Nonconvex energy minimization and dislocation structures in ductile single crystals

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Abstract

Plastically deformed crystals are often observed to develop intricate dislocation patterns such as the labyrinth, mosaic, fence and carpet structures. In this paper, such dislocation structures are given an energetic interpretation with the aid of direct methods of the calculus of variations. We formulate the theory in terms of deformation fields and regard the dislocations as manifestations of the incompatibility of the plastic deformation gradient field. Within this framework, we show that the incremental displacements of inelastic solids follow as minimizers of a suitably defined pseudoelastic energy function. In crystals exhibiting latent hardening, the energy function is nonconvex and has wells corresponding to single-slip deformations. This favors microstructures consisting locally of single slip. Deformation microstructures constructed in accordance with this prescription are shown to be in correspondence with several commonly observed dislocation structures. Finally, we show that a characteristic length scale can be built into the theory by taking into account the self energy of the dislocations. The extended theory leads to scaling laws which appear to be in good qualitative and quantitative agreement with observation. © 1999 Elsevier Science Ltd. All rights reserved.

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1. Introduction

Plastically deformed crystals are often observed to develop intricate dislocation structures such as: the dipolar wall, labyrinth and mosaic structures which arise in cylindrically deformed polycrystals and single crystals oriented for multiple slip (L'Esperance et al., 1986; Charsley, 1981; Rasmussen and Pedersen, 1980; Mecke

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and Blochwitz, 1982; Boulanger et al., 1985; Jin and Winter, 1984a; Ackermann et al., 1984; Wang and Mugharbi, 1984; Lepistö et al., 1986); the persistent slip bands in cyclically deformed crystals oriented for single slip (Woods, 1973; Winter, 1974; Mugharbi, 1978); the coplanar slip zones which develop during the stage I of hardening of FCC single crystals Higashida et al. (1986); and the fence and carpet structures characteristic of the early stages of stage II of hardening (Steed, 1966; Higashida et al., 1986), to name a few salient examples. The characterization of these and other dislocation structures from first principles of mechanics has long been a principal—albeit largely unfulfilled—aim of physical metallurgy.

It has been suggested that at least some of these structures can be understood as energy minimizers (Hansen and Kuhlmann-Wilsdorf, 1986; Laird et al., 1986; Laird et al., 1989). Neumann (1986) investigated the structure and stability of loop patches, such as are found in the matrix of single crystals oriented for single slip and cycled to saturation, by explicitly considering an ensemble of parallel straight edge dislocations and numerically minimizing their interaction energy. A similar approach has been followed in other recent studies of dislocation loop patches (Lubarda et al., 1993). In these investigations, the primary unknown is the equilibrium position of the discrete dislocations, and their motion, which is driven by their mutual interaction forces, is not explicitly related to the plastic deformation of the crystal. Consequently, the resulting structures cannot be interpreted as deformation microstructures in general.

Kocks (1986) pointed out that interactions between primary and secondary dislocations, which are responsible for latent hardening in single crystals, necessarily inhibit the simultaneous operation of more than one slip system over the same region of the crystal and, consequently, cause the slip activity to segregate into regions of single slip. Mobile dislocations belonging to two neighboring active systems meet at the interface between the corresponding single slip regions and interact strongly, e.g., through the formation of immobile sessile jogs. The accumulation of such trapped dislocations leads to the formation of dislocation walls. In general, these dislocation walls contain two types of glide dislocations and therefore are referred to as dipolar walls (e.g., Hansen and Kuhlmann-Wilsdorf, 1986). According to the energy minimization principle, the walls thus formed should tend to adopt energy minimizing configurations. The minimum condition was derived by Frank (1950) within the framework of linear elasticity. In turn, Hirth and Lothe (1968) (see also Bilde-Sorensen, 1986) found the dipolar walls which satisfy Frank's condition. Evidently, this theory relates the dislocation structures to plastic deformation processes only to the extent that the dislocation walls are required to be composed of glide dislocations.

Despite the valuable insights revealed by these studies, a comprehensive mathematical analysis of dislocation structures in plastically deformed crystals does not appear to have been attempted. In particular, the recently developed direct methods of the calculus of variations (e.g., D’Acerogna, 1989), including notions of weak convergence and effective behavior, have not been applied to ductile single crystals to the best of our knowledge. One of the primary goals of our work is to formulate the problem of the determination of dislocation structures as a nonconvex minimization problem. Because the constitutive behavior of ductile single crystals is inelastic, it is not immediately clear what—if any—minimum principle characterizes the stable equilibrium configurations of the crystal. Inelastic pseudoelastic energy densities may be better suited to incremental deformations of the crystal, and the principle reflects the inelastic and irreversible nature of the deformation.

The identification of an incremental energy functional for determining the equilibrium deformations of single crystals is a problem that is essentially geometrically speaking, ill-posed. Here geometrical softening is required for the operation of a system of latent hardening refers to the high rate of irreversible plastic strain. The activation of a secondary system (Hirth and Lothe, 1968; Franciosi et al., 1980; Bassani, 1986) is a phenomenon that is similar to the pseudoelastic energy density of primary hardening has wells corresponding to the activation of a single slip system followed by the energy of the crystal in essence, the energy associated with satisfying the requirements for a higher order slip system. The elastic deformation component of the energy of the crystal is described macroscopic value. A somewhat similar situation is given in Section 4 in terms of minimizing the energy.

As just stated, the determination of equilibrium is strictly a problem of compatibility and microstructural development, e.g., martensite (Ball and James, 1987; Muller, 1992; Bhattacharya, 1992). In Section 4, we primarily aim to characterize the equilibrium configurations of dislocation ensembles as the primary phase of the crystal. We expect that the energy-minimizing configuration of the deformation fields. Thus, while the equilibrium configuration in general, physically, the equilibrium configurations of dislocation ensembles is equivalent to a distribution of dislocations and is independent of the geometry of deformation.

In Section 4.1, interfaces between the crystallography. These interfaces are subjected to subsequent lamination, which results in a change of lamination. The general results are specialized to the case of crystals with the commonly observed dislocation wall structure. The equilibrium structures in cyclically deformed
equilibrium configurations of the crystals. We show, however, that a sequence of pseudoelastic energy densities may be defined which is minimized by the successive incremental deformations of the crystal. The incremental nature of the variational principle reflects the inelastic and irreversible nature of plastic deformations.

The identification of an incremental pseudoelastic energy confers the problem of determining the equilibrium deformations of ductile single crystals a variational character. It also reveals the following crucial insight: the pseudoelastic energy densities of crystals and undergoing geometrical softening or latent hardening are non-convex. Here geometrical softening refers to a reduction in the resolved shear stress required for the operation of a system induced by lattice rotations (Asaro, 1983); and latent hardening refers to a high rate of hardening of the primary system due to the activation of a secondary system (Kocks, 1964; Ramaswami et al., 1965; Kocks, 1966; Franciosi et al., 1980; Bassani and Wu, 1991a, b). In particular, we find that the pseudoelastic energy density of previously undeformed crystals possessing latent hardening has wells corresponding to those deformations which are attainable by the activation of a single slip system followed by a lattice or elastic rotation. Such crystals find it energetically favorable to deform locally in single slip. A strategy for minimizing the energy of the crystal is, in essence, to attempt to construct compatible deformations the following requirements: the plastic deformation field consists locally of single slip; the elastic deformation locally of a lattice rotation, which ensures the absence of “long-range stresses”; and the average deformation matches a prescribed macroscopic value. A somewhat more precise statement of this prescription is given in Section 4 in terms of minimizing sequences of deformations.

As just stated, the determination of microstructures in ductile single crystals is strictly a problem of compatibility and, as such, is in analogy to other problems of microstructural development, e.g., those arising in the crystallographic theory of martensite (Ball and James, 1987; Kohn, 1991; Bhattacharya, 1991; Kohn and Müller, 1992; Bhattacharya, 1992). It bears emphasis that the present theory seeks primarily to characterize the equilibrium deformations of ductile single crystals, and is therefore at variance with approaches which regard the disposition of discrete dislocation ensembles as the primary unknown. However, it should be carefully noted that the energy-minimizing dislocation structures may be deduced from the deformation fields. Thus, while the deformation gradient field must be compatible in some suitable sense, neither the elastic nor the plastic deformation fields need be compatible in general. Physically, the incompatibility of the plastic and elastic deformations is equivalent to a distribution of dislocations. The mathematical connection between dislocations and incompatibility is discussed in Section 4 and used subsequently to infer the geometry of dislocation structures.

In Section 4.1, interfaces between two single slip variants are characterized analytically. These interfaces are subsequently taken as the basic building block for sequential lamination, which results in the construction of complex wall structures. The general results are specialized to the FCC crystal class in Section 5. The predicted interfaces are of a precise crystallographic character and constitute a compendium of commonly observed dislocation walls, e.g., the \{100\} walls characteristic of the labyrinth structures in cyclically deformed crystals oriented for multiple slip (Charsley,
1981; Mecke and Blochwitz, 1982; Boulanger et al., 1985; Jin and Winter, 1984a; Ackermann et al., 1984; L’Esperance et al., 1986, which attests to the soundness of the theory. Many commonly observed dislocation structures consist of roughly parallel arrays of dislocation walls which, we argue, are instances of lamination. This includes coplanar slip zones such as observed by Higashida et al. (1986) to form during the stage I of hardening in Cu-1at.%Ge single crystals; the fence structures observed during the early stages of stage II of hardening in FCC crystals (Steed, 1966); and the parallel arrays of dipolar walls which develop in FCC crystals fatigued to saturation (Wang and Mugharbi, 1984; Yumen, 1989; Lepistö et al., 1986; Boutin, 1983; Dickson et al., 1986a, b). An instance of a possible rank-two laminate, or a laminate of laminates, is discussed in Section 5.4.

Finally, in Section 6 a nonlocal extension of the theory is derived by adding to the local free energy density of the crystal the self-energy density of the dislocations. This extension introduces an absolute microstructural length scale and permits to accord the dislocation walls a well-defined interfacial energy. On the basis of this interfacial energy, the spacing \( l \) of the dislocation walls is estimated. In the absence of branching the theory predicts the scaling laws \( l \sim L^{1/2} \) and \( l \sim \gamma^{-1/2} \) in terms of the grain size \( L \) and the slip \( \gamma \), respectively. This latter scaling relation is consistent with observations of the dependence of cell sizes on the applied strain (Bassim and Klassen, 1986). Simple estimates of the wall spacing in copper single crystals fatigued to saturation are also in the ballpark of experimental observation.

2. The variational formulation of inelastic problems

Our first objective is to devise a variational formulation for inelastic solids. In particular, we endeavor to formulate the boundary value problem of finite deformation plasticity as a sequence of incremental energy minimization problems. The appropriate definition of the energy function to be minimized is the principal aim of this section. We show that, when the constitutive equations are integrated along deformation histories which minimize the work of deformation, the resulting incremental stress-strain relations take a pseudoelastic form, with the work of deformation itself supplying the appropriate strain energy potential. This approach has been used in the past to derive deformation, or pseudoelastic, theories of plasticity (Martin and Pontier, 1966; Maier, 1969; Soechting and Lurie, 1969; Carter and Martin, 1976).

2.1. Field equations and constitutive framework

We begin by considering a general inelastic solid occupying a domain \( \Omega \) in its reference configuration. Deformations of the solid are described by deformation mappings \( \gamma(x) : \Omega \rightarrow R^3 \) with gradient

\[
F(x) = \nabla \gamma(x)
\]  

We adopt an internal variable formalism (Lubliner, 1972, 1973) to describe inelastic processes undergone by the solid an energy density \( \psi(F, \dot{q}) \) per unit unde

finite collection of internal variables: isothermal processes and omit the de

temperature. The local value of the functional relations in the form

\[
P = \frac{\partial \psi(F, \dot{q})}{\partial F}
\]

Here and in all subsequent discussion the fields on \( x \) for simplicity, and loc

hold at all material points \( x \in \Omega \). The

\[
\nabla \cdot P = 0
\]

In order to determine the evolution equations must be supplied. Assum

determined solely by the local therm

\[
\dot{q} = f(F, \dot{q})
\]

The second law of thermodynamics \( \dot{q} \) is:

\[
Q \cdot \dot{q} \geq 0
\]

where

\[
Q = -\frac{\partial \psi(F, \dot{q})}{\partial \dot{q}}
\]

are the thermodynamic “forces” which derive from an inelastic potential if it

\[
f = \frac{\partial \psi(Q, \dot{q})}{\partial Q}
\]

For single crystals, the concept of inelast
i.e., must remain invariant under the case in which the internal variables su

superimposed on the deformed con

\[
\phi(RF, \dot{q}) = \psi(F, \dot{q}), \quad \forall R \in SO
\]

A standard exercise (see, e.g., Gurt

d of \( \phi \) consistent with the requirement
processes undergone by the solid and postulate the existence of a Helmholtz free energy density \( \phi(F, q) \) per unit undeformed volume, where \( q \in P^n \) is some suitable finite collection of internal variables. For simplicity, we restrict our attention to isothermal processes and omit the dependence of \( \phi \) and all other state functions on temperature. The local value of the first Piola–Kirchhoff stress tensor follows from Coleman’s relations in the form

\[
P = \frac{\partial \phi(F, q)}{\partial F}
\]  

(2)

Here and in all subsequent discussions of local behavior, we omit the dependence of the fields on \( x \) for simplicity, and local relations such as (2) are tacitly presumed to hold at all material points \( x \in \Omega \). The equilibrium of the solid demands that

\[
\nabla \cdot P = 0
\]  

(3)

In order to determine the evolution of the internal variable field, suitable kinetic equations must be supplied. Assuming that the rate of the internal processes is determined solely by the local thermodynamic state, the general form of the kinetic equations is

\[
\dot{q} = f(F, q)
\]  

(4)

The second law of thermodynamics places the following restriction on the rate equations:

\[
Q \cdot \dot{q} \geq 0
\]  

(5)

where

\[
Q = -\frac{\partial \phi(F, q)}{\partial q}
\]  

(6)

are the thermodynamic “forces” conjugate to \( q \). The kinetic relations are said to derive from an inelastic potential if there exists a differentiable function \( \psi(Q, q) \) such that

\[
f = \frac{\partial \psi(Q, q)}{\partial Q}
\]  

(7)

For single crystals, the concept of inelastic potential was introduced by Rice (1975).

All the preceding constitutive relations are subject to material frame indifference, i.e., must remain invariant under superimposed rigid body motions. In the particular case in which the internal variables are scalars or remain unchanged under rotations superimposed on the deformed configuration, material frame indifference requires that

\[
\phi(RF, q) = \phi(F, q), \quad \forall R \in SO(3)
\]  

(8)

A standard exercise (see, e.g., Gurtin, 1981) then shows that the most general form of \( \phi \) consistent with the requirements of material frame indifference is

\[
\phi(F, q) = F^T \sigma F + \frac{1}{2} \lambda \text{tr} \sigma + \mu \text{det} \sigma - \psi(q)
\]  

This formulation for inelastic solids. In lary value problem of finite deformer results in a unified minimization problems. The \( \psi \) minimized is the principal aim of tive equations are integrated along rk of deformation, the resulting elastic form, with the work of deformation energy potential. This approach has pseudoelastic, theories of plasticity and interfacial layer (Bassim and Klassen, 1986). Single crystals fatigued to saturation ion.
\[ \phi = \phi(C, q), \quad C = F^T F \]  
\[ (9) \]

where \( C \) is the right Cauchy–Green deformation tensor.

2.2. Minimizing deformation paths

We shall assume sufficient regularity of the local deformation histories \( F(t) \) and the rates \( f(F, q) \) to ensure existence and uniqueness of continuously differentiable solutions \( q(t) \) of the local initial value problem

\[ \dot{q}(t) = f(F(t), q(t)), \quad q(0) = q_0 \]  
\[ (10) \]

over some time interval \([0, T]\). For instance, it suffices to assume that \( F(t) \) is a continuous function of \( t \in [0, T] \) and \( f(F, q) \) a continuous function of \( F \) satisfying the Lipschitz condition

\[ \|f(F, q) - f(F, q')\| \leq L\|q - q'\| \]  
\[ (11) \]

for all \( F, q \) and \( q', t \in [0, T] \), and some constant \( L \) (see, e.g., Gear, 1971). These conditions may reasonably be expected to be met, e.g., by most models of viscoelastic and viscoplastic behavior, including viscoplastic regularizations of rate-independent plasticity models (see Lubliner, 1972 for examples of these models; Ortiz, 1981, Chap. 3, for a discussion of the viscoplastic regularization). If the rates satisfy the Lipschitz condition (11), it then follows that problem (10) is well-posed with respect to the initial conditions, i.e., there exists a constant \( M \) such that

\[ \|q(t) - q'(t)\| \leq M\|q_0 - q'_0\| \]  
\[ (12) \]

for all \( q \) and \( q', t \in [0, T] \) (see, e.g., Gear, 1971).

In order to define an incremental pseudoplastic energy density, we consider the following auxiliary local problem. Let \( F(t) \) and \( q(t), t \in [0, T] \), be deformation and internal variable histories at the point under consideration. Suppose that the initial conditions \( F(0) \) and \( q(0) \) are known and the final deformation \( F(T) \) is prescribed. Then we wish to determine histories of deformation \( F(t) \), having the prescribed initial and terminal values \( F(0) \) and \( F(T) \), respectively, which minimize the work of deformation density

\[ W = \int_0^T P \cdot \dot{F} dt \]  
\[ (13) \]

In writing (13) it is tacitly understood that \( q(t) \) follows from \( F(t) \) by integration of the kinetic eqns (4). From relations (2) and (6), (13) may be recast as

\[ W = \int_0^T (\dot{\phi} + Q \cdot \dot{q}) dt \]  
\[ (14) \]

The first term is a perfect differental and integrates exactly, with the result

\[ W = [\phi]_0^T + \int_0^T Q \cdot \dot{q} dt \]

The minimizing deformation paths:

\[ \delta W = \left[ \frac{\partial \phi}{\partial F} \cdot \delta F + \frac{\partial \phi}{\partial q} \cdot \delta q \right]_0^T + \int_0^T \delta Q \cdot \dot{q} dt \]

Using (2) and the fact that \( \delta F(0) = \delta F(T) = 0 \),

\[ \delta W = P(T) \cdot \delta F(T) + \int_0^T [\delta Q] \cdot \dot{q} dt \]

An integration by parts of the second term

\[ \delta W = P(T) \cdot \delta F(T) + \int_0^T [\delta Q] \cdot \dot{q} dt \]

Finally, noting that \( \delta F(T) = 0 \), sir condition

\[ \delta W = \int_0^T [\delta Q] \cdot [\delta q - \dot{Q} \cdot \delta q] dt = 0 \]

which determines the minimizing deformation history.

2.3. Rate-independent behavior

The stationariness condition (19) is determined by the behavior. Let \( q(t) \) be the solution of \( F(t) \), and let \( s(t) \) be an absolutely \( \cdot \) \( t \in [0, T] \). The solid is said to be rate-independent to the deformation history \( F(s(t)) \) and independent are said to be rate dependent.

A rate-independent theory of inelastic deformation is one where the rate \( K \) on \( q \) is generally required in inelastic potential:

\[ \psi(Q, q) = I_{K_Q}(Q) = 0, \quad \text{if } Q = \infty, \quad \text{otherwise} \]

Here, \( I_{K_Q}(Q) \) is the indicator function. Evidently, this function is not differentiable, which precludes a direct application.
\[ W = [\phi]_0^T + \int_0^T \dot{Q} \cdot \dot{q} \, dt \]  

(15)

The minimizing deformation paths satisfy the stationarity condition

\[ \delta W = \left[ \frac{\partial \phi}{\partial F} \cdot \delta F + \frac{\partial \phi}{\partial \dot{q}} \cdot \delta \dot{q} \right]_0^T + \int_0^T \left[ \delta \dot{Q} \cdot \dot{q} + \dot{Q} \cdot \delta \dot{q} \right] \, dt = 0 \]  

(16)

Using (2) and the fact that \( \delta F(0) = 0 \), (16) reduces to

\[ \delta W = P(T) \cdot \delta F(T) + \int_0^T \left[ \delta \dot{Q} \cdot \dot{q} - \dot{Q} \cdot \delta \dot{q} \right] \, dt = 0 \]  

(17)

An integration by parts of the second term in the integrand and (6) gives

\[ \delta W = P(T) \cdot \delta F(T) + \int_0^T \left[ \delta \dot{Q} \cdot \dot{q} - \dot{Q} \cdot \delta \dot{q} \right] \, dt = 0 \]  

(18)

Finally, noting that \( \delta F(T) = 0 \), since \( F(T) \) is prescribed, results in the stationarity condition

\[ \delta W = \int_0^T \left[ \delta \dot{Q} \cdot \dot{q} - \dot{Q} \cdot \delta \dot{q} \right] \, dt = 0 \]  

(19)

which determines the minimizing deformation paths \( F(t) \).

2.3. Rate-independent behavior

The stationarity condition (19) simplifies further in the case of rate-independent behavior. Let \( q(t) \) be the solution of (10) corresponding to a deformation history \( F(t) \), and let \( s(t) \) be an absolutely continuous, monotonically increasing function of \( t \in [0, T] \). The solid is said to be rate-independent if the solution of (10) corresponding to the deformation history \( F(s(t)) \) is \( q(s(t)) \) for all \( F(t) \). Solids which are not rate independent are said to be rate dependent.

A rate-independent theory of inelastic behavior may be formulated by identifying an \( N \)-parameter family of convex sets \( K(q) \subseteq R^N \). The convex set \( K(q) \), which are allowed to have corners, define the elastic domain of the solid. As will become apparent in subsequent applications to finite-deformation plasticity, a explicit dependence of \( K \) on \( q \) is generally required in order to account for geometric effects. Introduce the inelastic potential:

\[ \psi(Q, q) = I_{K(q)}(Q) = 0, \quad \text{if} \ Q \in K(q) \]

\[ = \infty, \quad \text{otherwise} \]  

(20)

Here, \( I_{K(q)}(Q) \) is the indicator function of the convex set \( K(q) \) (Rockafellar, 1970). Evidently, this function is not differentiable with respect to \( Q \) in the ordinary sense, which precludes a direct application of (7). Nonetheless, it was noted by Moreau...
\[ f(Q, q) = \partial_q I_{K(q)}(Q) = \{ q \text{ s.t. } (Q - Q') \cdot q \geq 0, \quad \forall Q' \in K(q) \} \]  
\[ (21) \]

It follows from this definition that the rates \( f(Q, q) = 0 \) if \( Q \) belongs to the interior of \( K(q) \), while \( f(Q, q) \) is any element of the normal cone if \( Q \) is on the boundary \( \partial K(q) \) or \( K(q) \) (Ortiz, 1981), in agreement with the conventional definition of the flow rule in rate-independent plasticity. The subdifferential of a differentiable function coincides with its ordinary derivative. Therefore, (7) may be extended to the rate-independent case by simply interpreting derivatives with respect to \( Q \) in the sense of subdifferentials as required.

An alternative device for sidestepping the mathematical difficulties inherent to rate-independent behavior is to resort to a viscoplastic regularization. A particularly convenient procedure is furnished by the classical Yosida’s regularization of nonlinear semigroup theory (Yosida, 1965), leading to linear viscoplasticity. The relation between the Yosida regularization and linear viscoplasticiy was first noted by Ortiz (1981). Let \( P_{K(q)}(Q) \) denote the closest point projection of \( \mathcal{R}^n \) onto \( K(q) \). Thus,

\[ \| Q - P_{K(q)}(Q) \| = \min_{Q' \in K(q)} \| Q - Q' \| \]  
\[ (22) \]

for some suitable norm \( \| \cdot \| \). Then the Yosida or linear viscoplastic regularization of (20) is

\[ f_\varepsilon = \frac{1}{\varepsilon} [Q - P_{K(q)}(Q)] \]  
\[ (23) \]

where \( \varepsilon \) is a viscosity constant which plays the role of a small parameter. This class of kinetic equations satisfies all the regularity requirements assumed in Section 2.2.

In addition, it follows from general results of nonlinear semigroup theory (Crandall and Pazy, 1969, 1970; Ortiz, 1981) that the solutions \( q(t) \) of the initial value problem (10) corresponding to the kinetic relations (23) and the rate-independent solutions \( q^0(t) \) corresponding to (21) satisfy the bound:

\[ \| q(t) - q^0(t) \| \leq C \sqrt{\varepsilon t} \]  
\[ (24) \]

which shows that the linear viscoplastic solution converges to the rate-independent solution in the inviscid limit \( \varepsilon \to 0 \). Since \( \varepsilon \) sets the temporal scale, it additionally follows that the linear viscoplastic solution converges to the rate-independent solution in the quasistatic limit, i.e., for sufficiently slow deformation processes. These results show that the subdifferential formalism (21) required to represent rate-independent behavior, which necessitates the consideration of lower semi-continuous inelastic potentials of the form (20), may be conveniently sidestepped, if so desired, by con-

Considering slightly viscous regularizati behavior recovered in the limit of \( \varepsilon \)-

It is readily verified that, for rate-

\[ \delta Q \cdot \dot{q} = 0 \]

Thus, if \( Q(t) \) is in the interior of \( K \)

then \( \delta Q(t) \) must represent neutral \( \kappa \)
to \( K(q(t)) \) at \( Q(t) \). But, \( \dot{q}(t) \) lies w

consequently, (25) also holds. In vie

to

\[ \delta W = - \int_0^T \dot{q} \cdot \delta q \, dt = 0 \]

for rate-independent solids. Clearly

that \( Q(t) \) lies in the interior of \( K(q) \)

(26) is trivially satisfied. It thus fol-

2.4. Pseudoelastic incremental beha

Let \( W(F(T); F(0), q(0)) \) be the w

computed along a minimizing pat

variation \( \delta F(T) \) of the terminal defo

\( F(0), q(0)) \) is given by (18). But, s

along a minimizing path, the statio

\[ \delta W = P(T) \cdot \delta F(T) \]

This shows that \( W(F(T); F(0), q(0)) \)

\[ P(T) = \frac{\partial W(F(T); F(0), q(0))}{\partial F(T)} \]

which is the sought incremental co

(28) and hyperelastic constitutiva

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frame indifference that if \( F(t) \) is a r

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\( F(0), q(0)) \) satisfies material frame

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kinetic equations (4) along a mini

\[ q(T) = K(F(T); F(0), q(0)) \]

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equations (4) in the sense that
Considering slightly viscous regularizations of the form (23), with the rate-independent behavior recovered in the limit of $\varepsilon \to 0$.

It is readily verified that, for rate-independent solids,

$$
\delta Q \cdot \dot{q} = 0
$$

(25)

Thus, if $Q(t)$ is in the interior of $K(q(t))$, then $\dot{q}(t) = 0$ and (25) holds. If $\dot{q}(t) \neq 0$, then $\delta Q(t)$ must represent neutral loading and be contained within the tangent cone to $K(q(t))$ at $Q(t)$. But, $\dot{q}(t)$ lies within the normal cone to $K(q(t))$ at $Q(t)$ and, consequently, (25) also holds. In view of (25), the stationarity condition (19) reduces to

$$
\delta W = -\int_0^T \dot{Q} \cdot \delta q \, dt = 0
$$

(26)

for rate-independent solids. Clearly, for a purely elastic deformation history, such that $Q(t)$ lies in the interior of $K(q(t))$ for all $t \in [0, T]$, $\delta q(t)$ is necessarily zero and (26) is trivially satisfied. It thus follows that all elastic paths are extremal.

2.4. Pseudoelastic incremental behavior

Let $W(F(T); F(0), q(0))$ be the work of deformation per unit undeformed volume computed along a minimizing path joining $F(0)$ to $F(T)$. Consider now a small variation $P(T)$ of the terminal deformation. The corresponding variation of $W(F(T); F(0), q(0))$ is given by (18). But, since by assumption $W(F(T); F(0))$ is computed along a minimizing path, the stationarity condition (19) holds and (18) reduces to

$$
\delta W = P(T) \cdot \delta F(T)
$$

(27)

This shows that $W(F(T); F(0), q(0))$ is a pseudoelastic potential for $P(T)$, i.e.,

$$
P(T) = \frac{\partial W(F(T); F(0), q(0))}{\partial F(T)}
$$

(28)

which is the sought incremental constitutive relation. Despite the similarity between (28) and hyperelastic constitutive relations, the inelastic and history-dependent character of the material is clearly belied by the incremental form of $W(F(T); F(0), q(0))$ and its dependence on the initial conditions $(F(0), q(0))$. It follows from material frame indifference that if $F(t)$ is a minimizing path then $R(t)F(t)$ is also a minimizing path for any rigid motion $R(t) \in SO(3)$ and does the same work of deformation $W$ over the interval $[0, T]$. In particular, the pseudoelastic strain energy density $W(F(T); F(0), q(0))$ satisfies material frame indifference.

Besides leading to the incremental constitutive relations (28), an integration of the kinetic equations (4) along a minimizing deformation path yields a terminal value

$$
q(T) = K(F(T); F(0), q(0))
$$

(29)

of the internal variables. By construction, the mapping $K$ is consistent with the kinetic equations (4) in the sense that
\[ f(F(0), q(0)) = \left[ \frac{d}{dt} K(F(t); F(0), q(0)) \right]_{t=0} \]  

for all initial conditions \( F(0) \) and \( q(0) \). Additionally, because \( K(F(T); F(0), q(0)) \) is the exact integral of (4) along a minimizing path, it follows from (12) that \( K \) satisfies the Lipschitz condition

\[ \| K(F(T); F(0), q(0)) - K(F(T); F(0), q'(0)) \| \leq M \| q(0) - q'(0) \| \]  

which may be regarded as a stability condition (see, e.g., Gear, 1971, p. 55).

Evidently, actual deformation histories need not be minimizing paths. However, in order to approximate the effect of an arbitrary deformation history \( F(t), t \in [0, T] \), we may sample \( F(t) \) at discrete times \( t_n = n\Delta t, n = 0, 1, \ldots, N, \Delta t = T/N \), and apply the mapping (29) recursively to obtain the sequence

\[ q_{n+1} = K(F_{n+1}; F_n, q_n), \quad n = 0, \ldots, N-1 \]  

where \( F_n = F(t_n) \). At every step, the new stresses \( P_{n+1} \) derive from the pseudoelastic energy density \( W(F_{n+1}; F_n, q_n) \) as

\[ P_{n+1} = \frac{\partial W(F_{n+1}; F_n, q_n)}{\partial F_{n+1}} \]  

As expected, the response is history dependent, i.e., \( P_n \) depends not only on the terminal deformation \( F_N \) but on the complete history of deformation \( \{F_n, n = 0, \ldots, N\} \). While this incremental procedure is clearly approximate, it follows that the incremental internal variable history converges to the exact one as the number of steps increases. More precisely, the consistency and stability of \( K \), eqns (30) and (31), respectively, guarantee that

\[ q_{n+1} \to q(t), \quad \text{as } \Delta t \to 0 \]  

(see, e.g., Gear, 1971, p. 57).

2.5. Inelastic boundary value problems

The chief advantage of the incremental procedure just outlined is that the incremental stress-strain relations are pseudoelastic, which opens the way for the application of variational methods to inelastic solids. For the purposes at hand, it is sufficient to consider affine displacement boundary conditions of the form

\[ y(x, t) = F(t)x, \quad x \in \partial \Omega, \quad t \in [0, T] \]  

Since, by the divergence theorem, one has

\[ F(t) = \frac{1}{|\Omega|} \int_{\Omega} \nabla y(x, t) \, dx \]  

\( F(t) \) may be regarded as a prescribed history of average deformation. A dual picture, consisting of the application of tractions \( T(t) = F(t) \cdot n \) all around \( \partial \Omega \), has been developed by Ball et al. (1995). Here \( F(t) \) represents a history of average loading device.

In anticipation of the emergence of a deformation equilibrium and identify with the minimizers of the pseudoelastic

\[ E(y_{n+1}) = \int_{\Omega} W(\nabla y_{n+1}(x); y_{n+1}(x)) \]  

By definition, \( E(y_{n+1}) \) is the total work done from \( F_n(x) = \nabla y_n(x) \) to \( F_{n+1}(x) = \nabla y_{n+1}(x) \), \( x \in \Omega \). It should be carefully noted that \( E(y_{n+1}) \) is determined by the incremental procedure of the histories connecting \( F_n(x) \) to \( F_{n+1}(x) \), compatible in general. Let \( y_{n+1}(x) \) be

\[ E(y_{n+1}) = \inf_{y \in Y_{n+1}} \int_{\Omega} W(\nabla y(x)) \]  

where the infimum is taken over essential boundary conditions (35). In addition, let \( q_{n+1}(x) \) be obtained to \( (F_n(x), q_n(x)) \) with \( F_{n+1}(x) = \nabla y_{n+1}(x) \), relations (33), it is clear that the \( E \), the equilibrium equation (3) and its principle (38) and (3) are equivocal convergence property (34) of the under suitable technical conditions solutions \( y(x, t) \) and \( q(x, t) \) should.

The existence of minimizers of lack of it thereof—of the pseudoeig 1989). In particular, if \( F \) first begins \( (F_{n+1}) \), there may not exist any \( F \) often possible, however, to const which attain the minimum energy

\[ \lim E(y_{n+1}) = \inf_{y \in Y_{n+1}} \int_{\Omega} W(\nabla y) \]  

It should be carefully noted that the

\[ E(y_{n+1}) = \inf_{y \in Y_{n+1}} \int_{\Omega} W(\nabla y(x)) \]  

d a manifestation of the lack of lower
developed by Ball et al. (1995). Here \( n \) denotes the unit normal to \( \partial \Omega \). In this approach, \( \bar{P}(t) \) represents a history of average stress imparted to the solid by some suitable loading device.

In anticipation of the emergence of fine microstructures, we adopt a variational definition of equilibrium and identify the stable equilibrium deformations of the solid with the minimizers of the pseudoelastic energy

\[
E(y_{n+1}) = \int \Omega W(\nabla y_{n+1}(x); y_n(x), q_n(x)) \, dx
\]

By definition, \( E(y_{n+1}) \) is the total work of deformation done as the deformation jumps from \( F_n(x) = \nabla y_n(x) \) to \( F_{n+1}(x) = \nabla y_{n+1}(x) \) along local minimizing paths at all points \( x \in \Omega \). It should be carefully noted that, while the deformation gradients \( F_n(x) \) determined by the incremental procedure are compatible, the intervening deformation histories connecting \( F_n(x) \) to \( F_{n+1}(x) \) through local minimizing paths need not be compatible in general. Let \( y_{n+1}(x) \) be a solution of the variational problem:

\[
E(y_{n+1}) = \inf_{y \in F_{n+1}} \int \Omega W(\nabla y(x); y_n(x), q_n(x)) \, dx
\]

where the infimum is taken over some suitable space of functions satisfying the essential boundary conditions (35), e.g., \( Y_{n+1} = \{ y = F_{n+1} + y_n, y_n \in W_0^{1,\infty}(\Omega; \mathbb{R}^2) \} \).

In addition, let \( q_{n+1}(x) \) be obtained by applying the evolutionary mapping (32) locally to \( (F_n(x), q_n(x)) \) with \( F_{n+1}(x) = \nabla y_{n+1}(x) \) at every \( x \in \Omega \). In view of the potential relations (33), it is clear that the Euler–Lagrange equation corresponding to (38) is the equilibrium equation (3) and, consequently, for smooth solutions the minimum principle (38) and (3) are equivalent statements of equilibrium. In view of the local convergence property (34) of the incremental procedure, we may reasonably expect, under suitable technical conditions, global convergence of \( y_{n+1}(x) \) and \( q_{n+1}(x) \) to the solutions \( y(x, t) \) and \( q(x, t) \) should such solutions exist.

The existence of minimizers of (38) depends crucially on the quasiconvexity—or lack of it thereof—of the pseudoelastic strain energy density \( W \) (see, e.g., Dacorogna, 1989). In particular, if \( W \) first begins to lack quasiconvexity over the incremental step \( (t_n, t_{n+1}) \), there may not exist any energy-minimizing deformation \( y_{n+1}(x) \in Y_{n+1} \). It is often possible, however, to construct minimizing sequences of deformations \( y_{n+1}(x) \) which attain the minimum energy in the limit, i.e., such that

\[
\lim_{\theta} E(y_{n+1}^{\theta}) = \inf_{y \in F_{n+1}} \int \Omega W(\nabla y(x); y_n(x), q_n(x)) \, dx
\]

It should be carefully noted that the limit \( y_{n+1}^{\theta} \rightharpoonup y_{n+1} \) is not a minimizer in general, i.e.,

\[
E(y_{n+1}) > \inf_{y \in F_{n+1}} \int \Omega W(\nabla y(x); y_n(x), q_n(x)) \, dx
\]

a manifestation of the lack of lower semicontinuity of the functional \( E(y) \). Minimizing
sequences often exhibit increasingly fine detail and have been found to describe well
some commonly observed defects demonstrated in subsequent section.

3.1. Finite-deformation plasticity

Plastic solids are characterized by $F^p$, or “plastic” deformations, which in turn lead to the constitutive relation $F^p$, some degree of lattice

$$ F = F^0 F^p $$

and the free energy density follows

$$ \phi = \phi(F^0, \gamma) = \phi(F^{p-1}, \gamma) $$

where $\gamma$ is some suitable set of interatomic forces (e.g., quasiconvex function of the multiplicative elastic-plastic $k$ and further developed by others (1973; Hill and Rice, 1972; Mandel).

The free energy $\phi$ is subject to the constraint (41) that $F^p$ remains on $F$, as such a rotation is absorbed by the internal parameters $\gamma$ are small rotations, material frame indifference

$$ \phi(RF^p, \gamma) = \phi(F^p, \gamma), \quad \forall R \in S $$

A standard exercise (see, e.g., Gurtin & Sternberg, 1988) satisfies the requirements

$$ \phi = \phi(C^e, \gamma), \quad C^e = F^{pT} F^p = \gamma \text{ in accordance with (9).} \text{ In (44), } C^e \text{ is an independent } $$

tensor.

For the standpoint of the general theory, the internal variable set collected in the variables $q = \{F^p, \gamma\}$. A straightforward conjugate to $F^p$ as

$$ S = -\frac{\partial \phi}{\partial F^p} = F^{pT} \frac{\partial \phi}{\partial F^p} F^p. $$

It follows from material frame indifference that

3. Application to crystal plasticity

In this section, the preceding general framework is specialized to plastic solids and, as a further special case, to ductile single crystals. Simple models of geometrical softening and latent hardening are introduced which inevitably lead to nonconvex pseudoelastic strain energy densities. This lack of convexity in turn lies at the root
of some commonly observed deformation and dislocation structures in crystals, as demonstrated in subsequent sections.

### 3.1. Finite-deformation plasticity

Plastic solids are characterized by the existence of a certain class of deformations $F^p$, or "plastic" deformations, which leave the crystal lattice undistorted and unrotated, and, consequently, induce no long-range stresses. In addition to the plastic deformation $F^p$, some degree of lattice distortion $F^s$ may also be expected in general. One therefore has, locally,

$$F = F^p F^s$$

and the free energy density follows in the form

$$\phi = \phi(F^p, \gamma) = \phi(F F^p \gamma, \gamma)$$

where $\gamma$ is some suitable set of internal variables. We suppose that, for fixed $\gamma$, $\phi$ is a nice (e.g., quasiconvex) function of $F^p$ attaining a strict minimum for any $F^p \in SO(3)$. The multiplicative elastic-plastic kinematics (41) was first suggested by Lee (1969) and further developed by others (Teodosiu, 1969; Asaro and Rice, 1977; Havner, 1973; Hill and Rice, 1972; Mandel, 1972; Rice, 1971).

The free energy $\phi$ is subject to the requirement of material frame indifference. It is evident from (41) that $F^p$ remains unchanged upon the superposition of a rotation $R$ on $F$, i.e., such a rotation is absorbed by—and therefore solely affects—$F^p$. Assuming that the internal parameters $\gamma$ are scalar or also remain unchanged upon superimposed rotations, material frame indifference requires that

$$\phi(R F^p, \gamma) = \phi(F^p, \gamma), \quad \forall R \in SO(3)$$

A standard exercise (see, e.g., Gurin, 1981) then shows that the most general form of $\phi$, consistent with the requirements of material frame indifference is

$$\phi = \phi(C^\varepsilon, \gamma), \quad C^\varepsilon = F^{\varepsilon T} F^p = F^p \cdot T \cdot C F^p$$

in accordance with (9). In (44), $C^\varepsilon$ is the elastic right Cauchy–Green deformation tensor.

For the standpoint of the general theory developed in the preceding section, $F^p$ may be regarded as a set of distinguished internal variables, with the remainder of the internal variable set collected in the array $\gamma \in R^\varepsilon$. Thus, the complete set of internal variables is $\varphi = \{F^p, \gamma\}$. A straightforward calculation gives the thermodynamic force conjugate to $F^p$ as

$$S \equiv -\frac{\partial \phi}{\partial F^p} = F^{\varepsilon T} \frac{\partial \phi}{\partial F^p}(F^p) F^p$$

It follows from material frame indifference and representation (9) of the internal energy that
\[(SF^{\top}C^e)^\top = SF^{\top}C^e\] (46)
i.e., the tensor \(SF^{\top}C^e\) is symmetric. This places three algebraic constraints on \(S\). Additionally, the thermodynamic forces conjugate to \(\gamma\) are
\[-g = -\frac{\partial \psi}{\partial \gamma}\] (47)
The complete set of driving forces is \(Q = \{S, -g\}\). Assuming an inelastic potential of the form \(\psi(S, g; F^p, \gamma)\), the flow and hardening rules jointly follow from (7) in the form
\[F^p = \frac{\partial \psi}{\partial S}\] (48)
\[\gamma = -\frac{\partial \psi}{\partial g}\] (49)
where partial derivatives should be interpreted in the sense of subdifferentials in the rate-independent case.

3.2. Ductile single crystals

Next, we apply the general framework just outlined to ductile single crystals. Plastic deformations in single crystals are crystallographic in nature. The conventional kinetic relations for \(F^p\), or “flow rule”, are of the form (Rice, 1971)
\[F^p = \sum_{s=1}^{N} \gamma^s s^s \otimes m^s\] (50)
where \(\gamma^s \in R, s^s \in R^3,\) and \(m^s \in R^3\) are the slip strain, slip direction and slip-plane normal corresponding to slip system \(s\). Plastic irreversibility requires that
\[\gamma^s > 0\] (51)
A zero value of a slip rate \(\gamma^s(t)\) signifies that the corresponding slip system \(s\) is inactive at time \(t\). We note that the flow rule (50) allows for multiple slip, i.e., for simultaneous activity on more than one system over a region of the crystal. A pair \((s^s, m^s)\) is referred to as a “slip system”. For instance, in FCC crystals \(s^s\) is any cube face diagonal and \(m^s\) any cube diagonal, which gives the twenty-four slip systems enumerated in Table 1. For ease of reference, we adopt Schmid and Boas’ nomenclature (Schmid and Boas, 1961) for the slip systems of an FCC crystal, namely,

![Fig. 1. Slip systems of an FCC crystal and corresponding resolved shear stress.](image)
A \equiv (\bar{1}11), \quad B \equiv (111), \quad C \equiv (1\bar{1}1), \quad D \equiv (1\bar{1}1)\\1 \equiv [011], \quad 2 \equiv [0\bar{1}1], \quad 3 \equiv [10\bar{1}], \quad 4 \equiv [1\bar{1}0], \quad 5 \equiv [1\bar{1}0], \quad 6 \equiv [110]

cf Fig. 1. Note that we need to differentiate between pairs of slip systems of the form (+s, m) and (−s, m), as we have required that \( \gamma > 0 \). We shall denote by \( \mathcal{F} \) the collection of all slip systems available for plastic deformation. For processes of pure slip, one has \( s^a \cdot m^a = 0 \), which, in view of (50) gives \( \text{tr}(F^a F^{-1}) = 0 \) and plastic flow is volume-preserving.

The crystallographic flow rule (50) can be given the potential structure (48) as follows. Begin by introducing the resolved shear stress \( \tau^z \) on slip system \( z \) as

\[
\tau^z = (S^z F^p)^{-1} (s^z \otimes m^z)
\]

where the dot product \( A \cdot B \) between two matrices \( A \) and \( B \) is \( A_i B_j \). Following Rice (1975) we write the flow potential \( \psi \) as the sum of slip system contributions, i.e.,

\[
\psi(S, g; F^p, \gamma) = \sum_{z=1}^{n} \psi^z(S, g; F^p, \gamma)
\]

Next, we assume that the crystal obeys Schmidt's rule and write

\[
\psi^z = \psi^z(\tau^z - g^z)
\]

i.e., the slip system flow potential \( \psi^z \) depends on \((S, g; F^p, \gamma)\) solely through the corresponding resolved shear overstress \( \tau^z - g^z \). In this context, \( g^z \) takes on the significance of the critical resolved shear stress for the activation of slip system \( z \). Substitution of (53) and (54) into (48) and (49) gives

\[
\begin{array}{c|c|c|c|c|c}
C3 & C5 & D4 & D1 & D6 \\
\hline
[011] & \pm [\bar{1}0\bar{1}] & \pm [10\bar{1}] & \pm [0\bar{1}1] & \pm [110] \\
\hline
(\bar{1}\bar{1}1) & (\bar{1}11) & (\bar{1}11) & (1\bar{1}1) & (1\bar{1}1)
\end{array}
\]

Fig. 1. Slip systems of an FCC crystal and Schmid and Boas' nomenclature Schmid and Boas (1961).
\[ F^\gamma = \left( \sum_{a=1}^{N} \frac{\partial \psi^a}{\partial \tau^a} \otimes m^a \right) F^\gamma \]  

(55)

\[ \tau^a = -\frac{\partial \psi^a}{\partial g^a} = \frac{\partial \psi^a}{\partial \tau^a} \]  

(56)

Insertion (56) into (55) gives the standard crystallographic flow rule (50), as required.

3.3. Rate-independent behavior

In the particular case of a rate independent crystal, the slip system flow potential takes the form:

\[ \psi^a = 0, \text{ if } \tau^a - g^a \leq 0 \]

\[ = \infty, \text{ otherwise} \]  

(57)

Evidently, it follows from (52) that, for fixed \((g; F^\gamma, \gamma)\), the elastic domain \(K(F^\gamma) = \{ S \in \mathbb{R}^{3 \times 3} \text{ s.t. } \tau^a - g^a < 0, a = 1, \ldots, N \} \) when represented in \((SF^{\gamma})\)-space is the intersection of halfspaces and, therefore, is a convex set. Because of the orthogonality condition \(s^a \cdot m^a\), it follows that, in \((SF^{\gamma})\)-space, \(K\) is a cylinder coaxial with the hydrostatic axis. In view of (52), it is evident that the elastic domain depends on the current value of \(F^\gamma\), which may be regarded as a geometric effect. This illustrates the need for the explicit dependence of \(K(g)\) of the elastic domain on the internal variables allowed for in Section 2.3.

We now turn to the question of minimizing paths for single crystals. For a general plastic material, the incremental work of deformation per unit undeformed volume (13) takes the form

\[ W = [\phi]^\gamma + \int^T_0 (S \cdot F^\gamma - g \cdot \gamma) \, dt \]  

(58)

In the special case of single crystals, substitution of (50) into (58) gives

\[ W = [\phi]^\gamma + \int^T_0 [(\tau - g) \cdot \gamma] \, dt \]  

(59)

where we have grouped all the resolved shear stresses into the array \(\tau \in \mathbb{R}^N\). Proceeding as in the preceding section, the stationarity condition is found to be

\[ \delta W = \int^T_0 [(\delta \tau - \delta g) \cdot \gamma - (\tau - g) \cdot \delta \gamma] \, dt = 0 \]  

(60)

In the rate-independent limit (60) reduces to

\[ \int^T_0 (\tau - g) \cdot \delta \gamma \, dt = 0 \]

which determines the minimizing deformation.

If \(\tau^a - g^a < 0\) during \([t_1, t_2] \subset [0, T]\) for system \(a\), it follows that, necessarily, the corresponding term in (61) vanishes. To see this, suppose now that the crystal has attained the state of indifference, we can further restrict the problem \(F(t) = U(t)\). This leaves five independent variables. Assume that any arbitrary variation \(\delta U(t)\) is selected by a suitable choice of \(\delta U(t)\). The vanishing of \(\tau^a - g^a = 0\) for the active systems. Thus, constraint (51) can be expressed compactly as

\[ \tau^a(i) - g^a(t) \leq 0, \quad \text{and} \quad \gamma^a(t) \leq 0 \]

for all slip systems \(a = 1, \ldots, N\), which together with variational problems (Rockafellar, 1970) implies

\[ W = [\phi]^\gamma \]

i.e., the work of deformation along the path equals the change in free energy.

Next, we shall consider such pathwise time interval \([0, T]\) under consideration irreversibility constraint (51) and some weak step. The working assumption is, the active slip systems and relative slips \(\tau^a(t)\) for these paths,

\[ \gamma^a(t) = (1 - t/T)\gamma^a(0) + (t/T)\gamma^a(T) \]

and the flow rule (50) integrates to

\[ F^\gamma(t) = \exp \left\{ \sum_{a=1}^N [\gamma^a(t) - \gamma^a(0)] \right\} \]

In particular,

\[ F^\gamma(\gamma(T); F^\gamma(0), \gamma(0)) = \exp \left\{ \sum_{a=1}^N [\gamma^a(T) - \gamma^a(0)] \right\} \]

and the elastic right Cauchy–Green strain

\[ C^\gamma(\gamma(T), C(0); F^\gamma(0), \gamma(0)) = F^\gamma(0), \gamma(0)) \]
which determines the minimizing deformation paths.

If \( \tau^e - \dot{\gamma}^e < 0 \) during \([t_i, t_f] \subset [0, T] \), which corresponds to elastic unloading of the system \( x \), it follows that, necessarily, \( \delta \gamma^e = 0 \) in that time interval and the corresponding term in (61) vanishes. Thus, as expected, all elastic paths are stationary. Suppose now that the crystal has at least five independent slip systems and that we confine our attention to volume preserving deformation histories. By material time indifference, we can further restrict our attention to pure stretch deformations \( \mathbf{F}(t) = \mathbf{U}(t) \). This leaves five independent components of deformation. We shall assume that any arbitrary variation \( \delta \gamma(t) \) in the slip activity at time \( t \) can be attained by a suitable choice of \( \delta \mathbf{U}(t) \). The variations \( \delta \gamma(t) \) being arbitrary, (61) requires that \( \tau^e - \dot{\gamma}^e = 0 \) for the active systems. These requirements and the plastic irreversibility constraint (51) can be expressed compactly in Kuhn–Tucker form as

\[
\tau^e(t) - \dot{\gamma}^e(t) \leq 0, \quad \text{and} \quad \gamma^e(t) \geq 0, \quad \text{and} \quad [\tau^e(t) - \dot{\gamma}^e(t)] \gamma^e(t) = 0
\]

for all slip systems \( x = 1, \ldots, N \), which are the optimality conditions for constrained variational problems (Rockafellar, 1970). It follows from the third of (62) and (59) that

\[
W = [\phi]\mathbf{F}^0
\]

i.e., the work of deformation along a minimizing path in a rate-dependent single crystal equals the change in free energy.

Next, we shall consider such paths as result from constant slip rates \( \dot{\gamma}^e \) over the time interval \([0, T] \) under consideration. The slip rates are subject to the plastic irreversibility constraint (51) and some of them may vanish identically over the time step. The working assumption is, therefore, that the pattern of slip activity, i.e., the active slip systems and relative slip rates, remains constant throughout the interval \([0, T] \). For these paths,

\[
\gamma^e(t) = (1 - t/T)\gamma^e(0) + (t/T)\gamma^e(T)
\]

and the flow rule (50) integrates to

\[
\mathbf{F}^e(t) = \exp \left\{ \sum_{x=1}^N [\dot{\gamma}^e(t) - \gamma^e(0)] \mathbf{s}^x \otimes m^x \right\} \mathbf{F}^e(0)
\]

In particular,

\[
\mathbf{F}^e(\gamma(T); \mathbf{F}^e(0), \gamma(0)) = \exp \left\{ \sum_{x=1}^N \left[ \mathbf{s}^e(T) - \gamma^e(0) \right] \mathbf{s}^x \otimes m^x \right\} \mathbf{F}^e(0)
\]

and the elastic right Cauchy–Green deformation tensor at \( T \) takes the form

\[
\mathbf{C}^e(\gamma(T), \mathbf{C}(T); \mathbf{F}^e(0), \gamma(0)) = \mathbf{F}^{-T}(\gamma(T); \mathbf{F}^e(0), \gamma(0)) \mathbf{C}(T) \mathbf{F}^{e-1}(\gamma(T); \mathbf{F}^e(0), \gamma(0))
\]

(67)
where \( C(T) \) is given. If, in addition, the path is minimizing then the work of deformation follows from (63) and (44) in the form

\[
W(\gamma(T), C(T); F^e(0), \gamma(0)) = \phi(C_x(\gamma(T); F^e(0), \gamma(0)), \gamma(T)) - \phi(0) \tag{68}
\]

The terminal value \( \gamma(T) \) of the slip strains then follows from the minimum problem:

\[
W(C(T); F^e(0), \gamma(0)) = \min_{\gamma(0), \ldots, \gamma(N)} W(\gamma(T), C(T); F^e(0), \gamma(0)) \tag{69}
\]

Indeed, a trite calculation reveals that

\[
\frac{\partial W(\gamma(T), C(T); F^e(0), \gamma(0))}{\partial \gamma(T)} = \tau(T) - g(T) \tag{70}
\]

and, consequently, the Kuhn–Tucker optimality conditions corresponding to (69) are:

\[
\tau^*(T) - g^*(T) \leq 0, \quad \text{and} \quad \gamma^*(T) - \gamma^*(0) \geq 0
\]

and

\[
[\tau^*(T) - g^*(T)]_{\neq} \gamma^*(T) - \gamma^*(0) = 0 \tag{71}
\]

in accordance with (62).

Let \( \mathcal{A} \) be the collection of systems that are active during the time increment. Thus,

\[
\gamma^*(T) > \gamma^*(0) \quad \text{if} \quad x \in \mathcal{A} \tag{72}
\]

\[
\gamma^*(T) = \gamma^*(0) \quad \text{if} \quad x \notin \mathcal{A} \tag{73}
\]

Once problem (69) has been solved by \( \gamma(T) \), for given \( C(T) \) and appropriate initial conditions, the plastic deformation gradient history \( F^e(t), t \in [0, T] \) follows from (64) and (65); \( C(t) \) follows from the second of (44) in terms of the as yet unknown deformation history \( C(t) ; S(t) \) follows from (45) and (46); \( \tau(t) \) from (52); \( g(t) \) from (47) and (64); and, finally, the minimizing deformation history is any function \( C(t) \), with \( \det(C(t)) = 1 \), satisfying the conditions:

\[
\tau^*(t) = g^*(t) \quad \text{if} \quad x \in \mathcal{A} \tag{74}
\]

\[
\tau^*(t) < g^*(t) \quad \text{if} \quad x \notin \mathcal{A} \tag{75}
\]

provided that the ansatz (64) is correct and these constraints can indeed be simultaneously satisfied for all \( t \in [0, T] \). It should be noted that constraints (74) and (75) are satisfied at \( t = T \) by the choice of \( \gamma(T) \), and the question is, therefore, if the slip pattern can indeed be kept unchanged throughout the deformation increment.

The preceding construction reduces the determination of the pseudoplastic energy density \( W \) for rate-independent single crystals to a conventional convex minimization problem for the slip strains. The nature of \( W \) is illustrated in subsequent sections for two important examples: crystals undergoing geometrical softening; and crystals exhibiting latent hardening. In both cases, the corresponding energy density \( W \) is found to be nonconvex. The particular basis for constructing energy-minimizing well with observation.

3.4. Geometrical softening

The deformation of single crystals, correspondingly, in sizeable variations of systems. Consider, for simplicity, the appropriate conditions, the lattice shear stress on the active slip system unstable, a phenomenon known as g.

In order to illustrate the concept of convexity, we consider the case of in uniaxial tension, Fig. 2(a). To hardening and the elasticity of the case that the axis of loading is contained and the slip plane normal \( m \). We \( (x_1, x_2) \)-plane coincides with the \( (s, m) \) axis. The crystal then deforms in plane lattice rotation is the \( x_3 \)-axis. Let \( \theta \) be the angle from the \( x_1 \) axis and let \( \alpha \) be the angle:

\[
R = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}
\]

and

\[
R_s = \begin{pmatrix} \cos(\theta + \alpha) \\ \sin(\theta + \alpha) \\ 0 \end{pmatrix}, \quad R_m = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}
\]

The activation of the system requires

\[
\tau = \sigma \sin(\theta + \alpha) \cos(\theta + \alpha) = g
\]

where \( \sigma \) is the applied uniaxial stress. The deformation gradient is

\[
F = R[I + \gamma_s \otimes m]
\]

\[
= \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}
\]
minimizing then the work of deformation follows from the minimum problem:

\[ F(0) = F^\circ(0) \]

(68)

(69)

(70)

(71)

Thus, we have during the time increment. Thus,

\[ R = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \]

(76)

and

\[ R_s = \begin{pmatrix} \cos(\theta + \alpha) \\ \sin(\theta + \alpha) \\ 0 \end{pmatrix}, \quad R_m = \begin{pmatrix} -\sin(\theta + \alpha) \\ \cos(\theta + \alpha) \\ 0 \end{pmatrix} \]

(77)

The activation of the system requires

\[ \tau = \sigma \sin(\theta + \alpha) \cos(\theta + \alpha) = g \]

(78)

where \( \sigma \) is the applied uniaxial stress and \( g \) is the constant critical resolved shear stress. The deformation gradient is

\[ F = R[I + \gamma_s \otimes m] \]

(79)

found to be nonconvex. The particular well structure of \( W \) is subsequently taken as a basis for constructing energy-minimizing microstructures which agree remarkably well with observation.

3.4. Geometrical softening

The deformation of single crystals may result in large lattice rotations and, correspondingly, in sizeable variations in the resolved shear stresses acting on the slip systems. Consider, for simplicity, the case of a crystal oriented for single slip. Under the appropriate conditions, the lattice rotations may sufficiently increase the resolved shear stress on the active slip system to cause the behavior of the crystal to turn unstable, a phenomenon known as geometrical softening (Asaro, 1983).

In order to illustrate the concept of geometrical softening and its relation to lack of convexity, we consider the case of a single crystal oriented for single slip and loaded in uniaxial tension, Fig. 2(a). To further simplify the problem, we shall neglect hardening and the elasticity of the crystal, i.e., we take \( F^\circ = R \in \text{SO}(3) \), and assume that the axis of loading is contained within the plane defined by the slip direction \( s \) and the slip plane normal \( m \). We chose a cartesian reference frame in which the \((x_1, x_2)\)-plane coincides with the \((s, m)\) plane and the \( x_3 \)-axis is aligned with the loading axis. The crystal then deforms in plane strain within the \((x_1, x_2)\)-plane and the axis of lattice rotation is the \( x_3 \)-axis. Let \( \theta \) be the angle subtended by the initial slip direction \( s \) to the \( x_1 \)-axis, and let \( \alpha \) be the angle of lattice rotation, so that

\[ R = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \]

(76)
Assuming that the specimen stretches under the action of fixed grips furnishes the kinematic constraint

\[
\begin{pmatrix}
0 \\
1 \\
0
\end{pmatrix} = \begin{pmatrix}
0 \\
\lambda \\
0
\end{pmatrix}
\]  
(80)

where \(\lambda\) is a prescribed stretch ratio. Inserting (79) into (80) gives the identities

\[-\sin \alpha + \gamma \cos(\theta + \alpha) \cos \theta = 0, \quad \cos \alpha + \gamma \sin(\theta + \alpha) \cos \theta = \lambda\]  
(81)

From (78) and (81) we obtain

\[
\sigma = \frac{g}{\sin(\theta + \alpha) \cos(\theta + \alpha)}, \quad \gamma = \frac{\sin \alpha}{\cos(\theta + \alpha) \cos \theta}, \quad \dot{\lambda} = \cos \alpha + \frac{\sin \alpha \sin(\theta + \alpha)}{\cos(\theta + \alpha)}
\]  
(82)

parametrized in terms of \(\alpha\). The deformation power may be variously expressed as

\[
W = g\gamma = \sigma \frac{d \log \lambda}{d t}
\]  
(83)

which shows that \(W = g\gamma\).

The stress–strain curve of the crystal in terms of the work-conjugate variables \((\sigma, \log \lambda)\) can be obtained by eliminating \(\alpha\) from the first and third of (82). The stress–strain curve and work density function \(W(\log \lambda)\) corresponding to \(\theta = \pi/8\) and \(\alpha \in [0, \pi/4]\) are shown in Fig. 2(b). The lack of convexity of the work energy function is evident from the figure. In particular, we note that the stress–strain curve has the familiar up–down–up form of one-dimensional models of displacive phase transitions in solids (Ericksen, 1980; Silling, 1989). The equilibrium solutions led to by these models are presently well understood (Truskinovsky and Zanzotto, 1995, 1996) and, by analogy, we may expect crystals undergoing geometrical softening to develop fine microstructure. We shall return to this question in Section 5.2.

3.5. Latent hardening

Latent hardening tests (Kocks, 1964; Ramaswami et al., 1965; Kocks, 1966; Franciosi et al., 1980; Bassani and Wu, 1991a, b) have been widely used to investigate the hardening behavior of single crystals. In latent hardening experiments, the crystal is first oriented for single slip and loaded in uniaxial tension or compression. The crystal is subsequently cut into smaller specimens which are rotated and re-loaded so as to activate a secondary system, Fig. 3. This type of test enables a direct characterization of the hardening induced in secondary systems by plastic activity in the primary slip system, or latent hardening.

Latent hardening data is often reported in terms of the latent hardening ratio \(LHR = \tau_s/\tau_p\), where \(\tau_s\) and \(\tau_p\) denote the critical resolved shear stresses on the primary and secondary slip system, respectively. The values of the critical resolved shear stresses are typically obtained from experimental data (Franciosi et al. 1980) and the prestain \(\gamma_p\) on the primary system.
The action of fixed grips furnishes the

\[ (80) \]

\[
(\theta + x) \cos \theta = \lambda
\]

\[ (81) \]

\[
\lambda = \cos x + \frac{\sin x \sin(\theta + x)}{\cos(\theta + x)}
\]

\[ (82) \]

or may be variously expressed as

\[ (83) \]

of the work-conjugate variables corresponding to the first and third of (82). The convexity of the work energy function that the stress–strain curve has the models of displacive phase transitions for equilibrium solutions led to by these and Zanzotto, 1995, 1996 and, geometrical softening to develop fine Section 5.2.

![Diagram](image)

Fig. 2. (a) Single crystal oriented for single slip loaded in uniaxial tension, (b) stress–strain curve showing lack of convexity due to geometrical softening.

stresses are typically obtained from the stress–strain curve by backextrapolation. The experimental data (Franciosi et al., 1980) reveals that the LHR is a function of the prestrain \( \gamma_p \) on the primary system and the strength of the interaction between the primary and secondary systems. For well-annealed FCC crystals the LHR reduces to
latent-hardening, in the sense that the transition in breaking through the active slip lies between the primary and secondary systems. This conjecture is born out by the bifurcation analysis (Hill and Hutchinson, 1975) and found that, for such effects, the equations may change type from elliptic to parabolic and that this transition marks the inceptive crack size. For specimens subjected to uniaxial tension, these equations exhibit nonuniform slip patterns containing primary and secondary systems.

It should be carefully noted, however, that the Hutchinson type (1975) are based on the assumption that the “linear comparison solid” in Hill’s paper. This inevitably weakens the case for the conjecture between latent hardening and patchy slippage, as nonlinear analysis based on the energy release rate can account for such effects.

Fig. 3. Schematic representation of latent hardening tests, showing primary and secondary loading phases and definition of the latent hardening ratio.

Fig. 4. Instances of slip segregation into single phase.(b) from Rasmussen and Pedersen (1980), publisher.
latent-hardening, in the sense that the slip lines of the one system experience difficulty in breaking through the active slip lines of the other one” (Pierce et al., 1955, p. 337). This conjecture is born out by the bifurcation analysis and numerical simulations of Pierce et al. (1982). Thus, Pierce et al. (1982) applied Hill and Hutchinson’s bifurcation analysis (Hill and Hutchinson, 1975) to Asaro’s double-slip planar model of crystals (Asaro, 1979) and found that, for sufficiently strong latent hardening, the governing equations may change type from elliptic to parabolic. Pierce et al. (1982) reasoned that this transition marks the inception of patchy slip. Finite element simulations of specimens subjected to uniaxial tension carried out by Pierce et al. (1982) do indeed exhibit nonuniform slip patterns consisting of alternating regions of single slip on the primary and secondary systems.

It should be carefully noted, however, that bifurcation analyses of the Hill and Hutchinson type (1975) are based on the incremental behavior of the solid—the “linear comparison solid” in Hill’s parlance—and, consequently, are not fully nonlinear. This inevitably weakens the case for an unequivocal cause-and-effect relation between latent hardening and patchy slip. In subsequent sections, we carry out a nonlinear analysis based on the energy minimization theory developed in the fore-

Fig. 4. Instances of slip segregation into single-slip domains, or “patchy slip”. (a) From Saimoto (1963), (b) from Rasmussen and Pedersen (1980), (c) from Jin and Winter (1984b). Reprinted by permission of Publisher.
going. Within this framework, the transition to patchy slip arises as a consequence of the lack of convexity of the energy function in the presence of latent hardening. The well-structured nature of the pseudoelastic strain energy density suggests that crystals exhibiting latent hardening can reduce the work required to attain a prescribed average deformation by developing microstructures consisting of single-slip variants. Deformation structures based on this ansatz are constructed in subsequent sections.

In order to explicitly exhibit the relationship between latent hardening, lack of convexity and patchy slip, we resort to a simple model of latent hardening. In particular, we seek a model with the following attributes:

1. Parabolic hardening in single slip: $g(\gamma^\alpha) \sim \sqrt{\gamma^\alpha}$.
2. Off-diagonally dominant hardening matrix: $h^{\alpha \beta} > h^{\alpha \alpha}$, $\alpha, \beta = 1, \ldots, N$, $\beta \neq \alpha$.

where $h^{\alpha \beta}(\gamma) = \partial g^{\beta} / \partial \gamma^\alpha$ is the hardening matrix.

These two requirements roughly reflect the phenomenology of latent hardening summarized above. Evidently, the assumption of parabolic hardening can be trivially generalized to an arbitrary power-law dependence of $g^{\alpha}$ on $\gamma^\alpha$, but this generalization will not be pursued here. Begin by assuming an additive decomposition of the free energy of the form

$$\phi = W^r(C^r) + W^p(\gamma)$$

Implicit in this decomposition is the assumption, e.g., upon unloading, is not affected by the approximation for metals. We further assume purely elastic microstructures, a model of the form (84), the hardening relation

$$g^{\alpha} = \frac{\partial W^p(\gamma)}{\partial \gamma^\alpha}, \quad h^{\alpha \beta} = \frac{\partial^2 W^p(\gamma)}{\partial \gamma^\alpha \partial \gamma^\beta}$$

A class of functions $W^p(\gamma)$ which can be written

$$W^p = \frac{2}{3} \tau_0 \gamma_0 \left[ \sum_{s=1}^{N} \sum_{s=1}^{N} \alpha^{\alpha \beta} \frac{\gamma^{\beta}}{\gamma_0} \right]$$

where $\tau_0$ and $\gamma_0$ are a reference stress and reference hardening, respectively.

Experimentally determined values (Ott and Zaoui 1982) for FCC and BCC systems according to whether the dominant interaction coefficient $a_0$, fail to form junctions (interaction coefficient $a_1$), co-planar junctions (interaction coefficient $a_2$), or dominant hardening matrix $h^{\alpha \beta}$ as $h^{\alpha \beta} \alpha \beta$ gives $a_1/a_0 = 5.7$, $a_2/a_0 = 10.2$, $a_0/a_0 = 1$.

A simple geometrical model found by Cuitifio and Ortiz (1993). The model considers the number of dislocation intersections per unit volume of obstacles. A tritc calculation gives

$$n^{\beta} = \frac{2}{\pi} \sqrt{1 - (n^r m^p)^2}$$

In this simple model the slip systems stresses required to deform a well compared to those required for macroscopic 93 — in lieu of more detailed Ni$_3$Al single crystals.

The form of the pseudoelastic strain of particular interest. Begin by considering the undeformed state, i.e., set $F^r(0) = 0$.
\[ \phi = W^e(C^e) + W^p(\gamma) \]  \hspace{1cm} (84)

Implicit in this decomposition is the assumption that the elastic response of the solid, e.g., upon unloading, is not affected by internal processes, which is a good first approximation for metals. We further suppose that \( W^e \) is quasiconvex, which rules out purely elastic microstructures, and that \( W^p(y) \geq 0 \) and \( W^p(\gamma) = 0 \). For free energies of the form (84), the hardening relations and hardening matrix are

\[ g^e = \frac{\partial W^p(\gamma)}{\partial \gamma^e}, \quad h^{\alpha \beta} = \frac{\partial^2 W^p(\gamma)}{\partial \gamma^e \partial \gamma^\beta} \]  \hspace{1cm} (85)

A class of functions \( W^p(\gamma) \) which conforms to the requirements stated above is

\[ W^p = \frac{2}{3} \tau_0 \gamma_0 \left[ \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} \sigma^{\alpha \beta} \frac{\gamma^\alpha \gamma^\beta}{\gamma_0 \gamma_0} \right]^{1/4} \]  \hspace{1cm} (86)

where \( \tau_0 \) and \( \gamma_0 \) are a reference resolved shear stress and slip strain, respectively, and \( \sigma^{\alpha \beta} \) are interaction coefficients.

Experimentally determined values of the matrix \( \sigma^{\alpha \beta} \) have been given by Franciosi and Zaoui (1982) for FCC and BCC crystals. They classify the interactions between systems according to whether the dislocations belong to the same system (interaction coefficient \( a_0 \)), fail to form junctions (interaction coefficient \( a_1 \)), form Hirth locks (interaction coefficient \( a_2 \)), co-planar junctions (interaction coefficient \( a_3 \)), glissile junctions (interaction coefficient \( a_4 \)), or sessile Lomer–Cottrell locks (interaction coefficient \( a_5 \)), with \( 0 \leq a_0 \leq a_1 \leq a_2 \leq a_3 \). These order relations give an off-diagonally dominant hardening matrix \( h^{\alpha \beta} \) as required. For copper, a fit to the experimental data gives \( a_0/a_0 = 5.7, a_2/a_0 = 10.2, a_3/a_0 = 16.6 \) (Cuitiño and Ortiz, 1992).

A simple geometrical model for the interaction matrix \( \sigma^{\alpha \beta} \) has been proposed by Cuitiño and Ortiz (1993). The model is based on counting the number of forest dislocation intersections per unit area of the slip plane, which gives the density of point obstacles. A trite calculation gives

\[ \sigma^{\alpha \beta} = \frac{2}{\pi} \sqrt{1 - (m^\alpha \cdot m^\beta)^2} \]  \hspace{1cm} (87)

In this simple model the slip systems do not self-harden. Indeed, typical resolved shear stresses required to deform a well-annealed crystal in single slip tend to be small compared to those required for multiple slip and, for purposes of understanding the morphology of dislocation structures, they can conveniently and expeditiously be neglected to a first approximation. The relation (87) was used by Cuitiño and Ortiz (1993)—in lieu of more detailed experimental data—to describe the hardening of Ni3Al single crystals.

The form of the pseudoeelastic strain energy density (69) predicted by the model is of particular interest. Begin by considering a deformation increment from a previously undeformed state, i.e., set \( F(0) = I, \gamma(0) = 0 \). From (59), (84), (86) and the assumed
properties of \( W \), it is clear that \( W \geq 0 \). In addition, owing to the lack of self-hardening in model (87) one has \( W(F(T)) = 0 \) for any terminal deformation of the form

\[
F(T) = R(T)F^p(T), \quad F^p(T) = I + \gamma(T)s^a \otimes m^a
\]

i.e., for deformations consisting of single slip followed by an arbitrary lattice rotation \( F = R \in SO(3) \). Indeed, from the first of (88) one has \( C'(T) = I \) and, consequently, \( W^p(C'(T)) = 0 \) by the assumed properties of \( W \). Additionally, \( W^p = 0 \) as a consequence of the approximation \( a^a = 0 \). It therefore follows that all single-slip deformations constitute “wells”, or local minima, of the incremental strain energy density \( W \) of previously undeformed crystals exhibiting latent hardening. In particular, the energy density \( W \) is nonconvex, which foreshadows the development of fine microstructures.

To exhibit more explicitly the well structure induced by latent hardening, we consider the simple case of an FCC crystal deforming in plane strain within the plane determined by the directions [101] and [010]. The normal to this plane is in the [101] direction. Combinations of slip systems which result in plane-strain deformations with this geometry are the pair (111) [110] and (111) [010], which jointly gives rise to effective in-plane shear along the [121] direction, Fig. 5(a). Similarly, the systems (111) [110] and (111) [010] combine to produce effective in-plane slip along the [121] direction, Fig. 5(b). Finally, the joint operation of the pair of systems (111) [110] and (111) [010] results in the in-plane effective system [010] [110]. By material frame indiffERENCE and incompressibility, there are only two independent deformation components, which may be chosen to be \((e_{11} - e_{22}) \) and \( e_{12} \), where \( e = \log U \) is the logarithmic strain tensor. The corresponding energy function \( W \) is displayed in Fig. 5(c). The lack of convexity of \( W \) is immediately apparent. A section of \( W \) along a circle \( \|s\| = \text{const} \), centered at the origin exhibits multiple minima, or “wells”, corresponding to single-slip deformation modes. As noted earlier, due to the lack of self-hardening in the model, \( W \) vanishes identically at these minima.

Next, consider the incremental deformations over a time interval \([0, T]\) of a crystal that has been prestrained in single slip. In this case,

\[
F(0) = R(0)F^p(0), \quad F^p(0) = I + \gamma(0)s^a \otimes m^a
\]

for some slip system \( z \). Evidently, terminal deformations \( F(T) \) requiring the activation of a secondary system inevitably induce latent hardening and, consequently, lead to a \( W > 0 \). By contrast, a terminal deformation of the form (88), resulting from the continuing activation of the strained slip system, gives \( W = 0 \). Therefore, the only energy well available to a crystal prestrained in single slip corresponds to further single-slip on the prestrained slip system. This reduction in the number of wells due to prestraining in single slip may be regarded as a “training” of the crystal, which is subsequently conditioned to prefer a specific single slip for further deformation. We shall refer to deformation histories of form

\[
F(t) = R(t)F^p(t), \quad F^p(t) = I + \gamma(t)s^a \otimes m^a
\]

as “persistent single slip”. Note that the slip-strain history \( \gamma(t) \) is allowed to be arbitrary and, in particular, may exist without fatigued single crystals. From the above, \( W \) vanishes identically.

4. Dislocation structures

The models of geometrical softening presented in the preceding sections lead to nonconvex energy potentials. Under certain conditions, uniform deformation fields may be obtained by considering a macroscopic neighborhood of the displacement boundary conditions of an underlying microstructure, which is better in energetic terms than any other structure of the incremental strain energy.

For crystals exhibiting latent hardening, one may show that uniform deformations correspond to local energy minimizers. This suggests a search for local energy minimizers over \( \Omega \), namely, the minimizers of (35) which consist locally of persistently active slip.

\[
F^e(x, t) = R(x, t)F^p(x, t)
\]

over a subset \( \Omega \subset \Omega \). Note that this result is not inconsistent with the idea that the set of deformations, e.g. at the boundary of the grain, is not a single slip system. One may expect that the measure \( |\Omega - \Omega| \) can vanish. If, in addition, the energy function is such that the sequence \( F^p(x, t) \) converges weakly to a minimizer as \( t \to 0 \).

A fundamental question concerning the accommodation of deformation by the microstructure and the deformation history, the crystal is a hardener or a softener, is addressed early on, and subsequent averaging effect is necessary. The existence of a microstructure. Within the above framework, the conjecture is that, for crystals possessing a few or more independent slip systems, persistent single slip exist for any load gradients of the form

\[
F(t) = I + f(t)G
\]

where \( f(t) \) is any absolutely continuous function with a constant traceless matrix. A proof...
owing to the lack of self-hardening
deformation of the form
\begin{equation}
W = \frac{1}{2} m^T \sigma T m
\end{equation}
(88)
induced by an arbitrary lattice rotation
\( T \) has \( C^*(T) = I \) and, consequently, \( W^* = 0 \). As a conse-
quence, the following holds all single-slip defor-
mation the incremental strain energy density is
latent hardening. In particular, the existence
induces the development of fine micro-
expression of the form (35) of the
plane-strain within the plane normal to this plane is in the [101]
result in plane-strain deformations \((111)[110]\) and \((111)[010]\), which jointly gives rise to
Fig. 5(a). Similarly, the systems of
effectively in-plane slip along the [121]
\((111)[101]\) and \((111)[010]\). By material
only two independent deformation
\( \varepsilon_{12} \) and \( \varepsilon_{13} \), where \( \varepsilon = \log U \) is the
energy function \( W \) is displayed in Fig.
minima. A section of \( W \) along \( \varepsilon_{12} \) exhibits multiple minima, or “wells”,
minima. As noted earlier, due to the lack of
over a time interval \([0, T]\) of a crystal
\begin{equation}
F_i(x, t) = R_i(x, t)F^T_i(x, t)
\end{equation}
(91)
\begin{equation}
F_i^T(x, t) = I + \gamma_i(x, t)m_i(x) \otimes m_i(x), \quad (s_i(x), m_i(x)) \in S
\end{equation}
(92)
over a subset \( \Omega \subset \Omega \). Note that this is strictly a problem of compatibility. The reason
for not insisting on persistent single slip almost everywhere in \( \Omega \) is that compatibility of
deforations, e.g., at the boundary, will in general require the intro-
duction of boundary layers involving complex slip patterns and elastic strains. However, we
expect that the measure \( |\Omega - \Omega^*| \) can be made arbitrarily small be refining the micro-
structure. If, in addition, the energy density remains bounded almost everywhere, it
follows that the sequence \( F^{(n)}(x, t) = F^{(n)}(x, t) \) defines an incremental energy min-
\begin{equation}
F(t) = I + f(t)G
\end{equation}
(93)
where \( f(t) \) is any absolutely continuous function of time in the interval \([0, T]\), and \( G \)
is a constant traceless matrix. A plausibility argument supporting this conjecture is
4. Dislocation structures

The models of geometrical softening and latent hardening developed in the pre-
ceeding sections lead to nonconvex incremental energy densities. Under these
conditions, uniform deformation fields are not minimizers of (38) in general. Thus,
consider a macroscopic neighborhood \( \Omega \) of a ductile crystal subject to affine dis-
placement boundary conditions of the form (35). Then, the crystal can generally do
better in energetic terms than to deform uniformly over \( \Omega \) by exploiting the well
structure of the incremental strain energy density \( W \).

For crystals exhibiting latent hardening, the results given in the preceding section
show that uniform deformations consisting of persistent single slip are incremental
energy minimizers. This suggests a strategy for constructing more general approximate
energy minimizers over \( \Omega \), namely, to seek compatible deformation fields satisfying
(35) which consist locally of persistent single slip, i.e., which are of the form

The fundamental question concerns which average deformation histories \( \bar{F}(t) \) can be
accommodated by the microstructures just described. It is clear that, for any such
deforation history, the crystal is trained into a pattern of local persistent single slip early on, and subsequent average deformations must be compatible with the estab-
lished microstructure. Within the framework of linearized kinematics, a plausible
conjecture is that, for crystals possessing a sufficiently rich set \( S \) of slip systems, e.g.,
five or more independent slip systems, incremental energy minimizing sequences of
persistent single slip exist for any history of volume-preserving average deformation
gradients of the form
given in Section 4.3. The linearized kinematics framework is particularly relevant in high-cycle fatigue, where typical deformation amplitudes are of the order of $10^{-3}$. Indeed, many of the examples of microstructures given in Section 5 pertain to high-cycle fatigue of single crystals and polycrystals.

So far we have formulated the problem of microstructural development in ductile single crystals in terms of compatible deformation fields $F(x, t)$, and the mathematical description of dislocation structures has not as yet been addressed. However, the connection between deformation and dislocation structures is readily made. Thus, while $F(x, t)$ must be compatible, i.e., it must be a gradient for all $t \in [0, T]$ in some suitable weak sense, the plastic deformation field $F^p(x, t)$ is not subject to any such requirement. Physically, the incompatibility of $F^p(x, t)$ represents a distribution of dislocations within the crystal. To see this, let $\Gamma$ be a smooth closed circuit inscribed within the undeformed crystal, or Burgers circuit. Owing to the incompatibility of $F^p$, the vector

$$b(\Gamma) = \oint_{\Gamma} F^p \cdot \mathbf{dx}$$

(94)

is not zero in general but amounts to the vector sum of the undeformed or true Burgers vectors for all dislocations encircled by $\Gamma$. Let $\Sigma$ be any smooth surface bordering on $\Gamma$. Then, by Stokes' theorem,

$$b(\Gamma) = \oint_{\Sigma} (F^p \times \nabla) \cdot N \, dS$$

(95)

where $N$ is the unit normal to $\Sigma$ and $dS$ is the element of area. Following Nye (1953) (see also Mura, 1987), the dislocation density tensor is defined as

$$A = F^p \times \nabla$$

(96)

whereupon (95) can be rewritten as

$$b(\Gamma) = \oint_{\Sigma} A \cdot N \, dS$$

(97)

It is evident from (96) that $A$ is a measure of the incompatibility of $F^p$ and that, from a continuum perspective, dislocations are inextricably related to incompatibility. A direct consequence of definition (96) is that

$$A \cdot \nabla = 0$$

(98)

This identity embodies the physical requirement that dislocation lines cannot end abruptly in the interior of the crystal. Indeed, if the surface $\Sigma$ in (95) is closed, then an application of the divergence theorem and (98) shows that the net Burgers vector flux through the surface is zero, as required. Identity (98) also embodies Frank's rule for dislocation reactions.

The dislocation density tensor corresponding to a single dislocation line supported on a curve $C$ in $\Omega$ is

$$A(x) = b \otimes t(x) \delta_C(x)$$

where $b$ is the Burgers vector of the line Dirac-delta supported on $C$. Another distributed parallel dislocations, for $\rho > 0$

$$A = \rho b \otimes t$$

where $\rho$ is the dislocation length per unit length.

It follows from the fundamental model that describes not only deformation micromechanics well. However, it bears emphasis that investigations of low energy dislocation interaction tensors $A$, e.g., representing an ensemble, and seek to minimize the long-range energy—induced by $A$. By contrast, the unknown field and $A$ derives from this distribution is consistent with a history of stresses are absent from the calculation. $F^p$ is required to be locally a rotation.

### 4.1. Dislocation walls

In this and subsequent sections, we focus on the form (91) and (92), namely, if these structures suffice to explain and demonstrated in Section 5.

We begin by characterizing all possible deformed regions of the crystal using the martensitic theory of martensite, which were the interface as variants. The deformation

$$F^\pm(i) = R^\pm(i)(1 + \gamma^+(i)s^\pm \otimes s^\pm)$$

where the labels $\pm$ refer to the plus direction, the unit normal $N$. The active system is unchanged throughout the deformation, that the crystal is initially undeformed.

$$R^\pm(0) = I, \quad \gamma^+(0) = 0$$

and we shall require the functions $s^\pm$. In particular, we rule out unphysical change of slip strains.

Compatibility across the interface,

$$[F] = F^+ - F^- = [y_{\alpha\beta}] \otimes N$$

The rotation $R^-$ can be set to the...
framework is particularly relevant in amplitudes are of the order of $10^{-2}$. The
results given in Section 5 pertain to high-ductility microstructures.

Structural development in ductile materials is described by fields $F(x, t, \Gamma)$, and the mathematical formulation is addressed. However, the
behaviour of dislocation microstructures is readily made. Thus, a gradient for all $t \in [0, T]$ in some open set of $\mathcal{D}$ is not subject to any such
requirements. Thus, $F^\delta(x, t)$ represents a distribution of the form $F^\delta$, with $\delta$ being a smooth closed circuit inserted into $\mathcal{D}$.

Owing to the incompatibility of $F^\delta$, the surface integral of the derivatives of the $\delta$ function must vanish in $\mathcal{D}$, for any $t \in [0, T]$.

\begin{equation}
A(x) = b \otimes \delta_\epsilon(x) \tag{99}
\end{equation}

where $b$ is the Burgers vector of the dislocation, $t$ is the unit tangent to C and $\delta_\epsilon$ is the Dirac-delta supported on C. Another noteworthy special case is that of a linearly distributed parallel dislocations, for which

\begin{equation}
A = \rho b \otimes t \tag{100}
\end{equation}

where $\rho$ is the dislocation length per unit volume.

It follows from the fundamental relation (96) that representation (91) and (92) describes not only deformation microstructures but dislocation microstructures as well. However, it bears emphasis that the present approach is at variance with investigations of low energy dislocation structures which regard the dislocation density tensor $\mathbf{A}$, e.g., representing an ensemble of discrete dislocations, as the primary field, and seek to minimize the long-range stresses—of the corresponding elastic strain energy—induced by $\mathbf{A}$. By contrast, in the present approach $F^\delta$ is the primary unknown field and $\mathbf{A}$ derives from it through (96). In particular, the dislocation distribution is consistent with a history of plastic slip in the crystal. In addition, long-range stresses are absent from the crystal by construction, as the elastic deformation $F^\delta$ is required to be locally a rotation.

### 4.1. Dislocation walls

In this and subsequent sections, we proceed to describe some simple structures of the form (91) and (92), namely, interfaces and laminites. Despite their simplicity, these structures suffice to explain a number of experimental observations, as demonstrated in Section 5.

We begin by characterizing all possible planar interfaces separating two uniformly deformed regions of the crystal undergoing single slip. By analogy to the crystallographic theory of martensite, we shall refer to each of the regions separated by the interface as variants. The deformations of the variants are, therefore,

\begin{equation}
F^\pm(t) = R^\pm(t)(I + \gamma^\pm(t) s^\pm \otimes m^\pm), \quad (s^\pm, m^\pm) \in \mathcal{H}, \quad t \in [0, T] \tag{101}
\end{equation}

where the labels $\pm$ refer to the plus and minus sides of the interface as determined by the unit normal $\mathbf{N}$. The active systems in each of the variants are assumed to remain unchanged throughout the deformation. For definiteness we shall further suppose that the crystal is initially undeformed, i.e.,

\begin{equation}
R^\pm(0) = I, \quad \gamma^\pm(0) = 0 \tag{102}
\end{equation}

and we shall require the functions $R^\pm(t)$ and $\gamma^\pm(t)$ to be absolutely continuous. In particular, we rule out unphysical discrete jumps in either the lattice rotations or the slip strains.

Compatibility across the interface demands

\begin{equation}
[F] = F^+ - F^- = [\gamma_N] \otimes N \tag{103}
\end{equation}

The rotation $R^-$ can be set to the identity without loss of generality. Then, $R^+$ may
be regarded as the rotation of the (+) variant relative to the (−) variant. In addition, the slip strain $\gamma^-$ may conveniently be utilized to parametrize the motion instead of time. Then, the compatibility condition (103) must be satisfied for all values of $\gamma^-$. Equation (103) imposes four constraints on $[F]$, namely that the determinant and the three principal minors of $[F]$ vanish identically. Thus, for fixed $\gamma^-$, (103) defines a system of four nonlinear equations in the four unknowns $\gamma^+, R^+$. The problem is, therefore, to find all solutions $(\gamma^+, R^+)$ of this system of equations.

Of particular interest is the dislocation structure attendant to an interface. As noted in the foregoing, while the deformation gradients $F$ are required to be compatible at the interface in the sense of (103), the plastic deformations need not be compatible in general, and the incompatibility of $F^p$ is equivalent to a dislocation distribution of density (96). For interfaces, and application of (96) in a distributional sense gives

$$A(x) = -[[F^p]] \times N\delta_\Pi(x)$$

(104)

where $\Pi$ is the plane of the interface and $\delta_\Pi$ is the Dirac-delta supported on $\Pi$. As expected, the dislocations are confined to the interface and form a two-dimensional dislocation array. In the special case of variants undergoing single slip

$$A(x) = \gamma s \otimes m \times N\delta_\Pi(x)$$

$$= (\gamma^+ s^+) \otimes (N \times m^+) \delta_\Pi(x) - (\gamma^- s^-) \otimes (N \times m^-) \delta_\Pi(x)$$

(105)

A comparison of this density and (100) reveals that the dislocation wall comprises two bundles of parallel dislocations of line density, Burgers vector and direction

$$\rho^\pm = \frac{\gamma^\pm}{b} \delta_\Pi(x), \quad b^\pm = bs^\pm, \quad t^\pm = N \times m^\pm$$

(106)

respectively. In (106), $b$ is the magnitude of the Burgers vector. The dislocation density tensor can alternatively be computed from the jump in elastic part $F^e$ of the deformation gradient. Thus, inserting (41) into (104) and using (103) leads to

$$A(x) = ([F^e]) [F^+] \times N\delta_\Pi(x) = ([F^e]) [F^-] \times N\delta_\Pi(x)$$

(107)

In the absence of long-range stresses, $F^\pm = R^\pm \in SO(3)$, and one has

$$A(x) = ([R^\pm] [F^+]) \times N\delta_\Pi(x) = ([R^\pm] [F^-]) \times N\delta_\Pi(x)$$

(108)

which shows that the dislocation density tensor is related to the misorientation $[R^\pm]$ of the variants.

Two-dimensional dislocation arrangements of the type just described have been variously termed dislocation boundaries and dislocation walls. Dislocation arrays are often used as mathematical (Hirth and Lothe, 1968) representations of grain boundaries, but here the emphasis is on dislocation boundaries composed solely of glide dislocations. Because the walls contain dislocations belonging to two different slip systems, they are commonly termed dipolar walls. Planar dislocation walls of well-defined crystallographic orientations are often observed, e.g., as part of the labyrinth structures which develop in cyclically deformed crystals oriented for multiple slip (L'Esperance et al., 1986; Mecking and Winter, 1984a; Charsley, 1967). The structures observed during the early stage of slip (Steeds, 1966). Specific examples of the dislocation walls are presented in Section 5.

It has long been known (see, e.g., the work of Steeds) that dislocation walls do not induce low-energy dislocations or lines of low energy. Dislocation walls turn up ubiquitously in ensembles of discrete dislocations. As such, the dislocation wall is precisely those for which $F^\pm = R^\pm m^\pm$. It should be carefully noted that the precise density of dislocation walls is observed experimentally does not require the additional kinetic energy of the dislocations to be considered.

The enforcement of compatibility is useful in the analysis of the dislocation wall.

$$l = \nabla v = \dot{F} F^{-1}$$

be the spatial velocity gradient. For a straightforward calculation gives

$$l^\pm = \gamma^\pm (R^\pm s^\pm) \otimes (R^\pm m^\pm) + \dot{R}^\pm$$

Evidently, $l^\pm$ represent the superposition $(R^\pm s^\pm, R^\pm m^\pm)$ and incremental lattice twist of the compatibility condition (103) becomes

$$[\ell] = l^+ - l^- = [v_{\alpha}] \otimes n$$

where $n$ represents the current unit for preserving deformations, it follows

$$[v_{\alpha}] \cdot n = 0$$

The relation between $([v_{\alpha}], N)$ and $(\tilde{N}_{\alpha})$, with the result

$$[v_{\alpha}] = ([F^-])^{-T} N ([\dot{\gamma}_{\alpha}] - F^+ )$$

For variants undergoing single slip

$$\gamma^+(R^+ s^+) \otimes (R^+ m^+) + \dot{R}^+$$

The instantaneous lattice rotation is symmetric and skewsymmetric part
slip (L’Esperance et al., 1986; Mecke and Blochwitz, 1982; Ackermann et al., 1984; Jin and Winter, 1984a; Charsley, 1981; Boulanger et al., 1985); and in the “fence” structures observed during the early stages of stage II of hardening in FCC crystals (Steeds, 1966). Specific examples of dislocation walls observed in FCC crystals are presented in Section 5.

It has been long known (see, e.g., Nabarro, 1967) that certain infinite dislocation walls do not induce long-range elastic stresses in the crystal and, consequently, constitute low-energy dislocation structures. Not surprisingly, therefore, those dislocation walls turn up ubiquitously as energy minimizers in numerical simulations of ensembles of discrete dislocations (Neumann, 1986; Lubarda et al., 1993). In the present theory, the dislocation walls which are devoid of long-range stresses are precisely those for which \( F^\pm = R^\pm \in SO(3) \), as posited in (101). However, it should be carefully noted that the precise crystallographic nature of dislocation walls which is observed experimentally does not necessarily follow by simple minimization of the interaction energy of discrete dislocations, but, as demonstrated in Section 5.1, requires the additional kinematical assumption of persistent single slip in the variants.

The enforcement of compatibility at the interface in incremental or eulerian form proves useful in the analysis of certain interfaces. Let

\[
\begin{align*}
\dot{\mathbf{v}} &= \nabla \mathbf{v} = \dot{\mathbf{F}} \mathbf{F}^{-1} \\
I &= \dot{\mathbf{l}} + \dot{\mathbf{f}} = \dot{\mathbf{F}} \mathbf{F}^{-1}
\end{align*}
\]

be the spatial velocity gradient. For persistent single slip on both sides of the interface, a straightforward calculation gives

\[
I^\pm = \dot{\gamma}^\pm (R^\pm s^\pm) \otimes (R^\pm m^\pm) + \dot{R}^\pm (R^\pm)^{-1}
\]

(110)

Evidently, \( I^\pm \) represent the superposition of incremental slip on the rotated systems \((R^s s^\pm, R^s m^\pm)\) and incremental lattice rotations \( \dot{R}^\pm (R^\pm)^{-1} \). In a spatial setting, the compatibility condition (103) becomes

\[
\mathcal{L} = I^+ - I^- = [v_n] \otimes n
\]

(111)

where \( n \) represents the current unit normal to the plane of discontinuity. For volume-preserving deformations, it follows that \( \text{tr}(I^\pm) = 0 \), which in view of (111) necessitates

\[
[v_n] \cdot n = 0
\]

(112)

The relation between \( \langle [\mathbf{y}_N], N \rangle \) and \( \langle [v_n], n \rangle \) follows simply by inserting (109) into (111), with the result

\[
[v_n] = \| (F^-)^{-T} N \| \langle [\mathbf{y}_N], - \dot{\mathbf{F}}^- (F^-)^{-1} [\mathbf{y}_N] \rangle, \quad n = \frac{(F^-)^{-T} N}{\| (F^-)^{-T} N \|}
\]

(113)

For variants undergoing single slip, insertion of (110) into (111) gives

\[
\dot{\gamma}^+ (R^s s^\pm) \otimes (R^s m^\pm) + \dot{R}^+ (R^+)^{-1} - \dot{\gamma}^- s^- \otimes m^- = [v_n] \otimes n
\]

(114)

The instantaneous lattice rotation may be eliminated by decomposing (114) into symmetric and skewsymmetric parts, with the result

\[
\begin{align*}
\dot{\mathbf{y}}^\pm (R^s s^\pm) \otimes (R^s m^\pm) + \dot{R}^\pm (R^\pm)^{-1} - \dot{\gamma}^- s^- \otimes m^- &= [v_n] \otimes n \\
\dot{\mathbf{y}}^\pm (R^s s^\pm) \otimes (R^s m^\pm) + \dot{R}^\pm (R^\pm)^{-1} - \dot{\gamma}^- s^- \otimes m^- &= [v_n] \otimes n
\end{align*}
\]
\[
\gamma^+ \sym ([R^+ s^+ \otimes (R^+ m^+)] - \gamma^- \sym (s^- \otimes m^-)) \sym ([v_n] \otimes n)
\]

\[\gamma^+ \skw ([R^+ s^+ \otimes (R^+ m^+)] + \dot{R}^+ (R^+)^{-1} - \gamma^- \skw (s^- \otimes m^-) = \skw ([v_n] \otimes n)\]

Here
\[\sym A_{ij} = \frac{1}{2}(A_{ij} + A_{ji}), \quad \skw A_{ij} = \frac{1}{2}(A_{ij} - A_{ji})\]

signify the symmetric and skew-symmetric components of a tensor \(A\).

It therefore follows that a necessary condition for compatibility is that the left-hand side of (115) be the symmetric part of a traceless rank-one tensor. It is a simple matter to verify that a traceless symmetric second-order tensor over \(R^1\) is the symmetric part of a traceless rank-one tensor iff its determinant vanishes. To see this, let \(A = \sym (a \otimes n)\), with \(a \cdot n = 0\). Clearly, \(A(a \otimes n) = 0\), which shows that \(A\) is singular and, consequently, its determinant is zero. Conversely, let \(\det(A) = 0\). Since, in addition, \(\tr(A) = 0\) by assumption, the eigenvalues of \(A\) are of the form \(-\gamma/2, \gamma/2, 0\) for some \(\gamma \in R\). Let \(e_1, e_2, e_3\) be the corresponding eigenvectors and set \(a = \gamma s, \quad s = (e_3 \pm e_1)/\sqrt{2}, \quad m = (e_2 \mp e_1)/\sqrt{2}\). Then, \(\sym (a \otimes m) = -\gamma/2 e_1 \otimes e_1 + (\gamma/2) e_2 \otimes e_2 = A\), which completes the proof. It follows from this derivation that the symmetric part of a traceless rank-one tensor may be regarded as the small-strain tensor corresponding to an infinitesimal slip strain \(\gamma\) on the plane of normal \(m\) in the direction \(s\). It should be carefully noted that there are two equivalent representations of \(A\) obtained by exchanging the roles of \(s\) and \(m\).

An application of this result to (115) yields the condition
\[
\det ([\gamma^+ \sym ([R^+ s^+ \otimes (R^+ m^+)] - \gamma^- \sym (s^- \otimes m^-)] = 0
\]

which, after some trite algebra, reduces to the equation
\[
[R^+ s^+, R^+ m^+, s^-][R^+ s^+, R^+ m^+, m^-]\gamma^- = [s^-, m^-][s^-, m^-][s^-, m^-][s^-, m^-][\gamma^-]
\]

(119)

where \([a, b, c] = (a \times b) \cdot c\) is the triple product. The infinitesimal lattice rotation \(\hat{R}^+(R^+)^{-1}\) can be determined from (116) as follows. Let \((-\gamma/2, 0, 0)\) and \((e_1, e_2, e_3)\) be the eigenvalues and eigenvectors of \([\gamma^+ \sym ([R^+ s^+ \otimes (R^+ m^+)] - \gamma^- \sym (s^- \otimes m^-)]\).

Then,
\[
[v_n] = \gamma (e_2 \pm e_1)/\sqrt{2}
\]

(120)

\[n = (e_2 \mp e_1)/\sqrt{2}\]

(121)

and it follows from (117) that
\[
\omega^+ \equiv \dot{R}^+(R^+)^{-1} \pm \skw ([v_n] \otimes n) - \gamma^+ \skw ([R^+ s^+] \otimes (R^+ m^+)] + \gamma^- \skw (s^- \otimes m^-)
\]

(122)

We shall refer to interfaces such that
\[
[R^+ s^+, R^+] = [\gamma^+ s^+, \gamma^+ m^-]
\]

and
\[
[s^-, m^-] = [\gamma^- s^-, \gamma^- m^+]
\]

as "nondegenerate" interfaces. A similar result holds for \(i \in [0, T]\) and that \(\gamma^- (T)\) is a condition (102) define an initial traction that has two solutions, or branches, of nondegenerate cases eqn (119) is trivially satisfied but cannot be determined incrementally or continuously if enforced directly.

4.2. Simple laminates

Simple laminates reveal useful insights into the nature of such structures and furnish the basic building blocks that allow for the development of the characteristic dimension of the deformation gradient. Define the characteristic functions
\[
\chi^+ (\xi) = \begin{cases}
0, & \text{if } \xi \in [0, v^- l]
1, & \text{if } \xi \in [v^- l, l]
\end{cases}
\]

\[
\chi^- (\xi) = 1 - \chi^+ (\xi)
\]

with \(v^- \in [0, 1]\). Next extend these characteristic functions with those \(v^+\), \(v^-\), and \(v^0\) to the form (101) satisfied by the corresponding laminate of layer thicknesses \(t\). Let the deformation gradients, rotations and
\[
F_i(t, i) = \chi^+ (x \cdot N) F^+ (i) + \chi^- (x \cdot N) F^- (i) + \chi^0 (x \cdot N) F^0 (i)
\]

\[
F_i(t, i) = \chi^+ (x \cdot N) R^+ (i) + \chi^- (x \cdot N) R^- (i) + \chi^0 (x \cdot N) R^0 (i)
\]

\[
F_i(t, i) = \chi^+ (x \cdot N) (I + v^+ (i)) + \chi^- (x \cdot N) (I + v^- (i)) + \chi^0 (x \cdot N) (I + v^0 (i))
\]

respectively. By construction, this laminate has the characteristic function \(\chi^+ (x \cdot N) = 1\) and \(\chi^- (x \cdot N) = 0\), \(\chi^0 (x \cdot N) = 0\), and the laminate consists of an array of parallel disks.
We shall refer to interfaces such that
\[ [R^+ s^+, R^+ m^+, s^-][R^+ s^+, R^+ m^+, m^-] \neq 0, \]
and
\[ [s^-, m^-, R^+ s^+][s^-, m^-, R^+ m^+] \neq 0 \]  \hspace{1cm} (123)
as “nondegenerate” interfaces. Assuming that the nondegeneracy condition (123) holds for \( \tau \in [0, T] \) and that \( \gamma^-(t) \) is given, then eqns (119), (122) and the initial conditions (102) define an initial value problem for \( \gamma^+(t) \) and \( R^+(t) \). This problem has two solutions, or branches, depending on the choice of sign in eqn (122). In degenerate cases eqn (119) is trivially satisfied and the geometry of the interfaces cannot be determined incrementally. Instead, the jump condition (103) must be enforced directly.

4.2. Simple laminates

Simple laminates reveal useful insights into commonly observed deformation structures and furnish the basic building block for recursive lamination. Let \( L \) be a characteristic dimension of the domain \( \Omega \) of the crystal and let \( l \ll L, \varepsilon = l/L \ll 1 \). Define the characteristic functions \( \chi^\pm(\xi) : [0, l) \rightarrow R \) of the variants as
\[ \chi^+(\xi) = \begin{cases} 0, & \text{if } \xi \in [0, v^-l) \\ 1, & \text{if } \xi \in [v^-l, l) \end{cases} \]  \hspace{1cm} (124)
\[ \chi^-(\xi) = 1 - \chi^+(\xi) \]  \hspace{1cm} (125)
with \( v^- \in [0, 1] \). Next extend these functions to the whole real line by periodicity. In addition, let \( v^+ = 1 - v^- \), so that \( v^+ + v^- = 1 \). Next, consider two deformation histories \( F^+(t) \) of the form (101) satisfying the jump condition (103). Pairs of deformations of this form are exhaustively classified for FCC crystals in Section 5. Then, the corresponding laminate of layer thickness \( l \) and volume fractions \( v^\pm \) is characterized by deformation gradients, rotations and plastic deformations of the form
\[ F(x, t) = \chi^+(x \cdot N)F^+(t) + \chi^-(x \cdot N)F^-(t) \]  \hspace{1cm} (126)
\[ F^+(x, t) = \chi^+(x \cdot N)R^+(t) + \chi^-(x \cdot N)R^-(t) \]  \hspace{1cm} (127)
\[ F^-(x, t) = \chi^+(x \cdot N)(I + \gamma^+(t)s^+ \otimes m^+) + \chi^-(x \cdot N)(I + \gamma^-(t)s^- \otimes m^-) \]  \hspace{1cm} (128)
respectively. By construction, this deformation field is weakly compatible and, consequently, there is a continuous displacement field \( y(x, t) \) whose gradient is \( F(x, t) \) almost everywhere. The average deformation in the laminate is
\[ \mathcal{F}(t) = v^+ F^+(t) + v^- F^-(t) \]  \hspace{1cm} (129)
which is independent of \( \varepsilon \). The dislocation structure corresponding to laminates consists of an array of parallel dislocation walls of the type (104), i.e.,
\[ A(x, t) = \sum_{k=1}^{\infty} \left[ \gamma(t) s \otimes m \right] \times N[\delta(x \cdot N - kl) - \delta(x \cdot N - (v^+ + k)l)] \] (130)

Periodic arrays of dislocation walls of this type are very frequently found in FCC crystals, of Section 5.

Now let the crystal be subject to affine boundary conditions (35) with \( \bar{F}(t) \) given by (129). Clearly, the deformation field (126) is not affine at the boundary and, consequently, fails to be strictly compatible with \( \bar{F} \). Following Ball and James (1987), compatibility can be restored by the introduction of a narrow boundary layer of thickness \( l \). The details of the construction of the boundary layer may be found in Ball and James (1987). Let \( \Omega \) consist of \( \Omega \) with the boundary layer excluded. Then, by construction, the restriction of \( F \) to \( \Omega \) is of the form (126) and the incremental energy density \( W \) remains bounded within the boundary layer as \( \varepsilon \to 0 \), which ensures that \( F^0 = F_{ij} \) defines an incremental energy minimizing sequence.

4.3. Sequential lamination

From a macroscopic viewpoint, lamination effectively enriches the class of average deformation histories which are incremental energy minimizers, from the original class of persistent single slip histories (90) to deformation histories of the form (126). This process of enrichment may be continued recursively, leading to the definition of sequentially laminated microstructures. Treatments of sequential lamination may be found in Kohn and Strang (1986), Kohn (1991), Bhattacharya (1991, 1992) and Pedregal (1993). Experimental evidence of possible sequential lamination in FCC crystals is presented in Section 5.

Uniform deformations may conventionally be categorized as rank-zero laminates. Laminates of rank one have been explicitly defined in Section 4.2. Following Kohn (1991), a laminate of rank-\( r \) is a layered mixture of two rank-(\( r-1 \)) laminates, which affords an inductive definition of laminates of any rank. As noted by Kohn (1991), the construction of sequential laminates assumes a separation of scales: the length scale \( l \), of the rank-\( r \) layering satisfies \( l \ll l_{r-1} \).

Evidently, sequential laminates have a binary tree structure. The nodes of the tree are occupied by deformations histories \( F_i(t) \), \( i = 1, \ldots , n \), where \( n \) is the number of nodes, or order, of the tree. The root deformation is the average deformation history \( \bar{F}(t) \). Each node in the tree has either two children or none at all. Nodes with a common parent are called siblings. Nodes without children are called leaves. Nodes which are not leaves are said to be internal. The deformation histories of the children of node \( i \) will be denoted \( F^{\pm}_i(t) \). Each generation is called a level. The root occupies level 0 of the tree. The number of levels is the rank \( r \) of the tree. Level 0 contains at most \( 2^r \) nodes. The example in Fig. 6(a) represents a rank-three laminate of order eleven. The leaves of the tree are nodes 6–11. The children of, e.g., node 2 are nodes 4 and 5, with \( F^{+}_2(t) = F_4(t) \) and \( F^{-}_2(t) = F_5(t) \). The sequential laminate defined by the tree is shown in Fig. 6(b).

The deformation history \( F_i(t) \) of an internal node \( i \) is an average of the deformation histories \( F^{\pm}_j(t) \) of its children, i.e.,
are very frequently found in FCC

Finally, we consider energy minimizers, from the original form with rank-1 laminates, which may be redefined by assuming that the energy minimizers are now solutions of (35). Following Ball and James (1987), they all have the following form:

$$ (x \cdot N - (\nu + k)f) $$

which is the incremental form of the effective fracture energy. The solution of this equation is not affine at the boundary and, following Ball and James (1987), the effective fracture energy is identified as a narrow boundary layer of width $\varepsilon$. The effective fracture energy may be found in a region where the effective fracture energy is not affine at the boundary layer. Then, using the incremental form (126) and the incremental energy minimizers, we obtain a boundary layer as $\varepsilon \rightarrow 0$, which ensures existence of minimizers.

(b) Sequential Laminates

Sequential laminates are defined in Section 4.2. Following Kohn and Schlömerkemper (1990), sequential laminates are rank-$(r-1)$ laminates, which have the rank $r$. As noted by Kohn (1991), a rank-$r$ laminate is a laminate with a separation of scales: the length of the scale is $k$ and the scale of the structure. The nodes of the tree are numbered $1, 2, \ldots, n$, where $n$ is the number of children of the root. The average deformation history, if any, is defined as the average of the deformation history of the children or none at all. Nodes with no children are leaves. Nodes with children are called leaves. Nodes with children and deformation histories of the children are called levels. The root in the tree is called a level. The root occupies level 0, the leaves occupy level $r$ of the tree. Level 1 contains at least one node, which is a rank-three laminate of order 1. Levels 2 and more are laminates with children of, e.g., node 2 are nodes with no children.

Each level $i$ is an average of the deformation history.
\[ F_l(t) = v_l^- (t) F_l^+ (t) + v_l^+ (t) F_l^+ (t), \quad v_l^- (t) + v_l^+ (t) = 1 \] (131)

It therefore follows that the deformation history \( F_l(t) \) of an \( l \)-level node is the average deformation history of a \((r-l)\)-rank laminate. Additionally, siblings must be rank-one compatible, i.e.,

\[ F_l^+ (t) - F_l^- (t) = a_l (t) \otimes N_l (t), \quad |N_l (t)| = 1 \] (132)

We shall say that a sequential laminate is “persistent” if the interface normals \( N_l \) and volume fractions \( v_l^\pm \) are independent of time. In addition, we shall say that a sequential laminate undergoes persistent single slip if it is persistent and the deformation histories of all of its leaves are of the form (90).

Sequential lamination furnishes a plausibility argument in support of conjecture (93). We begin by considering a time-independent average deformation gradient \( \bar{F} \) and address the question of whether such deformation can be matched on average by a sequential laminate of finite rank in which all leaves deform in single slip. Since single-slip deformations are volume preserving, \( \bar{F} \) must itself necessarily be volume preserving for the laminate to be possible. Evidently, each leaf \( i \) in the laminate introduces the four degrees of freedom \( R_i \) and \( \gamma_i \). Additionally, each internal node \( i \) possesses the additional degree of freedom \( v_i^- \) or \( v_i^+ \), and introduces four rank-one compatibility constraints. Consequently, the number of independent degrees of freedom of the laminate is \( d = 4n_l - 3n_i \), where \( n_l \) is the number of leaves and \( n_i \) is the number of internal nodes. Matching the nine components of \( F \) on average requires \( d \geq 9 \). For a rank-one laminate, \( n_l = 2, n_i = 1, \) and \( d = 5 \). For a complete rank-two laminate, \( n_l = 4, n_i = 3, \) and \( d = 7 \). Thus, two levels of laminate are not sufficient to match an arbitrary average deformation gradient in general. By contrast, the two rank-three laminates shown in Fig. 6, have \( n_l = 6, n_i = 5, \) and \( d = 9 \) as required. It therefore follows that the number of degrees of freedom required to match an arbitrary average deformation gradient may be attained with three levels of laminate.

In general, the condition \( d \geq 9 \) is necessary but not sufficient for the existence of single-slip laminates matching any arbitrary volume-preserving average deformation gradient \( \bar{F} \) on average. Thus, in addition to having a sufficient number of degrees of freedom, the system of nonlinear eqns (131) and (132) in the leaf unknowns \( R_i, \gamma_i \) and the internal node unknowns \( v_i^-, a_i, \) and \( N_i \) must have solutions for arbitrary \( \bar{F} \). Physically, this in turn requires the crystal to possess a large enough class \( \mathcal{S} \) of independent slip systems. The crystallographic flow rule (50) requires five independent slip systems to match an arbitrary volume-preserving rate of deformation, but it is not known to us if this criterion is a sufficient condition for the existence of laminates as well.

Finally, we consider average deformation histories of the form (93) within the framework of linearized kinematics. Within this approximation, single-slip deformation gradients admit the representations: \( F = I + \omega + \gamma \text{sym}(a \otimes m) \), where \( \omega \) is a skewsymmetric tensor representing a small rotation. Let the laminate corresponding to the average deformation \( \bar{F} = I + G \) be determined by \( \omega \) and \( \gamma \), at the leaves, and \( v_l^- \), \( a_l \), and \( N_l \), at the internal nodes. Then, it follows immediately from the structure of equations (131) and (132) that the laminate corresponding to \( F = I + f(t)G \) is determined by \( f(t)\omega \) and \( f(t)\gamma \), at the leaves.

We note that the laminate undergoes persistent single-slip laminae for an average existence of a persistent single-slip slip history of the form \( \bar{F}(t) = I + f(t)G \). The deformation gradient \( \bar{F}(t) \) satisfies the condition (93). This formulation is thus compatible with the experimental observations reported by Smith et al. (1980) and Bilby et al. (1984). The geometry of these observations is illustrated in Fig. 7, where the lattice is represented by the unit cell.

5. Application to fcc crystals

The dislocation structures which are subjected to monotonic and cyclic loadings in the literature and, consequently, provide the basis for the foregoing. We adopt throughout this section the notation of Section 3.2. The slip systems of FCC crystals are described in Table 3.

5.1. Nondegenerate interfaces

We begin by considering interfaces of type \( R^+ \approx I \). Since all the slip systems of the systems meeting at the interface are of general type, for definiteness, we can assume:\n
Then, for each system \( (s^+, m^+) \in \mathcal{S} \) at \( R^+ = I \), leading to a complete set of constraints on the nature of the interface planes. The results of these calculations are summarized in Table 3, carefully noted that the roles of \( [u, r] \) and \( [v, s] \) are interchanged. The nature of the interface planes is now well-defined. The case of a pure shear (Ackermann et al., 1984) is a simplification of the theory of the interface planes.

A common test configuration involves a single crystal in a fatigued single crystal laboratory in a pure shear interface in Tables 2 and 3. In the literature, the highest level of interface is of the \{100\} type, characterized by the following orientations: (Rasmussen and Pedersen, 1982; L’Esperance et al., 1984; Boulander et al., 1985; Dickson, 1981). For instance, interface shown in Fig. 7(a), containing a single crystal that deforms in the [001] direction. The corresponding structure is also evident in Fig. 7(b), where the interface plane is oriented between [001] and [011]. For a [001] crystal such as tested...
We begin by considering interfaces which are nondegenerate at small strains, i.e., for $R^* \approx I$. Since all the slip systems in an FCC crystal are symmetry-related, one of the systems meeting at the interface, e.g., on the $(−)$ side, can be fixed without loss of generality. For definiteness, we choose $(s^{−}, m^{−}) = ([10\bar{1}], (11\bar{1})) \equiv B4$ throughout. Then, for each system $(s^{+}, m^{+}) \in \mathcal{S}$ the nondegeneracy condition (123) may be verified at $R^{+} = I$, leading to a complete enumeration of the nondegenerate interfaces of FCC crystals. The geometry of these interfaces then follows from (120) and (121). The results of these calculations are summarized in Tables 2 and 3. It should be carefully noted that the roles of $[e_{+}]$ and $n$ are interchangeable. The crystallographic nature of the interface planes is noteworthy. As demonstrated subsequently, Tables 2 and 3 is a compendium of commonly observed dislocation walls, which attests to the soundness of the theory.

A common test configuration involves the activation of a pair of orthogonal Burgers vectors in a fatigued single crystal, which corresponds to the B4–A3 and B4–C3 interfaces in Tables 2 and 3. In these cases, the interface normals predicted by the theory are of the $\{10\} \equiv \{10\}$ type, in agreement with experimentally observed wall orientations (Rasmussen and Pedersen, 1980; Lepistõ et al., 1984; Mecke and Blochwitz, 1982; L’Esperance et al., 1986; Ackerman et al., 1984; Wang and Mugharbi, 1984; Boulanger et al., 1985; Dickson et al., 1986a; Jin, 1987; Jin and Winter, 1984a, Charsley, 1981). For instance, Jin and Winter (1984a) have reported the labyrinth structure shown in Fig. 7(a), corresponding to cyclically deformed copper single crystals loaded in the [001] direction. The (010) section of the specimen shown in the figure clearly exhibits traces of (001) and (100) dislocation walls. A similar labyrinth structure is also evident in Fig. 7(b), corresponding to cyclically deformed copper single crystals oriented between [012] and [123], followed by in situ cyclic straining in pure shear (Ackermann et al., 1984).

For a [001] crystal such as tested by Jin and Winter (1984a), Fig. 7(a), the eight

5. Application to fcc crystals

The dislocation structures which arise in FCC single crystals and polycrystals subjected to monotonic and cyclic loading have been extensively documented in the literature and, consequently, provide a convenient test of the theory developed in the foregoing. We adopt throughout the Schmid and Boas nomenclature described in Section 3.2. The slip systems of FCC crystals are enumerated in Table 1.

5.1. Nondegenerate interfaces

We begin by considering interfaces which are nondegenerate at small strains, i.e., for $R^* \approx I$. Since all the slip systems in an FCC crystal are symmetry-related, one of the systems meeting at the interface, e.g., on the $(−)$ side, can be fixed without loss of generality. For definiteness, we choose $(s^{−}, m^{−}) = ([10\bar{1}], (11\bar{1})) \equiv B4$ throughout. Then, for each system $(s^{+}, m^{+}) \in \mathcal{S}$ the nondegeneracy condition (123) may be verified at $R^{+} = I$, leading to a complete enumeration of the nondegenerate interfaces of FCC crystals. The geometry of these interfaces then follows from (120) and (121). The results of these calculations are summarized in Tables 2 and 3. It should be carefully noted that the roles of $[e_{+}]$ and $n$ are interchangeable. The crystallographic nature of the interface planes is noteworthy. As demonstrated subsequently, Tables 2 and 3 is a compendium of commonly observed dislocation walls, which attests to the soundness of the theory.

A common test configuration involves the activation of a pair of orthogonal Burgers vectors in a fatigued single crystal, which corresponds to the B4–A3 and B4–C3 interfaces in Tables 2 and 3. In these cases, the interface normals predicted by the theory are of the $\{10\} \equiv \{10\}$ type, in agreement with experimentally observed wall orientations (Rasmussen and Pedersen, 1980; Lepistõ et al., 1984; Mecke and Blochwitz, 1982; L’Esperance et al., 1986; Ackerman et al., 1984; Wang and Mugharbi, 1984; Boulanger et al., 1985; Dickson et al., 1986a; Jin, 1987; Jin and Winter, 1984a, Charsley, 1981). For instance, Jin and Winter (1984a) have reported the labyrinth structure shown in Fig. 7(a), corresponding to cyclically deformed copper single crystals loaded in the [001] direction. The (010) section of the specimen shown in the figure clearly exhibits traces of (001) and (100) dislocation walls. A similar labyrinth structure is also evident in Fig. 7(b), corresponding to cyclically deformed copper single crystals oriented between [012] and [123], followed by in situ cyclic straining in pure shear (Ackermann et al., 1984).

For a [001] crystal such as tested by Jin and Winter (1984a), Fig. 7(a), the eight
Table 2
Geometry of nondegenerate interfaces between single-slip variants in FCC crystals at small strains (Part A). It should be carefully noted that the roles of \([v, a]\) and \(n\) are interchangeable.

<table>
<thead>
<tr>
<th>System (-) A2/System (+)</th>
<th>B4</th>
<th>B5</th>
<th>C5</th>
<th>C3</th>
<th>D6</th>
<th>D4</th>
<th>D1</th>
<th>C1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\gamma/\gamma')</td>
<td>2/3</td>
<td>2/3</td>
<td>1</td>
<td>3/2</td>
<td>3/2</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>([v, a])</td>
<td>[113]</td>
<td>[2T1]</td>
<td>[101]</td>
<td>[121]</td>
<td>[112]</td>
<td>[100]</td>
<td>[100]</td>
<td>[100]</td>
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<tr>
<td>(n)</td>
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<td>[1T3]</td>
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<td>[3T1]</td>
<td>[1T1]</td>
<td>[1T1]</td>
<td>[1T1]</td>
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</tbody>
</table>

<table>
<thead>
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<th>B2</th>
<th>C5</th>
<th>D6</th>
<th>D4</th>
<th>D1</th>
<th>C1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\gamma/\gamma')</td>
<td>1</td>
<td>3/2</td>
<td>2/3</td>
<td>1</td>
<td>3/2</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>([v, a])</td>
<td>[1F0]</td>
<td>[1T1]</td>
<td>[211]</td>
<td>[121]</td>
<td>[112]</td>
<td>[001]</td>
<td>[111]</td>
<td>[311]</td>
</tr>
<tr>
<td>(n)</td>
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<td>[0T1]</td>
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<td>[3T1]</td>
<td>[3T1]</td>
<td>[0T1]</td>
<td>[0T1]</td>
<td>[0T1]</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>System (-) A6/System (+)</th>
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<th>B5</th>
<th>B2</th>
<th>C5</th>
<th>C3</th>
<th>D4</th>
<th>D1</th>
<th>C1</th>
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</thead>
<tbody>
<tr>
<td>(\gamma/\gamma')</td>
<td>1</td>
<td>3/2</td>
<td>2/3</td>
<td>1</td>
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<td>1</td>
</tr>
<tr>
<td>([v, a])</td>
<td>[010]</td>
<td>[0T1]</td>
<td>[211]</td>
<td>[121]</td>
<td>[112]</td>
<td>[001]</td>
<td>[111]</td>
<td>[311]</td>
</tr>
<tr>
<td>(n)</td>
<td>[111]</td>
<td>[001]</td>
<td>[211]</td>
<td>[121]</td>
<td>[112]</td>
<td>[001]</td>
<td>[111]</td>
<td>[311]</td>
</tr>
</tbody>
</table>

The geometries of the B4–A3, B2–A1, and B5–A1 interfaces are particularly noteworthy, as they conform to the Schmid factor \(\varepsilon = 0.40825\). The interfaces leading to (001) dislocation walls are: B4–C3, B2–C1, A3–D4, and D1–A2; the interfaces giving (100) dislocation walls are: B4–A3, B2–D1, B2–C1, C3–D4, D1–A2, and C1–A2. The geometry of the B4–C3 interface is shown in Fig. 8(a). It is noteworthy that the Burgers vectors involved are mutually orthogonal, a feature that has long been thought to be characteristic of labyrinth structures. Both sets of interfacial dislocations have the common direction [1T1], in accordance with (106). The remaining (001)-interfaces are related to the B4–C3 interface by symmetry operations in the cubic symmetry group which leave the loading direction [001] and the wall plane (001) invariant. Thus, the A2–D1 interface is obtained from the B4–C3 interface by a 90° rotation about the [001] axis; the B2–C1 interface is obtained from the B4–C3 interface by a reflection about the (1T1) plane; and the A3–D4 interface is obtained from the B2–C1 interface by a 90° rotation about the [001] axis.
Table 3
Geometry of nondegenerate interfaces between single-slip variants in FCC crystals at small strains (Part B). It should be carefully noted that the roles of [vₓ] and n are interchangeable.

<table>
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<tr>
<th>System (-) C1/System (+)</th>
<th>B4</th>
<th>B5</th>
<th>B2</th>
<th>A3</th>
<th>D6</th>
<th>D4</th>
<th>A6</th>
<th>A2</th>
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<td>vₓ [-3/2]</td>
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<td></td>
<td></td>
<td></td>
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<td></td>
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<tr>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>n</td>
<td>(110)</td>
<td></td>
<td>(010)</td>
<td></td>
<td>(001)</td>
<td></td>
<td>(111)</td>
<td></td>
</tr>
<tr>
<td>System (-) C3/System (+)</td>
<td>B4</td>
<td>B5</td>
<td>B2</td>
<td>D6</td>
<td>D4</td>
<td>A6</td>
<td>A2</td>
<td></td>
</tr>
<tr>
<td>vₓ [-1]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3/2</td>
<td></td>
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<td></td>
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<tr>
<td>[111]</td>
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<tr>
<td>n</td>
<td>(100)</td>
<td></td>
<td>(111)</td>
<td></td>
<td>(110)</td>
<td></td>
<td>(001)</td>
<td></td>
</tr>
<tr>
<td>System (-) C5/System (+)</td>
<td>B4</td>
<td>B2</td>
<td>A3</td>
<td>D6</td>
<td>D4</td>
<td>A6</td>
<td>A2</td>
<td></td>
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<tr>
<td>vₓ [2/3]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1</td>
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<td>[111]</td>
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<tr>
<td>n</td>
<td>(100)</td>
<td></td>
<td>(111)</td>
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<td>(010)</td>
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<td>(001)</td>
<td></td>
</tr>
<tr>
<td>System (-) D1/System (+)</td>
<td>B4</td>
<td>B5</td>
<td>B2</td>
<td>A3</td>
<td>C5</td>
<td>A6</td>
<td>A2</td>
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<tr>
<td>vₓ [2/3]</td>
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<td>3/2</td>
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<tr>
<td>n</td>
<td>(100)</td>
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<td>(111)</td>
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<td>(010)</td>
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<td>(001)</td>
<td></td>
</tr>
<tr>
<td>System (-) D4/System (+)</td>
<td>B5</td>
<td>B2</td>
<td>A3</td>
<td>C5</td>
<td>A6</td>
<td>C1</td>
<td>A2</td>
<td></td>
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<tr>
<td>vₓ [2/3]</td>
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<td>3/2</td>
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<td>[111]</td>
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<tr>
<td>n</td>
<td>(100)</td>
<td></td>
<td>(111)</td>
<td></td>
<td>(010)</td>
<td></td>
<td>(001)</td>
<td></td>
</tr>
</tbody>
</table>

The geometries of the B4–A3, B2–D1 and B2–C1 interfaces are shown in Fig. 8b–d. As before, the Burgers vectors of the active systems are mutually orthogonal. In the B4–A3 interface, both sets of interfacial dislocations have the common direction [011], in accordance with (106). The B2–D1 and B2–C1 interfaces contain two families of orthogonal screw dislocations along the [011] and [011] directions. The remaining (100)-interfaces are obtained from the B4–A3, B2–D1 and B2–C1 interfaces by the application of symmetry operations in the cubic symmetry group which leave the loading direction [010] and the wall plane (001) invariant. Thus, the C3–D4 and C1–A2 interfaces are obtained from the B4–A3 and B2–D1 interfaces by the application of 180° rotations about the [010] axis; and the D1–A2 interface follows from the B2–C1 interface by the application of a reflection about the (100) plane.

Other theoretically predicted interfaces are also born out by observation. Thus, Jin (1987) observed a labyrinth structure in cyclically deformed copper single crystals loaded in the [011] direction. Figure 9(a) shows a (011)-section of the specimen.
Traces of two sets of dislocation walls along the [100] and [011] directions are clearly apparent in the figure. All dislocation wall traces are of comparable width, which is suggestive of (011) and (100) walls perpendicular to the (011) plane. Jin (1987) noted that the most highly stressed slip planes for this configuration are B4, B5, A3 and A6. Walls of (011) orientation are consistent with B4–A6 and B5–A3 interfaces, while (100)-walls correspond to the B4–A3 and B5–A6 interfaces. A similar structure was observed by Charsley (1981), Fig. 9(b), in polycrystalline copper alloys fatigued to saturation.
Fig. 8. (a) Geometry of the B4–C3 interface, (b) geometry of the B4–A3 interface, (c) geometry of the B2–D1 interface, (d) geometry of the B2–C1 interface.
Fig. 8 (continued)
Fig. 9. Further examples of the labyrinth structure. (a) (0\(\overline{1}\))-section of copper single crystal cycled in the [011] direction, Jin (1987), (b) polycrystalline Cu–Ni alloy fatigued to saturation, Charsley (1981). Reprinted by permission of Publisher.

Observations of Jin (1983) and Jin and Winter (1984b) of dislocation structures on (1\(\overline{1}\)1) foils of a copper single crystal cyclically deformed along the [\(\overline{1}\)12] axis show dislocation wall traces in the [110] and [\(\overline{1}\)12] directions. For this loading axis, the highest resolved shear stresses occur on systems B4 and C1, with a Schmid factor of 0.40825. The two types of B4–C1 interfaces correspond to (1\(\overline{1}\)1) and (110) dislocation walls, Table 2. These walls intersect the (1\(\overline{1}\)) plane along the [110] and [\(\overline{1}\)12] directions, respectively, in agreement with observation. In polycrystalline copper, walls of the {110} type have also been found by Boutin (1983) and by Wang and Mugharbi...
Fig. 10. (101) wall structure in fatigued polycrystalline copper, Wang and Mugharbi (1984). Reprinted by permission of Publisher.

Lepistö et al. (1986) reported wall structures in copper single-crystals cycled in the [T11] direction. In this orientation, the systems B4, B5, C5, D4, D1 and C1 are all potentially active with a common Schmid factor of 0.27217. A (12T) section of the specimen revealed an arrangement of parallel dislocation wall traces in the [101] direction, Fig. 12. These traces are consistent with B4–C5 and D4–C1 interfaces, which give (131) walls; and B4–C1 and C5–D4 interfaces, which result in (1T1) walls. Walls of the {113} type have also been observed by Boutin (1983), Dickson et al. (1986a), Dickson et al. (1986b), Fig. 13(a) and by Liu et al. Yumen (1989) in polycrystalline copper.

5.2. Degenerate interfaces

Next we seek to characterize the degenerate interfaces of FCC crystals. These interfaces fall into three categories: interfaces between coplanar systems with coincident normals \( m^+ = m^- \) and different slip directions \( s^+ \neq s^- \); interfaces between cross-glide systems having coincident slip directions \( s^+ = s^- \) and different normals \( m^+ \neq m^- \); and interfaces involving one single slip system, i.e., such that \( m^+ = m^- \) and \( s^+ = s^- \). In all these cases, eqn (119) is trivially satisfied and the jump condition (103) must be directly enforced in order to ascertain the geometry of the interface.

Pairs of coplanar systems having a common normal satisfy (103) with

\[
R^+ = R^- = R, \quad [\gamma_{\parallel}] = \gamma^+ s^+ - \gamma^- s^-, \quad N = m^+ = m^- = m
\]  \hspace{1cm} (133)

In these interfaces, the slip strains \( \gamma^\pm \) are not constrained by compatibility and may
interfaces of FCC crystals. These interactions with coincidences \( s^+ \neq s^- \); interfaces between \( s^+ = s^- \) and different normals to the slip system, i.e., such that \( m^+ = m^- \) are typically satisfied and the jump condition determines the geometry of the interface.

Normal satisfy (103) with

\[
m^+ = m^- = m
\]

(133)

strained by compatibility and may

---

**Fig. 11.** (11̅1) wall structure in fatigued polycrystalline copper, Yumen (1989). Reprinted by permission of Publisher.

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**Fig. 12.** (12̅1) section of fatigued [11̅1] single crystal showing possible (13̅1) or (11̅1) wall structure, Lepistö et al. (1986). Reprinted by permission of Publisher.
Fig. 13. (a) Detail of fatigued polycrystalline copper showing $\bar{1}01$ walls (region A) and either $\bar{1}12$ or $\bar{1}11$ walls (region B) (Boutin, 1983; Dickson et al., 1986a; Dickson et al., 1986b). (b) Rank-two laminate predicted by the theory. Reprinted by permission of Publisher.

Fig. 14. Cu-1at. % Ge alloy crystal oriented $\bar{3}2\bar{1}$-oriented crystal. (a) Coplanar slip zone configuration due to secondary dislocation. Reprinted by permission of Publisher.
be chosen arbitrarily. Evidently, coplanar interfaces are parallel to the common slip plane. Coplanar slip zones have been observed by Higashida et al. to form during the stage I of hardening in a Cu-1at %Ge single crystal loaded in monotonic tension near the [321] direction, Fig. 14(a). For a crystal in this orien-

Fig. 14. Cu-1at %Ge alloy crystal oriented near [321] and deformed monotonically to 30% strain, Higashida et al. (1986). (a) Coplanar slip zones revealed by etch pits on the conjugate plane, (b) etch pit configuration due to secondary dislocations in the vicinity of kink bands. Reprinted by permission of Publisher.
tation, the primary slip system is C3, with a Schmid factor of 0.46657. However, Higashida et al. (1986) observed that the systems C1 and C5 are predominantly active in coplanar slip zones, while the activity of the more loaded primary system C3 is largely inhibited. Indeed, the joint activation of the C1 and C5 systems does result in an energetic advantage over the activation of system C3, as demonstrated subsequently in Section 5.3.

Similarly, pairs of cross-glide systems having a common slip direction satisfy (103) with

\[
R^+ = R^- \equiv R, \quad [\gamma_{xy}] = \|\gamma^+ m^+ - \gamma^- m^-\| s, \quad N = \frac{\gamma^+ m^+ - \gamma^- m^-}{\|\gamma^+ m^+ - \gamma^- m^-\|} \tag{134}
\]

where we write \( s \equiv s^+ = s^- \). As in the coplanar case, the slip strains \( \gamma^\pm \) are not constrained by compatibility and may be chosen arbitrarily.

Finally, we consider interfaces involving nontrivial rank-one connections of a slip system with itself. Evidently, a class of interfaces of this type can be constructed as in the coplanar case, leading to

\[
R^+ = R^- \equiv R, \quad [\gamma_{xy}] = (\gamma^+ - \gamma^-) s, \quad N = m \tag{135}
\]

It should be noted that in this case the plastic deformation \( F^{\pm} \) are themselves rank-one compatible and, in view of (104), the interfaces are free of dislocations. The dislocations are either pushed out to infinity or bind tightly to form dense walls of zero net Burgers vector, such as the rungs in the ladder structure which arises in single crystals oriented for single slip and fatigued to saturation, Fig. 15. Such walls are invisible within the present continuum description of dislocations, and regions of the crystal containing them are indistinguishable from the defect-free crystal.

The matrix-persistent slip band (PSB) boundaries in cyclically deformed single crystals oriented for single slip constitute a prime example of this type of interface (e.g., Mugharbi et al., 1979; Wang and Mugharbi, 1984). Fig. 15. The planes of the PSBs are ostensibly parallel to primary slip plane, in accordance with (135). It bears emphasis, however, that the inhomogeneous character of slip in this structure cannot be explained on the basis of latent hardening, as only one system is kinematically necessary to match the average strain. An alternative explanation may be based on the geometrical softening phenomenon discussed in Section 3.4. We shall return to this question in Section 5.3.

A complementary class of single-system interfaces can be constructed as follows. Choose the interface normal \( N = s \), i.e., any vector of type \( \langle 100 \rangle \), and impart slip strains \( \gamma^\pm = \pm \tan \theta \) on both sides of the interface, Fig. 16(a). Restore compatibility by effecting rotations \( R^\pm = Q R(s \times m; \pm \theta) \). Here, the notation \( R(e; z) \) is used to denote a rotation about an axis \( e \) through and angle \( z \), and \( Q \) is an arbitrary rotation. Since the planes on both sides of the interface remain unstretched along the \( s \times m \) direction and stretch by the same amount in the \( m \) direction, the rotated crystals fit compatibly, Fig. 16(b). The resulting deformations are

\[
F^{\pm} = Q R(s \times m; \pm \theta)[I \pm \tan \theta s \otimes m] \tag{136}
\]

Thus the variant deformations correspond to

\[
[I \pm \tan \theta m \otimes s][\cos \theta \otimes \mp s + \sec \theta m] = 2 \sin \theta Q m, \quad N = s
\]

The deformations (136) of the variant
amid factor of 0.46657. However, C1 and C5 are predominantly active. The more loaded primary system C3 is the C1 and C5 systems does result in an independent C3, as demonstrated subsequently in Section 3.4. Common slip direction satisfy (103)

\[ N = \frac{\gamma^+ m^+ - \gamma^- m^-}{\|\gamma^+ m^+ - \gamma^- m^-\|} \]  

In this case, the slip strains \( \gamma \) are not arbitrary.

Irregular rank-one connections of a slip surface of this type can be constructed as in (135)

\[ F^\pm \] are themselves rank-one deformation, and walls are dislocations which are free of dislocations. The blame for this is the formation of dense walls of dislocations which arises in single saturation, Fig. 15. Such walls are free of dislocations, and regions of the crystal are dislocation-free crystal.

Figures in cyclically deformed single crystals in accordance with (135). It bears out that only one system is kinematically equivalent explanation may be based on the definition of Section 3.4. We shall return to this point.

Fig. 15. Views of the (121) section of Cu crystals oriented for single slip and fatigued to saturation at room temperature revealing matrix and persistent slip bands (PSB). (a) From Mugharhi et al. (1979), (b) from Wang and Mugharbi (1984). Reprinted by permission of Publisher.

\[ j^N = 2 \sin \theta Qm, \quad N = s \]  

The deformations (136) of the variants can alternatively be rewritten as

\[ F^\pm = Q[\cos \theta s \otimes s + \sec \theta m \otimes m + (s \times m) \otimes (s \times m)] [I \pm \sin \theta \cos \theta m \otimes s] \]

\[ = Q[I \pm \tan \theta m \otimes s][\cos \theta s \otimes s][\cos \theta s \otimes s + \sec \theta m \otimes m + (s \times m) \otimes (s \times m)] \]

Thus the variant deformations consist of the composition of slip strains of magnitude
\[ \gamma = \pm \sin \theta \cos \theta \text{ on the plane of normal } s \text{ in the direction } m, \]

followed by stretches of magnitude \( \cos \theta \) and \( \sec \theta \) in the directions \( s \) and \( m \), respectively, followed by an arbitrary rotation \( Q \); or, equivalently, the composition of stretches of magnitude \( \cos \theta \) and \( \sec \theta \) in the directions \( s \) and \( m \), respectively, followed by slip strains of magnitude \( \gamma = \pm \tan \theta \) on the plane of normal \( s \) in the direction \( m \), followed by an arbitrary rotation \( Q \). The dislocation density tensor (104) evaluates to

\[ A(x) = 2 \tan \theta s \otimes (s \times m) \delta_1(x) \]

which represents a planar array of parallel edge dislocations, or tilt boundary.

This type of interface arises in the so-called "fence" structures observed during the early stages of stage II of hardening in FCC crystals (Steeds, 1966), Fig. 17. Because

\[ \gamma = \|v^+ \gamma^+ s^+ + v^- \gamma^- s^-\|, \]

the dislocation walls are normal to, sometimes termed "kinks", and the dislocation walls (Higashida et al., 1986). Higashida et al. observed that at the onset of stage II of hardening in monotonic tension near the [321] orientation, the primary slip systems of the kink bands were revealed by deforming the specimen.

Fig. 16. Schematic of kink formation. (a) Slip strains \( \gamma^+ = \pm \tan \theta \), (b) rotations through \( \pm \tan \theta \).

5.3. Simple laminates

By lamination of single-slip variants of the deformation \( \dot{F} \) while remaining essentially parallel, for coplanar variants the average deformation

\[ \dot{F} = R(I + \gamma s \otimes m) \]

with

\[ \gamma = \|v^+ \gamma^+ s^+ + v^- \gamma^- s^-\|, \]

This represents a single-slip deformation in direction \( s \). Evidently, by varying the fractions \( v^\pm \), any effective slip direction of coplanar laminates effectively extends all systems \( (s, m) \) consisting of a cut through \( m \).

As noted in Section 5.2, coplanar dislocation walls loaded in monotonic tension near the [321] orientation, the slip direction gives rise to the maximum Schmid factor direction of a prescribed deformation, which is close to atomistic results (38). Higashida et al. observed that slip was predominantly active in nearly equal slip directions [527] and that the ability of coplanar slip zones to exhibit an energetic advantage which

Likewise, for cross-slip variants of the deformation of the laminate is of the form

\[ \gamma = \|v^+ \gamma^+ m^+ + v^- \gamma^- m^-\|, \]
the dislocation walls are normal to the primary slip direction, eqn (137), they are sometimes termed “kinks”, and the resulting deformation structures “kink bands” (Higashida et al., 1986). Higashida et al. (1986) observed the emergence of kink bands at the onset of stage II of hardening in a Cu-1at.%Ge single crystal loaded in monotonic tension near the [321] direction. As noted above, for a crystal in this orientation, the primary slip system active is C3. In a (111)-section of the specimen, the kink bands were revealed by dense etch-pit arrays normal to the Burgers vector, Fig. 14(b).

5.3. Simple laminates

By lamination of single-slip variants, crystals can attain a larger class of average deformations \( \mathbf{F} \) while remaining essentially free of long-range stresses. For instance, for coplanar variants the average deformation of the corresponding laminate is

\[
\mathbf{F} = R(I + \gamma s \otimes m)
\]

with

\[
\gamma = \|v^+\gamma^+s^+ + v^-\gamma^-s^-\|, \quad s = \frac{v^+\gamma^+s^+ + v^-\gamma^-s^-}{\|v^+\gamma^+s^+ + v^-\gamma^-s^-\|}
\]

This represents a single-slip deformation on the common plane \( m \) in the effective slip direction \( s \). Evidently, by varying the slip activities \( \gamma^\pm \) of the systems and their volume fractions \( v^\pm \), any effective slip direction \( s \) orthogonal to \( m \) can be achieved. Thus, coplanar laminates effectively extend the crystallographic slip-system set \( \mathcal{S} \) to include all systems \((s, m)\) consisting of a cube diagonal \( m \) and any direction \( s \) orthogonal to \( m \).

As noted in Section 5.2, coplanar slip zones have been observed by Higashida et al. (1986) to form during the stage I of hardening in a Cu-1at.%Ge single crystal loaded in monotonic tension near the [321] direction, Fig. 14(a). For a crystal in this orientation, the slip direction giving the maximum Schmid factor is [527] which, evidently, is not a crystallographic slip direction. It should be noted that slip in the maximum Schmid factor direction minimizes the work \( W \) required to attain a given prescribed deformation, which in turn is in accordance with the minimum principle (38). Higashida et al. observed that the primary coplanar slip systems C1 and C5 are predominantly active in nearly equal amounts in the coplanar slip zones. The optimal slip direction [527] can be effectively attained as in eqn (142) through the combined operation of the systems C1 and C5 with \( \gamma_{C1} = \gamma_{C2} \) and \( \nu_{C1} = 7/12, \nu_{C5} = 5/12 \). This ability of coplanar slip zones to effectively match the optimal slip direction confers them an energetic advantage which explains their occurrence in actual crystals.

Likewise, for cross-glide variants having a common Burgers vector the average deformation of the laminate is of the same form (133) with

\[
\gamma = \|v^+\gamma^+m^+ + v^-\gamma^-m^-\|, \quad m = \frac{v^+\gamma^+m^+ + v^-\gamma^-m^-}{\|v^+\gamma^+m^+ + v^-\gamma^-m^-\|}
\]
Thus, the average deformation is of the single-slip type on the effective plane \( m \) along the common slip direction \( s \). By varying the slip activities \( \gamma^\pm \) of the systems and their volume fractions \( v^\pm \), any effective normal \( m \) orthogonal to \( s \) can be achieved and, consequently, cross-glide laminates effectively extend the crystallographic slip-system set \( \mathcal{S} \) to include all systems \((s,m)\) consisting of a cube-face diagonal \( s \) and any normal \( m \) orthogonal to \( s \).

Finally, we turn to single-system laminates. We begin by considering the “slip-bond” geometry in which the interfaces are parallel to the slip plane. As noted in Section 5.3, a prime example of this type of laminated is furnished by the matrix-PSB structure characteristic of single crystals oriented for single slip and fatigued to saturation (Ng, Mugharbi et al., 1979; Wang and Mugharbi, 1984), Fig. 15. In this microstructure, the average deformation is carried almost completely by the PSB's, and the matrix remains nearly undeformed by comparison. The average deformation is again of the form (141), with

\[
\gamma = v^+ \gamma^+ + v^- \gamma^-
\]

(144)

where \( v^\pm \) and \( \gamma^\pm \) are the volume fractions and slip strains in the matrix and PSB. A similar deformation pattern is observed in the form of slip bands during the stage I hardening of most FCC crystals (Fourie and Wilsdorf, 1959). Equation (144) is the basic kinematic relation underlying the so-called “two-phase model” of cyclic deformation (Wintz, 1974).

Evidently, slip-band structures cannot be caused by latent hardening, as only one system is in operation in those structures. A plausible alternative mechanism is geometrical softening, Section 3.4, which results in the up-down-up stress-strain curve characteristic of displacive phase transitions, Fig. 2(b). Under these conditions, the work of deformation of the crystal is minimized by the development of two phases—the matrix and the bands—which jointly operate at the Maxwell stress (Ericksen, 1980). This stress is determined by the equal-area rule, i.e., the two regions demarcated by the Maxwell line and the stress-strain curve must be identical, Fig. 2(b). We note that the Maxwell stress may be considerably lower than that required for the operation of the slip system. The strains of the phases are those corresponding to the intersections of the Maxwell line with the ascending, or stable, parts of the stress–strain curve. In crystals which are elastically stiff, the matrix strain determined by this construction is small, in keeping with observation (Mugharbi, 1978), and approaches zero in the rigid–plastic limit. The volume fractions of the two phases follow from Gibbs rule.

For kink interfaces, the average deformation follows from (138) and (139) in the form

\[
F = Q[\cos \theta s \otimes s + \sec \theta m \otimes m + (s \times m) \otimes (s \times m)]
\]

\[
[1 + (v^+ - v^-) \sin \theta \cos \theta m \otimes s] = Q[I + (v^+ - v^-) \tan \theta m \otimes s]
\]

\[
[\cos \theta s \otimes + \sec \theta m \otimes m + (s \times m) \otimes (s \times m)]
\]

(146)

where, as before, \( v^\pm \) are the volume fractions occupied by the + and − variants,

respectively, with \( v^+ + v^- = 1 \). It follows that deformation which can be attained by such a combination of a slip strain of magnitude \( s \) in the direction \( m \), followed by stresses \( s \) and \( m \), respectively, followed by a composition of stretches of magnitude \( \pm \theta \) in both variants, for which both variants are mixed, deformation takes the form: 

\[
\mathcal{F} = \{\cos \theta, \sec \theta, 1\} \text{ and principal rotation. A clear example of this is observed during the early stages of stage II}
\]

17. The alternating ±\( \theta \) misorientations of the theory, eqn (136), are evident in the

As noted in Section 4.2, the dislocation network consists of an array of parallel dislocation walls, with the exception of assemblage of flat sheets, as observed to occur in roughly parallel sets of lamina. In the case of polycrystals, which inevitably develop, as noted in Section 4.3, the slip requires several levels of lamina, more likely to arise in polycrystals.

The geometry of the dislocation structure is a much in the same way as the geometry of the climb. We begin by analyzing the fine laminae, which are of roughly equal thickness, in the specimen of orthogonal to both sets of planes \( (110) \) are \( (121) \) in polycrystal A and
respectively, with \( v^+ + v^- = 1 \). It follows from (145) and (146) that the average deformation which can be attained by a single-system laminate consists of the composition of a slip strain of magnitude \( \gamma = (v^+ - v^-) \sin \theta \cos \theta \) on the plane of normal \( s \) in the direction \( m \), followed by stretches of magnitude \( \cos \theta \) and \( \sec \theta \) in the directions \( s \) and \( m \), respectively, followed by an arbitrary rotation \( Q \); or, alternatively, the composition of stretches of magnitude \( \cos \theta \) and \( \sec \theta \) in the directions \( s \) and \( m \), respectively, followed by a slip strain of magnitude \( \gamma = (v^+ - v^-) \tan \theta \) on the plane of normal \( s \) in the direction \( m \), followed by an arbitrary rotation \( Q \). In the special case in which both variants are mixed in equal proportions, i.e., \( v^+ = v^- \), the average deformation takes the form: \( \bar{F} = QU \), where \( U \) is a stretch tensor with principal stretches \( \{\cos \theta, \sec \theta, 1\} \) and principal directions \( \{s, m, s \times m\} \), and \( Q \) is an arbitrary rotation. A clear example of this type of lamination is the fence structures observed during the early stages of stage II of hardening in FCC crystals (Steeds, 1966), Fig. 17. The alternating \( \pm \theta \) misorientations about an axis in the slip plane predicted by the theory, eqn (136), are evident in the figure.

As noted in Section 4.2, the dislocation structure corresponding to first-order laminates consists of an array of parallel dislocation walls of the type (130). With the exception of labyrinth structures, all the dislocation walls discussed in Section 5.3 are observed to occur in roughly parallel arrays and, therefore, provide further examples of lamination, see Figs 10–11(a), 14, 15, 17.

### 5.4. Sequential laminates

A few of the dislocation structures reported in the literature may arguably be interpreted as instances of sequential lamination. For instance, Fig. 18 shows a detail of an interior grain in a polycrystalline copper specimen tested in fatigue by Rasmussen and Pedersen (1980). A set of nearly horizontal fine laminates occupying nearly vertical parallel bands separated by other bands of cell structures is clearly visible in the figure, which would appear to furnish an example of a rank-two laminate. Another seeming example of a rank-two laminate is revealed by Fig. 13(a), which shows a region of extended wall structure observed by Boutin (1983) in a fatigued polycrystalline copper. The structure consists of \((101)\) walls (region A) and either \((112)\) or \((112)\) walls (region B). These two types of laminates may be seen to occupy roughly horizontal alternating bands in Fig. 13(a), which may be regarded as defining the first level of the laminate. It is interesting to note that both examples correspond to polycrystals, which inevitably develop complex deformations at the single grain level. Indeed, as noted in Section 4.3, the accommodation of general deformations by single slip requires several levels of lamination and, consequently, sequential laminates are more likely to arise in polycrystals.

The geometry of the dislocation structure shown in Fig. 13(a) may be ascertained much in the same way as the geometry of interfaces was determined in Section 4.1. We begin by analyzing the fine laminates A and B. Since the wall traces in Fig. 13(a) are of roughly equal thickness, it seems reasonable to presume that the section of the figure of orthogonal to both sets of walls, i.e., a \((1\overline{1}1)\) section. The wall traces on the \((1\overline{1}1)\) are [121] in laminate A and [110] in laminate B. Interfaces leading to \((101)\) walls
degrees of freedom $\tilde{R}^{-}(R^{-})^{-1}$ and $\tilde{\gamma}^{-}$. This leaves four resulting from (111). This leaves for $\tilde{R}^{-}(R^{-})^{-1}$ and $\tilde{\gamma}^{-}$. The average degrees of freedom from relations (111), (119), (120), $\varepsilon_{\Lambda}^{A}(\varepsilon_{\Lambda}^{A})^{-1}$ and $\varepsilon_{\Lambda}^{B}$. In computing $\nu^{-} = \nu^{+} = 1/2$, as suggested by the number of degrees of freedom, e.g., $\varepsilon_{\Lambda}^{A}(\varepsilon_{\Lambda}^{A})^{-1}$ and $\varepsilon_{\Lambda}^{B}$, deformation rates $\varepsilon_{\Lambda}^{A,B}$ are subject to replacements four constraints which suffice of these equations is now identical to equations of the form (120) and A straightforward calculation gives which on the (111) plane is $[-1.06\, 1.06]$ and $[0.1, 0, 5]$. The geometry predicts agreement between theory and observations considerable irregularities and uncertainties. It is conceivable that a better agreement, considering a different combination pursued here.

It is interesting to note that the transition layers separating regions of the wall spacing in the deformations of the A and B bands may to prevent long-range stresses, the introduction of elastically strained regions of the microstructure, which tend to increase the layers, and the self-energy of the dislocation, is addressed in the next section.

6. Dislocation self-energy and scalar strain

The precise manner in which resistances and cell sizes, scale with various considerable study. For instance, based on the assumption of "similar a stress $\tau$ will be stable under a stress by Staker and Holt (1972) and has $\tau_{c}$ (Staker and Holt, 1972; Kuhlman-Winter and Merve, 1982; Holt, 1970). A of materials and deformations, study of the mean dislocation line density.

Fig. 18. Nested bands of wall structure in a matrix of disoriented cells in polycrystal Cu fatigued to saturation, Rasmussen and Pedersen (1980). Reprinted by permission of Publisher.

are A2--C5 and A6--C1; interfaces resulting in (T12) walls are A6--D1 and A6--D4; and interfaces giving (T13) walls are C5--D1 and B5--D4. Assume that the walls in the B laminate are of the (T12) type and that the A and B interfaces are A6--C1 and A6--D4, respectively. As noted in Section 4.1, each of the A and B laminates has the eight
degrees of freedom \( \mathbf{R}^{\pm}(\mathbf{R}^{\pm})^{-1} \) and \( \gamma^{\pm} \), and is subject to four compatibility conditions resulting from (111). This leaves four effective degrees of freedom per laminate, e.g., \( \mathbf{R}^{-}(\mathbf{R}^{-})^{-1} \) and \( \gamma^{-} \). The average deformation rates \( I_{A,B} \) of laminates A and B follow from relations (111), (119), (120) and (121) in terms of the degrees of freedom \( \tilde{R}_{\chi,\nu}(\tilde{R}_{\chi,\nu})^{-1} \) and \( \tilde{\gamma}_{\chi,\nu} \). In computing averages, we assume equal volume fractions \( v^{-} = v^{+} = 1/2 \), as suggested by the widths of the variants in Fig. 13(a). Four degrees of freedom, e.g., \( \tilde{R}_{\chi}(\tilde{R}_{\chi})^{-1} \) and \( \tilde{\gamma}_{\chi} \), can be fixed without loss of generality. The deformation rates \( I_{A,B} \) are subject to the rank-one compatibility condition (111). This places four constraints which suffice to determine \( \tilde{R}_{A}(\tilde{R}_{A})^{-1} \) and \( \tilde{\gamma}_{A} \). The treatment of these equations is now identical to that given in Section 4.1 to interfaces, leading to equations of the form (120) and (121) giving the orientation of the A–B interface. A straightforward calculation gives \( n_{A,B} = (0.534523, 0.801785, 0.267262) \), the trace of which on the (111) plane is \([-1.06904, 0.267262, 1.33631] \), or, approximately \((2, 3, 1)\) and \([4, 1, 5]\). The geometry predicted by the theory is shown in Fig. 13(b). The agreement between theory and observation may be deemed satisfactory in view of the considerable irregularities and uncertainty in the experimentally observed structure. It is conceivable that a better agreement with experiment might be obtained by considering a different combination of interfaces, but such a possibility will not be pursued here.

It is interesting to note that the dislocation walls bend or split within narrow transition layers separating regions A and B. The thickness of these layers is of the order of the wall spacing in the second-level fine laminates. While average deformations of the A and B bands may be expected to be rank-one compatible, as required to prevent long-range stresses, the strict compatibility within the bands requires the introduction of elastically strained boundary layers. The trade-off between refinement of the microstructure, which tends to decrease the elastic energy in the boundary layers, and the self-energy of the dislocation walls, which tends to increase with refinement, is addressed in the next section.

6. Dislocation self-energy and scaling

The precise manner in which microstructural dimensions, such as laminate thicknesses and cell sizes, scale with various macroscopic variables has been the subject of considerable study. For instance, a widely accepted theory of cell size evolution is based on the assumption of “similitude”, i.e., to wit, that a structure which is stable under a stress \( \tau \) will be stable under a stress \( 2\tau \) when shrunk to one-half its size. This similitude conjecture has been verified experimentally for a number of materials (Hansen, 1969; Staker and Holt, 1972) and has been justified on the basis of energy minimization (Staker and Holt, 1972; Kuhlmann-Wilsdorf, 1970; Kuhlmann-Wilsdorf and van der Merwe, 1982; Holt, 1970). Another scaling relation which holds for a wide range of materials and deformations states that the flow stress \( \tau \) scales with the square root of the mean dislocation line density \( \rho \) (Otte and Hren, 1966; Mecking and Kocks,
This law, in conjunction with similitude, implies that the dislocation cell size scales as $1/\sqrt{\rho}$.

The theory developed in the foregoing is purely local, i.e., it lacks an intrinsic length scale. As a consequence, the local theory furnishes no information regarding absolute microstructural dimensions or scaling laws such as just described. While a detailed study of these issues is beyond the scope of the present paper, it is nevertheless of some immediate interest to demonstrate how the local theory can be extended in a physically meaningful manner so as to incorporate an intrinsic length scale compatible with the crystal lattice parameter. In the local theory, dislocations are regarded as being continuously distributed with density $A(x)$ given by (96). The free energy density is given by (42) which accounts for the long-range elastic distortions of the lattice and, therefore, suffices to compute the dislocation interaction energy. However, the free energy density (42) does not account for the self-energy of the dislocations. Indeed, this energy scales with the dislocation length, the estimation of which requires the consideration of discrete dislocation lines and, consequently, an explicit acknowledgement of the discreteness of the lattice.

A nonlocal extension of the theory can be obtained—in the spirit of the so-called “sharp-interface” approximation (Modica, 1987; Sternberg, 1988)—simply by adding to the free energy density (42) the self-energy density of the dislocations, which we proceed to calculate. On the scale of the lattice, plastic slip occurs on discrete crystallographic planes in integer multiples of the Burgers vector (Fonseca, 1987, 1988; Chipot and Kinderlehrer, 1988). Consider a dislocation loop $C$ of Burgers vector $b$ on a slip plane of normal $m$. For simplicity, suppose that the crystal has slipped by $b$ over the area $\Sigma$ of the slip plane bounded by $C$. The corresponding microscopic plastic deformation is

$$F^p = I + b \otimes m \delta(x \cdot m)$$

where $\Sigma$ is the characteristic function of $\Sigma$ on the slip plane $x \cdot m = 0$. Inserting this expression into (96), a straightforward calculation gives

$$A(x) = b \otimes (v \times m) \delta_C(x)$$

where $v$ is the unit normal to $C$ within the slip plane and $\delta_C(x)$ is the Dirac delta supported on $C$. The dislocation length contained in a volume $\Omega$ of the crystal is, therefore,

$$L = \int_\Omega \frac{|A|}{|b|} \, dx$$

Let $T$ denote the dislocation self-energy per unit length, or dislocation line tension. Assume, for simplicity, that $T$ is independent of the orientation of the dislocation line. A commonly used expression for $T$ is Kuhlmann-Wilsdorf (1989):
implies that the dislocation cell size is local, i.e., it lacks an intrinsic length. No information regarding absolute size is just described. While a detailed present paper, it is nevertheless of local theory can be extended in a finite an intrinsic length scale compared to the local theory, dislocations are density $A(x)$ given by (96). The free energy of the long-range elastic distortions is the dislocation interaction energy, which accounts for the self-energy of the dislocation length, the estimation of annihilation lines and, consequently, an atom lattice.

Therein—in the spirit of the so-called (Attenberg, 1988)—simply by adding density of the dislocations, which form, plastic slip occurs on discrete Burgers vector (Fonseca, 1987), a dislocation loop $C$ of Burgers vector, suppose that the crystal has occurred by $C$. The corresponding slip plane $x,m = 0$. Inserting this gives

(147)

(148)

(149)

plane and $\delta_{r}(x)$ is the Dirac delta in a volume $\Omega$ of the crystal is,

(150)

where $\mu$ is an average shear modulus and $C$ is a constant of the order of 0.3. The assumption of a well-defined line tension permits writing the self-energy of the dislocations as

$$T = C\mu|b|^{2}$$

which, in view of (96), can be put in the form

$$E_{\text{self}} = \oint_{\Omega} \frac{T|A|}{|b|} \, dx$$

(151)

(152)

In this simple model, the self-energy density is

$$\phi_{\text{self}}(F^{p} \times \nabla) = \frac{1}{|b|} |F^{p} \times \nabla|$$

(153)

and the total free energy density follows from (42) and (153) as

$$\phi_{\text{total}} = \phi_{\text{F}}(F^{p-1},y) + \phi_{\text{self}}(F^{p} \times \nabla)$$

(154)

which replaces (42). By way of example, consider a planar interface $\Pi$ separating two uniformly deformed regions of the crystal. In view of (104), the corresponding self-energy density is

$$\phi_{\text{self}}(x) = \frac{T}{|b|} |[F^{p}] \times N| \delta_{\Pi}(x)$$

(155)

Thus, the scalar

$$\Gamma = \frac{T}{|b|} |[F^{p}] \times N|$$

(156)

plays the role of a surface energy for the interface. This is in close analogy to crystallographic twinning, where a surface energy can be assigned to the twin boundaries. We note that, in view of (150) and (156), the surface energy $\Gamma$ vanishes in the formal limit of $|b| \to 0$.

Evidently, the self-energy $\phi_{\text{self}}(F^{p} \times \nabla)$ depends on the plastic deformation gradient and its inclusion in (154) renders the theory nonlocal. While in the local theory a periodic microstructure $F^{p}(x)$ can be scaled to $F^{p}(x/\xi)$ without affecting the energy density, the self-energy density is magnified by a factor of $1/\xi$. Thus, in the nonlocal theory an energy cost is incurred when the scale of the microstructure is refined. This type of energy trade-offs have been extensively investigated in other contexts such as the mathematical theory of martensitic transformations (Ball and James, 1987), and thin films (Giota and Ortiz, 1994). In particular, Kohn and Müller have shown that
surface energy (Kohn and Müller, 1992), in addition to setting an absolute length scale, can also influence the morphology of the microstructures, e.g., by promoting twin branching.

Dislocation walls in parallel arrays are often observed to be fairly uniformly spaced at a distance \( l \) of the order of 1 \( \mu \text{m} \). Consideration of the dislocation self-energies yields a simple estimate of \( l \). For simplicity, we assume that the geometry of the interfaces is not affected by the dislocation self-energy. From the standpoint of the local theory, a dislocation structure such as shown in Fig. 13(a) may be regarded as a member of a minimizing sequence \( E_{\varepsilon}(x) \) of compatible deformations, with \( \varepsilon = l/L \) and \( L \) a characteristic macroscopic dimension of the crystal such as the grain size. As mentioned earlier, compatibility between two laminates, or between a laminate and the boundary, generally requires the introduction of boundary layers of thickness \( \sim l \) at their interface. The elastic energy in these boundary layers is of the order of \( \mu \gamma^{2} L^{3} l \), where \( \gamma \) is a representative slip strain. From (150) and (156), the surface energy density \( \Gamma \) is of the order of \( C_{\mu} \mu \gamma^{2} / l \), while the surface energy of the crystal is of the order of \( C_{\mu} \mu [b] \gamma L^{3} / l \). Assuming additivity of energies, the total energy of the crystal follows as

\[
E_{\text{total}} = C_{1} \mu \gamma^{2} L^{3} l + C_{2} \mu [b] \gamma L^{3} / l \quad (157)
\]

for some constants \( C_{1} \) and \( C_{2} \) of order unity. Minimization of \( E_{\text{total}} \) with respect to \( l \) gives

\[
l = C_{3} \sqrt{|b| L / \gamma} \quad (158)
\]

whereupon (157) becomes

\[
E_{\text{total}} = C_{4} \mu \sqrt{|b| \gamma^{3/2} L^{5/2}} \quad (159)
\]

for some constants \( C_{3} \) and \( C_{4} \) of order unity.

The scaling law \( l \sim \gamma^{-1/2} \) is consistent with observations of the dependence of cell sizes on the applied strain (Bassim and Klassen, 1986). The scaling laws \( l \sim L^{3/2}, E_{\text{total}} \sim L^{5/2} \) were derived by Ball and James for martensite and can be improved by a self-similar construction involving branching (Ball and James, 1987; Kohn and Müller, 1992). Using \( |b| = 2.56 \times 10^{-10} \text{ m}, \gamma = 2.5 \times 10^{-3} \text{ and } L = 10^{-5} \text{ m}, \) as representative of fatigue in copper, (158) gives \( l \sim 10^{-6} \text{ m}, \) which is in the ballpark of experimental observation.

7. Summary and discussion

Dislocation structures have been variously investigated by considering ensembles of discrete dislocations and minimizing their interaction energy (Neumann, 1986;

Lubarda et al., 1993); or by seeking a condition (Frank, 1950; Hirth and Lothe, 1960) pursued a different line of inquiry based on the Euler equation. These methods seek to characterize solutions as solutions of the Euler equation with the majority of investigations. The primary emphasis on deformation theory of the manifestations of the incompatibility of crystal plasticity, the energy function of single slip deformations. This favored approach has been shown to be in correspondence with various deformation microstructural studies. Several deformation microstructures that have been shown to be in correspondence with the theory by taking into account the scale of are in agreement with observation.

It is noteworthy that the fundamental dislocation structures is the lack of increases. The connection between lack of increase and is presently well-established in a number of studies, micromagnetics, liquid a, surface tension, existence of the energy function has turned out to be existence of uniqueness of solutions placed on a misunderstanding about the nature of micromechanical applications, it has the fundamental problem and, consequently, guarantees conditions (e.g., Dacorogna, 1989). For, in theory, the energy function is to be microstructural development concept, in which Drucker's postulates. This new concept, departure from classical plasticity.

A number of open questions remain with us what rules—if any—governing whether cell structures may also be. The determination of energy-minimizing single slip, in addition to, it would be a question of a mathematical investigation of the microstructure.
Lubarda et al., 1993); or by seeking dipolar walls satisfying Frank’s minimum energy condition (Frank, 1950; Hirth and Lothe, 1968; Bilde-Sorensen, 1986). Here we have pursued a different line of inquiry based on direct methods of the calculus of variations. These methods seek to characterize solutions directly as energy minimizers, instead of as solutions of the Euler equations of the energy functional. We part company with the majority of investigations of low energy dislocation structures by placing primary emphasis on deformation microstructures and regarding the dislocations as manifestations of the incompatibility of the plastic deformation gradient field. Within this framework, we show that the incremental displacements of inelastic solids follow as minimizers of a suitably defined pseudoelastic energy function. In crystals exhibiting latent hardening, the energy function is nonconvex and has wells corresponding to single slip deformations. This favors microstructures consisting locally of single slip. Several deformation microstructures constructed in accordance with this prescription have been shown to be in correspondence with commonly observed dislocation structures. Finally, we have shown that a characteristic length scale can be built into the theory by taking into account the self energy of the dislocations. The extended theory leads to scaling laws which appear to be in good qualitative and quantitative agreement with observation.

It is noteworthy that the fundamental factor determining the development of dislocation structures is the lack of convexity of the incremental energy functional. The connection between lack of convexity and the emergence of fine microstructure is presently well-established in a number of applications such as martensitic transformations, micromagnetics, liquid crystals and thin films. From this perspective, the overriding emphasis once placed on formulating constitutive restrictions guaranteeing existence and uniqueness of solutions of boundary value problems seems somewhat misplaced. For instance, Drucker’s celebrated postulates (see, e.g., Lubliner, 1990) are equivalent to the assumption of convexity of the incremental boundary value problem and, consequently, guarantee existence, uniqueness and regularity of classical minimizers (e.g., Dacorogna, 1989). Thus, while convexity may be desirable in structural applications, it has the unfortunate effect of ruling out solutions with fine microstructure. Therefore, the case of primary interest as regards the investigation of microstructural development concerns precisely those materials which do not obey Drucker’s postulates. This new constitutive paradigm represents a sharp—and refreshing—departure from classical plasticity theory.

A number of open questions remain to be addressed. For instance, it is not known to us what rules—if any—govern the turns and bends in labyrinth structures; or whether cell structures may also be understood as compatible arrangements of regions of single slip. In addition, it would be desirable to have constructions enabling the determination of energy-minimizing microstructures for general deformation histories. The question of scaling laws and their relation to nonlocal extensions of the theory has merely been touched upon in this paper and is in need of much further development. These present uncertainties notwithstanding, it is hoped that the theory formulated in this paper will provide a convenient basis for a rigorous and systematic mathematical investigation of the effective behavior of ductile single crystals with microstructure.
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References


A numerical analysis of the deformation of aluminum and dispersion strengthened aluminum products drawn at room-temperature. Transactions of the Metallurgical Society of the AIME 245, 2061–2067.


The formation of deformation bands in f.c.c. crystals. Materials Science and Engineering 81, 239–258.


Dislocation structures in cyclically deformed copper crystals. Philosophical Magazine 32, 1173–1176.


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In the title of Section 3.3, the title should read

3.3. Asymptotic behaviour of $\tilde{W}_+$.

In equations (30) to (33) and (35) read $\tilde{W}_1^1$, $\tilde{W}_2^1$, etc. instead of $W_1^1$. 

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