjugate forces for any given θ and H , and that conditions for the forces to be linear in σ are met, each Ω surface may be shown to be convex, in that a plane which is tangent to the surface at any point will never cross it. Indeed, if we consider two different stress states σ^A, σ^B but the same plastic state H and θ ,

$$\sum (f_\alpha^A - f_\alpha^B) [(d\xi_\alpha/dt)^A - (d\xi_\alpha/dt)^B] \geq 0 \quad (2.89)$$

by the assumed monotonicity of the rate law. But by eqns. (2.47, 48) which apply when the forces are linear (in which case $d\epsilon^P/dt = d^P \epsilon/dt$), the inequality becomes, successively

$$\Sigma (\sigma_{ij}^A - \sigma_{ij}^B) \epsilon_{\alpha, ij}^1 [(d\epsilon_{\alpha}^A/dt)^A - (d\epsilon_{\alpha}^B/dt)^B] \geq 0$$

$$(\sigma_{ij}^A - \sigma_{ij}^B) [(d^P \epsilon_{ij}^A/dt)^A - (d^P \epsilon_{ij}^B/dt)^B] \geq 0 \quad (2.90)$$

This, in combination with eqn. (2.86), proves the convexity of Ω surfaces (see Rice, 1970).

Often the kinetic relation of eqn. (2.84) is strongly non-linear: At any given H and θ , an essentially zero $d\gamma/dt$ results for a certain range of τ values, whereas $d\gamma/dt$ takes on very large magnitudes for values of τ only slightly beyond the limits of this range. Of course, these limits change with accumulating H . Evidently, if we consider a restricted range of deformation rates, then the resulting behavior is well described by a time-independent idealization in which the limits represent critical shear stresses for yielding a slip system, and in which the changes in the limits with H represent strain hardening.

Within this time-independent model, we may take state B in the preceding inequality to coincide with a point within the elastic domain at the current H and A to lie on the current yield surface. Thus it reduces to the classical inequality of maximum plastic work,

$$(\sigma_{ij}^A - \sigma_{ij}^B) (d^P \epsilon_{ij}^A/dt)^A \geq 0, \quad (2.91)$$

except that the present form, in conjugate deformation variables, is properly invariant to rigid rotations in going from A to B , under the tacit assumption of small elastic lattice stretches between the two states. This inequality is well known to lead to the time independent normality structure discussed in connection with eqns. (2.35,36) and also to require that all yield surfaces be convex. Rice (1971) and Hill and Rice (1973) have further shown, in fact, that validity of the inequality (2.89), in the time-independent theory, implies the Il'yushin inequality, and hence normality in conjugate variables, without regard to the magnitude of elastic deformations.

By directly adopting the time-independent idealization in connection with a somewhat more restricted crystalline slip model than necessitated in the present framework, Hill (1967), Mandel (1966), and Rice (1966) independently derived such results on plastic normality and convexity as just discussed.

They show that the plastic strain increment $d^P \epsilon$ has the di-

rection of the outward normal to the current macroscopic yield surface in σ space when that surface is smooth, and a direction within the cone of limiting normals at a vertex. In fact, as Hill has emphasized, a vertex is usually to be expected, within the model, on subsequent yield surfaces at points of sustained deformation. This is because the macroscopic yield surface is the envelope of an infinite family of yield planes in σ space, each corresponding to a critical shear stress on a local slip system. These planes may translate as residual stress contributions to τ build up and as direct or latent hardening occurs, but their normals remain of fixed orientation. Every individual plane corresponding to a slip system active in the sustained deformation must pass through the current stress state, and this creates the vertex. Hill has also proposed that vertex-free large offset "yield surfaces" can be interpreted as families of plastic limit states as defined in terms of the local distribution of hardness in a polycrystalline aggregate. This is tantamount to treating the material as rigid-plastic, as in a study by Bishop and Hill (1951).

Rice (1970) has discussed the time-independent idealization in terms of a clustering of Ω surfaces outside the non-yielding domain of σ space. Also, he has shown that if the relation between $d\gamma/dt$ and τ on each slip system is continuous, then the Ω surfaces do not contain vertices except possibly when a surface corresponds to zero strain rate. This latter case arises when a non-yielding domain, in which $\Omega = \text{constant}$, exists.

The dual potential to Ω is of some utility. Let us suppose that the relation of $d^P \epsilon/dt$ to σ is invertible to the extent that a function (Rice, 1973)

$$\Lambda = \Lambda(d^P \epsilon/dt, \theta, H) = \sigma_{ij} d^P \epsilon_{ij} / dt - \Omega \quad (2.92)$$

may be defined. Then by eqn. (2.86) when θ and H are considered fixed,

$$d\Lambda = \sigma_{ij} d(d^P \epsilon_{ij} / dt), \quad \text{or} \quad \sigma_{ij} = \frac{\partial \Lambda(d^P \epsilon/dt, \theta, H)}{\partial (d^P \epsilon_{ij} / dt)} \quad (2.93)$$

if components of $d^P \epsilon/dt$ can be varied independently. Usually they cannot be, because plastic straining is incompressible. In this case it is easy to see that the differential form of eqn. (2.93)₁ allows solution for the deviatoric part of σ .

By using eqns. (2.43,87) and by writing r_α for $d\varepsilon_\alpha/dt$ and integrating by parts, the microstructural interpretation of Λ is

$$\Lambda = \frac{1}{V} \Sigma \left[\int_0^{r_\alpha} f_\alpha(r_\alpha, \theta, H) dr_\alpha - (f_\alpha - \sigma_{ij} \frac{\partial f_\alpha}{\partial \sigma_{ij}}) r_\alpha \right], \quad (2.94)$$

where, for purposes of the integration at fixed θ, H , the kinetic law given by eqn. (2.83) is supposed to have been inverted to obtain f in terms of r . Of course, when f is linear in σ this becomes

$$\Lambda = \frac{1}{V} \Sigma \left[\int_0^{r_\alpha} f_\alpha(r_\alpha, \theta, H) dr_\alpha - f_\alpha^0(\theta, H) r_\alpha \right], \quad (2.95)$$

where f_α^0 is now the value of f_α when $\sigma = 0$. This would, for example, take the form

$$\Lambda = \frac{1}{V} \int_V \Sigma \left[\int_0^{\eta^{(k)}} \tau^{(k)}(\eta^{(k)}, \theta, H) d\eta^{(k)} - \tau_0^{(k)}(\theta, H) \eta^{(k)} \right] dV \quad (2.96)$$

for the slip model which averages out the individual dislocations, where $\eta^{(k)}$ is written for $d\gamma^{(k)}/dt$, and where the rate law of eqn. (2.84) is supposed to have been inverted in the integrand.

For the time-independent idealization, f_α^f will have a definite value (namely, the current yield value) if the associated r_α or $d\varepsilon_\alpha/dt$ is non-zero. Hence each of the integrals in eqn. (2.94) amounts in a term $f_\alpha r_\alpha$, and so

$$\Lambda = \frac{1}{V} \Sigma \sigma_{ij} \frac{\partial f_\alpha}{\partial \sigma_{ij}} \dot{r}_\alpha = \sigma_{ij} d^p \varepsilon_{ij} / dt \quad (2.97)$$

by eqn. (2.43). Thus eqn. (2.93) reproduces a known result for time-independent materials satisfying the normality rule: that components of σ are derivatives of the rate of plastic working with respect to corresponding components of $d^p \varepsilon / dt$. This identification of Λ could also be developed directly from eqn. (2.92) in the rate-insensitive limit.

2.8 THE AVERAGING PROBLEM; POLYCRYSTAL MODELS

The general framework must be completed by some procedure of averaging a given set of rate relations over all the local sites of rearrangement within a material sample, to arrive finally at specific macroscopic representations of constitutive laws. Here we shall examine some approaches to the averaging problem for the plastic behavior of polycrystalline aggregates deforming by slip, on the assumption that kinetic relations of the kind (2.84) are given, a priori, from dislocation dynamics considerations and/or experiment for the operative slip systems within the individual crystals of the aggregate. Of course, these relations are not known precisely in general and very simple forms have been employed in the studies under review. Nevertheless, they do presumably show the manner in which constraints of neighboring grains and induced residual stresses affect the macroscopic constitutive behavior of polycrystals. All the discussion of this section is carried on within a small displacement gradient approximation, for which distinctions between stress and deformation measures of different kinds and their rates are ignored. Further, elastic moduli are taken to be uninfluenced by slip.

Local stress and strain fields within individual crystalline elements of the aggregate are denoted by s and e . The plastic strain is given in terms of the local shears γ by

$$e_{ij}^p = \Sigma \mu_{ij}^{(k)} \gamma^{(k)}, \quad (2.98)$$

where the summation extends over all operative slip systems of the element and where

$$\mu_{ij} = \frac{1}{2} (n_i m_j + n_j m_i), \quad (2.99)$$

with n and m being unit vectors describing the slip plane normal and slip direction for a given system. The mechanical shearing stress acting on a given system is

$$\tau^{(k)} = s_{ij} \mu_{ij}^{(k)}; \quad (2.100)$$

this differs from the thermodynamic shear stress of eqn. (2.54) only in that the latter contains an additional part accounting for energy which would remain stored in the dislocation substructure even if the local stress were reduced to zero ($s \rightarrow 0$).

Hence τ as we now use it includes the long range residual shear stress as well as that induced elastically by σ , and called $\bar{\tau}$ earlier.

Taylor (1938) and Bishop and Hill (1951) considered a single phase polycrystal and neglected elastic strains (rigid-plastic model), further supposing that each individual grain sustains the macroscopic strain ϵ^P of the aggregate. While their considerations were for time-independent behavior only, we can in fact consider the general time-dependent case, presuming that by inversion of eqn. (2.84), rate laws are given in the form (isothermal for simplicity)

$$\tau^{(k)} = \tau^{(k)}(\eta^{(k)}, H), \quad \text{where } \eta^{(k)} = d\gamma^{(k)}/dt \quad (2.101)$$

The procedure is to directly calculate the potential Λ from eqn. (2.96) as

$$\Lambda = \frac{1}{V} \int_V \Sigma \left[\int_0^{\eta^{(k)}} \tau^{(k)}(\eta^{(k)}, H) d\eta^{(k)} \right] dV. \quad (2.102)$$

Now the term with $\tau_0^{(k)}$ of eqn. (2.96) has seemingly disappeared. This is because its part representing stored energy in the dislocation substructure has already been incorporated, due to the discussion following eqn. (2.100), and because the remaining long-range residual stress part does no net work on the $d\gamma$'s by the principle of virtual work, which can here be applied because elastic strains are neglected and hence the γ 's give the total strain and correspond to a compatible deformation field.

To calculate each $\eta^{(k)}$ of an individual grain so that Λ may be computed, one recognizes that these are to be constrained by the approximation that each grain sustains the same strain. Hence

$$\Sigma \mu_{ij}^{(k)} \eta^{(k)} = d\epsilon^P/dt \quad (2.103)$$

for each. We must further choose the η 's so that the associated set of τ 's as computed from eqn. (2.101) are, in fact, derivable from a local stress field s by eqn. (2.100). The correct η 's are given by minimizing the bracketed terms in eqn. (2.102) subject to the constraint of eqn. (2.103), for by the method of Lagrange multipliers, this is equivalent to

$$\delta \left\{ \left[\Sigma \int_0^{\eta^{(k)}} \tau^{(k)}(\eta^{(k)}, H) d\eta^{(k)} \right] - \lambda_{ij} \left[\Sigma \mu_{ij}^{(k)} \eta^{(k)} \right] \right\} = 0, \\ \text{or } \left\{ \tau^{(k)}(\eta^{(k)}, H) - \lambda_{ij} \mu_{ij}^{(k)} \right\} \delta \eta^{(k)} = 0, \quad (2.104)$$

where λ_{ij} are the multipliers. Evidently, the equation is solved when

$$\tau^{(k)} = \lambda_{ij} \mu_{ij}^{(k)}, \quad (2.105)$$

which is the same as saying that the τ 's are derivable from a stress field. In fact, $\lambda = s$.

By performing this constrained minimization, the bracketed term of eqn. (2.102) is determined as a function of $d\epsilon^P/dt$ for each grain orientation. The remaining volume integral means that Λ is given by the average of this function over all grain orientations, and σ is computed from eqn. (2.93). The time-independent version of this general approach is exactly that employed by Bishop and Hill (1951). The net result is that Taylor orientation factors have been determined showing, for example, that the flow stress of an fcc polycrystal loaded in simple tension is approximately 3 times the corresponding shear strength on its $(111)[\bar{1}10]$ slip systems (assumed equal for all). Lin (1957) has further extended this approach to the elastic-plastic case by assuming that the total strain is constant in each grain; this allows an estimate of the entire stress-strain curve. Of course, the constraint that each grain deforms the same makes it impossible for stress equilibrium to hold and also causes an overestimate of the resistance to flow.

Batdorf and Budiansky (1949) have proposed a slip theory of plasticity which, if reinterpreted in the present context, can be seen as complementing the above approach by assuming that each individual grain carries the same stress, equal to σ . Hence eqn. (2.100) becomes

$$\tau^{(k)} = \sigma_{ij} \mu_{ij}^{(k)} \quad (2.106)$$

and with this together with rate laws of the type (2.84), phrased in terms of the mechanical shear stress, one may directly calculate Ω from eqn. (2.88) as the average over all

orientations of the flow potential which an individual grain would have, if subjected to the stress σ . The corresponding plastic strain rate is then given by eqn. (2.86). Of course, this approach does not satisfy displacement continuity between adjacent grains, nor can it account for development of residual stresses which tend to build up preferentially on the systems of greatest slipping; hence it underestimates the resistance to flow.

Recently Clough and Simmons (1973) have proposed an approach to rate-dependent flow which, on examination, may be seen as amounting to the formalism outlined above with a rate law for which $d\gamma/dt$ varies as a hyperbolic sine of τ , with no effect of H on the relation. The original Batdorf-Budiansky application was to rate-independent slip, with hardening of active systems, but no latent hardening or reverse hardening. This led to a pronounced vertex at the current load point. Also, for any stress path which continuously activated every slip system, once initially activated, the total strain was seen to depend only on the stress -- i.e., 'deformation theory' applied (Budiansky, 1959).

Lin and Ito (1965,1966) analyzed by methods of three dimensional elasticity the behavior of a polycrystalline model of $4 \times 4 \times 4$ square blocks, each containing one permissible set of slip planes with three equally spaced slip directions. Orientations were chosen to simulate a macroscopically isotropic polycrystal. They showed that a vertex formed at the current load point when a zero offset strain definition of yield was adopted, but they also showed that this vertex became a rounded bulge when a small but finite offset definition was used.

The bulk of work on predicting elastic-plastic behavior of polycrystals has been based on the self-consistent model of Kröner (1961) and Budiansky and Wu (1962). It considers s and e to take on constant values within each grain. Apart from any constitutive connection between the two, these are related to σ and ϵ by the same formulae that would apply if the grain were a homogeneous spherical inclusion imbedded in an infinite homogeneous matrix, having the overall elastic properties of the aggregate, and carrying the remotely uniform fields σ and ϵ . Thus, if these overall properties are isotropic with shear modulus G and Poisson ratio ν ,

$$s_{ij} = \sigma_{ij} - \frac{3-5\nu}{4-5\nu} G \delta_{ij} (e_{kk} - \epsilon_{kk}) - \frac{7-5\nu}{4-5\nu} G (e_{ij} - \epsilon_{ij}) \quad (2.107)$$

Here, ϵ, σ are volume averages of e, s ,

$$\epsilon_{ij} = \frac{1}{V} \int_V e_{ij} dV, \quad \sigma_{ij} = \frac{1}{V} \int_V s_{ij} dV \quad (2.108)$$

and the first of these will imply the second by eqn. (2.107).

Now, in the special case when each grain is idealized as being elastically isotropic with the same constants ν and G eqn. (2.107) may be re-written solely in terms of plastic strain as

$$s_{ij} = \sigma_{ij} - \frac{2}{15} \frac{7-5\nu}{1-\nu} G (e_{ij}^P - \epsilon_{ij}^P), \quad (2.109)$$

and in this case, although not generally (Rice, 1970; Hill, 1971), ϵ^P is the volume average of e^P . Hence, using eqns. (2.98,100) the shear stress associated with a slip system in a given grain, having the orientation parameter $\mu^{(k)}$, is

$$\tau^{(k)} = \sigma_{ij} \mu_{ij}^{(k)} - \frac{2}{15} \frac{7-5\nu}{1-\nu} G \left[\sum \mu_{ij}^{(\ell)} \mu_{ij}^{(k)} \gamma^{(\ell)} - \frac{1}{V} \int_V \sum \mu_{ij}^{(\ell)'} \mu_{ij}^{(k)'} \gamma^{(\ell)'} dV' \right], \quad (2.110)$$

where the first sum, on (ℓ) , extends over all slip systems of the same grain and the second, on $(\ell)'$, extends over all systems of every grain as it is encountered in the volume integral (or orientation average); the primes distinguish those variable quantities in the integration. This gives an explicit representation for the long range residual stress, as a linear function of all the γ 's in all the grains. The procedure is then to solve the kinetic relations for the γ 's, given a history of σ variation, and to thereby compute ϵ^P .

Hutchinson (1964) has applied this procedure to time-independent calculations, both without hardening and with Taylor hardening, for fcc and bcc polycrystals. His results include the calculation of Bauschinger effects and of the response to proportional loading under combined stress. Bui (1970) has adopted the model to compute subsequent yield surfaces and shows a clear vertex formation. Kocks (1970) has given an extensive general survey of work with the self-consistent model and with the Taylor model in predicting the yield behavior of polycrystals, including experimental comparisons. Brown (1970a) and Zarka (1972) have considered time dependent behavior; the former has adopted a power law relation between $d\gamma/dt$ and τ for fcc polycrystals, and has computed the

surfaces of constant flow potential in tension-torsion stress space for various deformation histories. These seem, to a fair approximation, to show kinematic translation without much shape change. Brown (1970b) has also attempted direct experimental measurement of Ω surfaces. These, for an aluminum alloy at elevated temperature, seem to show the same pronounced anisotropy as did the lower temperature yield surface for tension-torsion specimens of the same material.

Hill (1965) has suggested a more elaborate self-consistent model which is intended to take account of directional weaknesses developing with continuing deformation in a time-independent plastic framework; the corresponding generalization for time-dependence is, however, unclear. Recently Hutchinson (1970) has given an extensive review, contrasting the Hill model with that of Kroner-Budiansky-Wu. The latter gives limit states which agree with the Taylor model, and are thus overestimates, whereas the Hill model seems to give lower values. Hutchinson also calculates the plastic moduli governing increments of shear after tensile loading. These are considerably nearer to the predictions of 'deformation' theory than to those of a 'flow' theory with a smooth yield surface, although the theory itself is, of course, of the flow type.

Similar averaging procedures, to obtain macroscopic constitutive laws, could presumably be carried out for other of the internal variable and conjugate force sets of Section 2.6. The point which must be achieved, in general, is the development of an equation analogous to (2.110), which expresses the forces f_α in terms of the macroscopic stress σ and the various microstructure parameters whose increments are measured by the $d\xi$'s. These, together with a kinetic relation of, say, the type (2.83) relating $d\xi/dt$ to f enable one to write differential equations for $d\xi/dt$ in which σ enters as a forcing function. The resulting macroscopic plastic strain rate is expressed in terms of the f 's and $d\xi/dt$'s by eqn. (2.43), or by eqn. (2.48) when appropriate, and this is in the form of a volume average expression. As for the self-consistent crystalline slip models, the balance of the analysis consists of carrying out the averaging over all sites and their orientations within a representative material sample to arrive finally at specific macroscopic constitutive relations.

Judging from the progress with slip models as just reviewed, this general procedure does seem to reveal many of the observed features of combined stress behavior, including Bauschinger effects, kinematic like translation of yield and flow potential surfaces, tendency toward vertex formation on small offset yield surfaces, etc. However, the computations involved in estimating

the constitutive response to even simple deformation histories are quite complex and involve large storage requirements since, e.g., shears γ on all systems of crystals of all the representative orientations chosen for the calculation must be analyzed in each step. Indeed, when each dy/dt is expressed in terms of its associated τ , eqn. (2.110) becomes a large system of coupled, non-linear differential equations.

Thus the use of averaging procedures that involve, even with substantial approximations, a direct calculation from micro-scale models entails substantial complexity, and this would seem overwhelming if required in each increment of deformation for each element of, say, a finite element computer formulation for some structural problem involving inhomogeneous deformation. This means that any reasonably direct prediction of material response is unlikely to displace the phenomenological and less rigorously based structure-parameter models, discussed in subsequent chapters, as a basis for practical calculation. A brief discussion of this type of approach follows.

2.9 PHENOMENOLOGICAL AND MACROSCOPIC STRUCTURE-PARAMETER FORMULATIONS

There is an extensive literature on purely phenomenological approaches to constitutive laws within the time-independent plasticity idealization (see reviews by Drucker, 1956; and Naghdi, 1960) and some attempts at generalization to the time-dependent range have been made. Here we examine a simple formulation, intended for problems of time-dependent plastic flow under variable temperature and non-proportional stressing, which incorporates and generalizes, in what seems to be a physically acceptable form, notions such as kinematic and isotropic hardening as developed in the time-independent theory. We deal with initially isotropic materials.

Taking the viewpoint that the instantaneous plastic strain rate $d^P\varepsilon/dt$ is some function of σ, θ and the current plastic state H , we can define a rest stress tensor λ_{ij} (see Rice, 1970; Ahlquist and Nix, 1969) associated with θ and H as that for which $d^P\varepsilon/dt$ vanishes when $\sigma = \lambda$. The tensor λ is approximately interpretable as a macroscopic structure parameter, or internal variable, that measures the intensity of residual stress contributions to the forces f . As seen in eqn. (2.47) and in the slip and diffusion examples of Section 2.6, these typically have a form in which there is a term directly

proportional to σ plus another term of long and short range residual stress origin, the latter being reflected by λ . Still, λ is not purely a structure parameter because its definition, as the stress corresponding instantaneously to a null plastic strain rate, involves the kinetic relations as well. For this reason, and also because temperature alterations can cause residual stresses in heterogeneous materials, λ will vary at least slightly with θ at a given H .

Now, λ can be taken as a measure of the anisotropy that has been induced by plastic deformation. It is known within the time-independent framework, however, that when offset strains of the order 1/2 to 2% are taken to define yield, subsequent yield surfaces in stress space are essentially isotropic, with little evidence of the pronounced anisotropy that shows on small offset yield surfaces. Thus there is need for a further scalar structure parameter, called ρ here, which characterizes the intrinsic resistance to flow that exists apart from anisotropic and related strain transient effects (see the chapter by Hart et al.). We may think of ρ as denoting a parameter such as the net dislocation density, or some average measure of the kind b/L where L is a distance between strong dislocation pinning points, or instead just as the flow stress (suitably averaged among directions to free the definition of anisotropy) at some fixed temperature, sufficiently low that creep effects are absent. This single parameter characterization would seem suitable so long as the deformation is not so large as to induce significant preferred orientation and texturing.

The balance of the discussion is done within the conventional small displacement gradient approximation. All that is said can, however, be taken to apply as well for large plastic deformations, within the limitation of texturing, by using the procedure outlined at the end of Section 2.3 and taking F^P there to correspond to a pure deformation. In that case σ is to be interpreted as the stress conjugate to logarithmic strain based on a reference state instantaneously coincident with the elastically unloaded state, or as R^{TR} to the order of the approximation, and the rates $d\sigma/dt$ and $d\epsilon/dt$ are interpreted as discussed there in terms of $\mathcal{D}T/\mathcal{D}t$ and D .

The assumption made is that the instantaneous $d^P\epsilon/dt$ depends only on (i) the stress difference $\sigma - \lambda$, (ii) temperature θ , and (iii) the scalar structure parameter ρ . The assumption (i) is, of course, far too simply to closely match either observed behavior or the predictions of detailed microscale models for general loading paths, particularly in

the neighborhood of yield surface vertices or sharply rounded portions of flow potential surfaces. It does, however, comprise a suitably simple basis for applications to stress analysis.

It is assumed that the microscale mechanisms of deformation are such that the flow potential Ω exists and, from (i) above, it is clear that this can be stress-state dependent only through the three invariants of the stress difference $\sigma - \lambda$.

If, however, the plastic response $d^P\epsilon/dt$ is volume preserving, or conversely if the microscale forces are uninfluenced by hydrostatic stress of the levels considered, then Ω depends only on the second and third invariants of the deviatoric part of $\sigma - \lambda$. This means that any hydrostatic part of λ is without effect and λ can therefore be taken as a deviatoric tensor. It usually constitutes a suitable approximation to assume, as in the Prandtl-Reuss equations, that there is a dependence only on the second deviatoric invariant, which can be expressed as an equivalent shear stress τ_{eq} :

$$\tau_{eq} = \tau_{eq}(\sigma - \lambda) = \left[\frac{1}{2} (\sigma'_{ij} - \lambda_{ij})(\sigma'_{ij} - \lambda_{ij}) \right]^{1/2},$$

$$\text{where } \sigma'_{ij} = \sigma_{ij} - \frac{1}{3} \delta_{ij} \sigma_{kk}. \quad (2.111)$$

Thus we arrive at the form

$$\Omega = \Omega[\tau_{eq}(\sigma - \lambda), \theta, \rho], \quad (2.112)$$

and there follows from eqn. (2.86) the plastic strain rate

$$d^P\epsilon_{ij}/dt = \frac{\sigma'_{ij} - \lambda_{ij}}{2 \tau_{eq}(\sigma - \lambda)} \frac{\partial \Omega[\tau_{eq}, \theta, \rho]}{\partial \tau_{eq}}. \quad (2.113)$$

Note that the explicit dependence of Ω on τ_{eq} at different states θ and ρ can be determined experimentally by examining the variation of instantaneous plastic strain rate with stress at various stages throughout a program of uniaxial tension and compression, or of pure shear deformation, provided results are fitted to the assumed symmetric dependence on $\sigma - \lambda$.

The constitutive description must be completed by a specification of equations governing alterations in the structure parameters λ and ρ . This is perhaps the most arbitrary part, and there is little hope of including all possible ef-

facts. An appealing form for ρ is

$$\frac{d\rho}{dt} = h(\rho, \theta) \left[\frac{d^p \epsilon_{ij}}{dt} \frac{d^p \epsilon_{ij}}{dt} \right]^{1/2} + \beta(\rho, \theta) \lambda_{ij} \frac{d^p \epsilon_{ij}}{dt} - r(\rho, \theta), \quad (2.114)$$

where h represents an intrinsic rate of "hardening", the same for all directions, and β represents the extent to which the hardening induced by a strain increment is biased by its direction relative to the current rest stress. In fact, the first two terms are independent of the time scale and contribute net hardening rates

$$h(\rho, \theta) + \beta(\rho, \theta) [\lambda_{ij} \lambda_{ij}]^{1/2}, \quad h(\rho, \theta) - \beta(\rho, \theta) [\lambda_{ij} \lambda_{ij}]^{1/2}$$

when $d^p \epsilon$ is respectively co-directional and oppositely directed to λ . The minus sign in the latter form may be thought of as representing the annihilation of dislocations that have not spread widely from their sources, but rather have been blocked by obstacles in the deformation that produced λ . The last term $r(\rho, \theta)$ of eqn. (2.14) is the temperature-dependent rate of hardness recovery. Provided that λ can be ascertained, the functions h and β can be determined in principle by loading a tensile specimen to a given hardness state ρ , and then measuring the increments of ρ due to rapid increments of further loading and reverse compressive loading, both done on a time scale for which the recovery effect is negligible. Also, $r(\rho, \theta)$ is accessible either from recovery studies or from observed values of ρ and the strain rate in states of steady creep at various temperatures, provided that these correspond to $\rho = \text{constant}$.

It is plausible that λ be chosen codirectional with σ' in a program of proportional stressing, commencing from a state at which $\lambda = 0$. Further, λ should approach some saturation magnitude, with ongoing deformation, that increases with increasing σ' , and is here supposed to take the form

$$\lambda_{ij}^{\text{sat}} = q(\rho, \theta) \sigma'_{ij}, \quad (2.115)$$

where $0 \leq q < 1$, although the saturation magnitude itself may never be attained if σ' increases indefinitely. A simple man-

ner of describing the change in λ is by writing

$$\frac{d\lambda_{ij}}{dt} = p(\rho, \theta) \left[\lambda_{ij}^{\text{sat}} - \lambda_{ij} \right] \left[\frac{d^p \epsilon_{ij}}{dt} \frac{d^p \epsilon_{ij}}{dt} \right]^{1/2} \quad (2.116)$$

so that changes in λ always follow the direction from λ to the instantaneous saturation value associated with the current state. It is seen that p is a relaxation parameter when phrased in terms of plastic strain arc length

$$\ell = \int_0^t \left[\frac{d^p \epsilon_{ij}}{dt} \frac{d^p \epsilon_{ij}}{dt} \right]^{1/2} dt. \quad (2.117)$$

For example, if p and q are taken as constant during some program of creep deformation at constant stress σ , commencing from a state at $t = 0$ for which $\lambda = \lambda^0$, then

$$\lambda_{ij} = e^{-p\ell} \lambda_{ij}^0 + (1 - e^{-p\ell}) q \sigma'_{ij}, \quad (2.118)$$

and this shows the decay of prior influences as the new saturation state, appropriate to σ , is approached. Evidently, p would have to be of a magnitude so that prior memory is lost in strains ℓ of order 1/2 to 2%. As it stands, eqn. (2.116) has no time scale, but λ like ρ should be subject to recovery at high temperature and one way of incorporating this is by adding a term proportional to $-\lambda$ in eqn. (2.116).

For an application of the formulation, consider isothermal deformation and suppose that $d^p \epsilon/dt$ in eqn. (2.112) varies from negligible to very large values as τ_{eq} is increased

through a certain critical magnitude, dependent on the current plastic state. Thus the time-independent idealization is adopted and we interpret the structure parameter ρ , for convenience, as the critical stress magnitude for flow. In the notation of eqn. (2.35), the yield condition is then $F \equiv \tau_{eq}(\sigma - \lambda) - \rho = 0$, and eqn. (2.112) is now replaced by

$$d^p \epsilon_{ij} = \frac{\sigma'_{ij} - \lambda_{ij}}{2 \tau_{eq}(\sigma - \lambda)} d\lambda = \frac{1}{\sqrt{2}} N_{ij} d\lambda, \quad (2.119)$$

where N is the indicated unit tensor ($N_{ij} N_{ij} = 1$) giving the direction of stressing relative to λ . We solve for $d\lambda$ in

the standard way (e.g. Naghdi, 1960), writing $dF = 0$ during a plastic deformation process and expressing $d\rho$ and $d\lambda$ as in eqns. (2.114,116), ignoring the recovery term in the former. This results in

$$d^p \epsilon_{ij} = \frac{1}{E_t} N_{ij} N_{k\ell} d\sigma_{k\ell} \quad , \quad \text{for } N_{k\ell} d\sigma_{k\ell} \geq 0 \quad , \quad (2.120)$$

where the total or overall hardening rate E_t is given by

$$E_t = \sqrt{2} (h + p q \rho) - [-\sqrt{2} \beta + p(1-q)] N_{ij} \lambda_{ij} \quad , \quad (2.121)$$

and where explicit relations for the change in ρ and λ during a deformation process with $N d\sigma \geq 0$ are

$$d\rho = \frac{1}{E_t} [h + \beta N_{ij} \lambda_{ij}] N_{k\ell} d\sigma_{k\ell} \quad (2.122)$$

$$d\lambda_{ij} = \frac{p}{E_t} [\sqrt{2} q \rho N_{ij} - (1-q) \lambda_{ij}] N_{k\ell} d\sigma_{k\ell} \quad (2.123)$$

Examining eqn. (2.121) for E_t , we see that a result of the formulation is anisotropy of the overall hardening, depending on the direction N of the stress difference $\sigma - \lambda$ at flow relative to the direction of λ . Indeed, unless the bias parameter β in eqns. (2.114,122) is large by comparison to unity, the dominant term in the latter part of the expression for E_t is that containing p , since from the discussion following eqn. (2.118), this would have to be very much larger than unity. Thus, when the rest stress λ is near its saturation level [i.e. the bracketed term in eqn. (2.123) vanishes], the anisotropy is most pronounced, with the greatest differences being between the E_t for continued stressing in the direction of λ and that for reversed stressing. The former is of order h , whereas the latter is of order $h + 2 p q \rho$.

It is also of interest to note that the anisotropic effects represented by λ are indeed transient, and that large amounts of deformation under a fixed stressing direction result ultimately in strain increments that become normal to an isotropic hardening "yield" surface. This surface is of the form $\tau_{eq}(\sigma) = \text{constant}$, and has an apparent hardening rate of order h in all directions, when saturation conditions have been achieved. However, it is not an actual yield surface, but

rather an envelope of individual yield surfaces of the kind $\tau_{eq}(\sigma - \lambda) = \text{constant}$, each being generated by a different loading history and each exhibiting a pronounced anisotropy of hardening.

There are many issues to be further explored here, concerning both the general formulation and the assignment of specific forms to the functions involved. An interesting question of the former kind is the following: Given an initially isotropic material in which the plastic state is assumed to be fully characterized by a scalar ρ and second order tensor λ , what is the most general possible class of flow and structure parameter equations? The present efforts have generated a member of the class, but others are possible that could, for example, model substantial shape distortions in flow potential and yield surfaces.

2.10 SUMMARY

This chapter has presented the basis in continuum mechanics and thermodynamics for constitutive descriptions of plasticity, with special attention being given to the connection between macroscopic formulations and deformation mechanisms as operative on the microscale. Conjugate stress and strain measures have been introduced in Sections 2.2 and 2.3, and procedures outlined there for materially objective formulations of elastic-plastic constitutive equations at large or small deformations. Further, the thermodynamic framework for inelastic constitutive laws, as set by the existence of potentials governing purely elastic response, has been reviewed in Section 2.4 and second law restrictions have been stated.

Section 2.5 has presented the general procedure by which structural rearrangements, on the microscale, of the elements of a representative material sample can be related to its macroscopic plastic deformation. This involves the thermodynamic forces f conjugate to the extents $d\xi$ of the rearrangements, and each f is shown to be a "plastic potential" for the macroscopic strain induced by its associated $d\xi$ [eqn. (2.43)]. The procedure is applied in Section 2.6 to inelastic deformation arising from crystalline slip, diffusion, phase changes, and micro-cracking, and the appropriate $d\xi$'s and f 's are identified in each case.

In Section 2.7 it is remarked that kinetic relations for crystalline slip in accord with a Schmid resolved shear stress dependence, and also for linear diffusion with Onsager coefficient symmetry, fall into the general class for which a given rate $d\xi/dt$ is stress state dependent only through its conjugate f . All microscale kinetic laws of this class are

shown to lead to a unifying normality structure in macroscopic constitutive relations, for which components of the instantaneous plastic strain rate are given by derivatives of a scalar flow potential on corresponding stress components. Associated results in terms of normality to yield surfaces are demonstrated within the time-independent idealization of crystalline slip.

The problem of averaging microscale kinetic relations over all sites within a representative material sample, to arrive at specific macroscopic constitutive descriptions, is illustrated in Section 2.8 by review of procedures for predicting the behavior of polycrystals deforming by slip. It is suggested that polycrystal models of the type considered seem capable of modelling some of the real complexities of path dependence in plastic response and of shape distortions of flow potential or yield surfaces, but the necessary computations are very extensive, even for simple deformation paths. Thus considerable interest remains in phenomenological and less rigorously based structure parameter formulations. A class of such constitutive relations is presented in Section 2.9, where the effect of prior deformation on an initially isotropic material is taken to be represented by a single scalar hardness parameter and by a rest stress tensor, the latter coinciding with the stress state at which the instantaneous plastic strain rate vanishes.

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