MD-Vol. 32

MICROSTRUCTURAL CHARACTERIZATION IN CONSTITUTIVE MODELING OF METALS AND GRANULAR MEDIA

edited by
G. Z. VOYIADJIIS

MD-Vol. 32

MICROSTRUCTURAL CHARACTERIZATION IN CONSTITUTIVE MODELING OF METALS AND GRANULAR MEDIA

presented at
THE ASME SUMMER MECHANICS AND MATERIALS CONFERENCES
TEMPE, ARIZONA
APRIL 28–MAY 1, 1992

sponsored by
THE MATERIALS DIVISION, ASME

edited by
GEORGE Z. VOYIADJIS
LOUISIANA STATE UNIVERSITY

THE AMERICAN SOCIETY OF MECHANICAL ENGINEERS
345 East 47th Street • United Engineering Center • New York, N.Y. 10017

ISBN No. 0-7918-0906-4

Library of Congress
Catalog Number 92-53838

FOREWORD

Constitutive modeling with microstructural effects is becoming increasingly important in structural and granular materials. More sophisticated methods that utilize the microstructure of the material are being favored more and more as opposed to the available macrostructural models. More important is the effective correlation between the microstructural and macrostructural points of view in such a way as to lead to modeling that can be used in practical applications. The primary purpose of this symposium is to examine the latest research in the microstructural characterization in constitutive modeling of metals and soils.

Consideration of the microstructure in the constitutive modeling of materials takes several forms. Some of these forms involve the study of dislocations in crystals and polycrystalline aggregates and/or the inclusion of the plastic spin in materials that undergo plastic deformation. This is especially important for crystals undergoing multiaxial deformation and for materials subjected to large inelastic deformation. In addition, the microstructure plays an important role in the constitutive modeling of granular materials.

Constitutive modeling of materials based on macroscopic analyses is widely available in the literature. This macroscopic description of material behavior provides satisfactory answers to many problems and predicts stresses or strains that are acceptable for practical application. However, the methods based on this description are not reliable and involve large factors of safety. Furthermore, the results using these methods become questionable when problems of large inelastic deformation are encountered. This is clearly demonstrated by studying the problem of finite simple shear of elastoplastic materials. Several papers have appeared recently in the literature dealing with this topic. In fact, some new developments in this area are included in this symposium. It has been well known that using the Jaumann stress rate in analyzing the simple shear kinematically hardening material leads to oscillatory stress distributions even though the shear strain is monotonically increasing. Several remedies have been suggested to solve this discrepancy utilizing different techniques. It is noticed that the most successful solution to this problem have utilized, to some extent, the microstructure. In particular, the introduction of the plastic spin has been shown to have a microstructural connection. The same remark holds for those methods dealing with the use of modified spin tensors in the corotational stress rate equations, although in this case, the microstructural connection is not clear or has not yet been established.

Dislocation theory has been utilized successfully in the microstructural characterization in the constitutive modeling of metals. Recently, researchers have shown a link between the dislocation theory and continuum theory based on the physics of plastic deformation. In particular, the plastic spin has been directly correlated to the study of continuously distributed straight edge dislocations.

The articles appearing in this symposium reflect the recent trends in the microstructural constitutive modeling of metals and granular materials. These involve several aspects of microstructural characterization ranging from dislocations in crystals to the micromechanics of large inelastic deformation. It is noticed that much research effort is directed towards the effects of anisotropy in the constitutive models. These effects are reflected through the study of polycrystalline aggregates and large plastic deformation. In the constitutive modeling of metals, much emphasis is placed on large inelastic deformation, the plastic spin, texture development and polycrystalline aggregates. The microstructural characterization of granular materials is displayed using several approaches utilizing indentical spheres and elliptical particles. In these cases, the effects of the microstructure are studied through numerical simulations and cone penetration tests.

It is hoped that the symposium gives a comprehensive overview of the recent trends in research in the microstructural constitutive modeling of metals and granular materials. The editor wishes to thank the authors for their contributions. Indeed, the time and effort invested in preparing these manuscripts is gratefully appreciated.

George Z. Voyiadjis

CONTENTS

MICROSTRUCTURAL MODELING OF METALS

Mechanics Aspects in Micro- and Nano-Scales
Elias C. Aifantis 1

Some Aspects of the Macroscopic Plastic Spin During Texture Development in Polycrystalline Metals
Erik van der Giessen 5

Simulation of Dislocation Configurations in the Presence of Inclusions
A. N. Gulluoglu and C. S. Hartley 21

Stress State Dependence of Finite Strain Inelasticity
Matthew P. Miller and David L. McDowell 27

A Model for Elastoplastic Materials With Anisotropic and Vertex Effects
Hussein M. Zbib 45

MICROSTRUCTURAL MODELING OF GRANULAR MATERIAL

Microstructural Characterization in Constitutive Modelling of Granular Material
Ching S. Chang 55

Effects of Stress History on Cone Penetration Tests in Sand: A Micromechanical Study
An-Bin Huang, Max Y. Ma, and Jong S. Lee 69

Relationship of Porosity and Elastic Properties for Consolidated Granular Aggregates
Anil Misra 81

Numerical Simulations of Granular Soil Using Elliptical Particles
Tang-Tat Ng 95

Anisotropic Distortional Yield Model for Granular Media
George Z. Voyiadjis, Ganesh Thiagarajan, and Emmanuel Petrakis 119

Author Index 135

MD-Vol. 32, Microstructural Characterization in
Constitutive Modeling of Metals and Granular Media
ASME 1992

MECHANICS ASPECTS IN MICRO- AND NANO-SCALES

Elias C. Aifantis*
Michigan Technological University
Houghton, Michigan

ABSTRACT

In this lecture a discussion of various mechanics aspects as they apply to the modelling of mechanical phenomena occurring at the nano and micro scales is given. Emphasis is placed on the description of relevant chemo-mechanical instabilities and their effect on pattern formation, and on developing a framework where pattern-forming instabilities at one scale will manifest explicitly on the occurrence of instabilities and corresponding patterns at another scale. Attention is restricted, in particular, on the understanding of the mechanisms of deformation and localization at the nano-, micro-, and macro-level, as well as on determining the degree of coupling between them and its effect on the overall macroscopic response. To accomplish this, all three regimes of deformation (i.e. prelocalization, postlocalization, and fracture) are considered. At the nanoscale (~10 - 100 nm grain size) recent results suggest that plastic deformation occurs via the rearrangement and production of free volume associated with nanopores at triple grain boundary junctions, but also direct grain boundary "stretching" and "rotation" and "nano damage" development has been observed. At the microscale (~10 - 100 μm grain size) the usual deformation mechanism is dislocation motion and production within the grains, while grain boundaries may act as obstacles or sources to dislocation evolution. Moreover, "micro damage" development is another mechanism of irreversible deformation, either independent or indirectly related to dislocation processes. Modelling of the evolution, stability, localization, pattern formation, and interaction of the nano and micro deformation mechanisms and of their influence on the macro (~0.1 - 1.0 mm) scale may result into a rational approach for synthesis and design of nano (or micro) phase materials and composites. For example, the determination of possible wavelengths occurring at the nanoscale and their effect on the spacing of deformation bands and crack patterns occurring at the micro and macro scales may provide a new approach for controlling and optimizing the mechanical behavior of manmade materials.

A problem for connecting "micro" to "macro" scales based on the concept of "normal" and "excited" states has been proposed by the author in the last decade. As a result of this program, "standard" and "non-standard" models of macroscopic plasticity were obtained on the basis of crystal slip and dislocation motion, and a justification for introducing higher order gradients

*Aristotle University of Thessaloniki
Thessaloniki GR, Greece

of strain into respective constitutive equations was provided. The physically based "non-standard" plasticity models have led to a direct interpretation of axial effects in torsion. The higher order gradients have led to a direct interpretation of measurements pertaining to shear bands widths and spacings. The notion of "normal" and "excited" states is extended to describe deformation mechanisms occurring at the nanoscale. Nanostructural materials exhibit a large surface-to-volume ratio and, as a result, the material element may be viewed as a superposition of "surface" and "bulk" continua with each one supporting its own mechanical (stress and strain) fields and also allowed to exchange effective mass and momentum with the other. As in the case of micro-macro transition, the approach can now provide a framework for the nano-micro-macro transition. As an example, the development of nanodamage is documented from experimental results obtained recently by the MTU group and then a set of partial differential equations modelling nanodamage evolution is derived.

In concluding, a suggestive mathematical framework is outlined below to indicate a possible apparatus to address the question of nano-micro-macro transition. A starting point will be to decompose the strain rate $\underset{\sim}{D}$ (the symmetric part of the velocity gradient) as follows

$$\underset{\sim}{D} = \underset{\sim}{D}_{\mathcal{L}} + \underset{\sim}{D}_{\ell}$$

where $\underset{\sim}{D}_{\mathcal{L}}$ is associated with a long-wavelength and $\underset{\sim}{D}_{\ell}$ is associated with a short-wavelength of co-existing deformation processes. The symbols $\mathcal{L}$ and ℓ may represent either macro and micro or micro and nano scales. In cases where all three scales need to be addressed simultaneously, a third strain rate quantity should be included the above equation. To fix ideas, $\mathcal{L}$ is identified with the macro scale and ℓ is related to the micro scale, for simplicity. The strain $\underset{\sim}{D}_{\mathcal{L}}$ is the one usually appearing in continuum plasticity formulations whereas $\underset{\sim}{D}_{\ell}$ is neglected. Within the length scale $\mathcal{L}$ characterizing the macroscale, the microstrain $\underset{\sim}{D}_{\mathcal{L}}$ may be spatially periodic and thus its mean value becomes zero without contributing to the overall strain. This is true for "stable" situations where the two length scales $\mathcal{L}$ and ℓ may be treated independently. Near instability, however, a strong coupling between the two length scales $\mathcal{L}$ and ℓ takes place and the deformation processes occurring at the microscale set the stage for the evolution of deformation at the macroscale. For example, the average spacing between micro-deformation bands may define a macroscopic bending stiffness for the analysis of macro-shear bands. Moreover, the patterning of microstructural variables and related "adiabatic elimination" of the micro-deformation or short-wave length variable $\underset{\sim}{D}_{\ell}$ can lead to a higher-order evolution equation for the intensity γ of the macro-deformation variable $\underset{\sim}{D}_{\mathcal{L}}$ of the general form

$$\dot{\gamma} = g(\gamma, \tau) + d(q^2 + \nabla^2)^2\gamma,$$

where g is a strain-production function related to dislocation production within the elementary volume, d is a phenomenlogical coefficient, and q a preferred wave number associated with the spacing of micro-deformation field. This equation is similar to the "slow-mode dynamics" equation derived for fluid and chemical systems and its stability analysis will provide certain information on the connection between the spatial features of micro- and macro-deformation patterns. A similar approach may be adopted for making a connection between nancoscales and microscales, as well as for the more general question of addressing the nano-micro-macro transition. Various classes of nano-micro-macro deformation phenomena are discussed on the basis of the aforementioned approach ranging from deformation and shear bands to nanodamage development and zig-zag cracking.

REFERENCES

1. E.C. Aifantis, On the Role of Gradients in the Localization of Deformation and Fracture, Int. J. Engng. Sci. (in press).

2. S.A. Hackney, W.W. Milligan, and E.C. Aifantis, Ductility in Nanocrystalline Gold, Preprint.

ACKNOWLEDGEMENT

Fruitful discussions with my collaborators Steve Hackney and Walter Milligan are gratefully acknowledged, especially in the area of processing and mechanical testing of nanophase materials and composites. The support of US Airforce under grant AFOSR-91-0421 is also acknowledged.

MD-Vol. 32, Microstructural Characterization in
Constitutive Modeling of Metals and Granular Media
ASME 1992

SOME ASPECTS OF THE MACROSCOPIC PLASTIC SPIN DURING TEXTURE DEVELOPMENT IN POLYCRYSTALLINE METALS

Erik van der Giessen
Engineering Mechanics Laboratory
Delft University of Technology
Delft, Netherlands

ABSTRACT

The macroscopic plastic spin in polycrystalline metals due to crystallographic texture development is identified, and defined on the basis of crystal plasticity theory. The plastic spin in cubic polycrystals during large strain, planar stationary deformation processes is computed from simulations using a Taylor-Bishop-Hill approach. The effects of crystal structure and initial anisotropy in pre-textured materials are discussed. The macroscopic plastic spin according to a very much simplified 2-D model for slip on (infinitely) many slip systems in a polycrystal is also discussed, and the analytical results are compared with those of the Taylor simulations. A few aspects are examined of a constitutive description of the plastic spin which utilizes nonsymmetric tensors as internal variables.

INTRODUCTION

The plastic spin has recently been identified as a key concept in the macroscopic constitutive description of large elastoplastic deformations of materials which exhibit deformation-induced anisotropy. As a constitutive entity added to the usual continuum framework, the plastic spin governs the rotation of the directions of anisotropy during the deformation process. With very few exceptions, the applications to the macroscopic constitutive description of polycrystalline metals have been limited to modeling the deformation-induced anisotropy in terms of a kinematic hardening model. Correspondingly, the constitutive equation for the plastic spin has so far been formulated mainly within the framework of kinematic hardening (e.g. Dafalias, 1983; Loret, 1983; Van der Giessen, 1989b); such approaches have been critically examined in (Van der Giessen, 1991). Following suggestions by Mandel (1982), Van der Giessen and Van Houtte (1990, 1991) proposed instead to explicitly identify the macroscopic plastic spin for metals on the basis of the key physical mechanism for deformation-induced anisotropy, namely crystallograhic texture development. The macroscopic plastic spin can then be defined in a physically sound way on the basis of crystal plasticity theories as a volume average over the polycrystal of the slip-induced plastic spin for each crystallite.

In the present paper, following a brief recapitulation of the constitutive framework that we work in, we further develop this concept of a micromechanics based plastic spin associated with texture development. The identification of the plastic spin on the various size scales — single slip system, single crystal, polycrystal — is carefully presented, and results are given for the macroscopic plastic spin obtained from numerical simulations using the Taylor-Bishop-Hill model to perform the volume averaging.

We proceed by briefly presenting some issues related to the routes that are currently being followed in order to incorporate this macroscopic plastic spin concept into macroscopic phenomenological plasticity models. One of these routes is based on a very much simplified model proposed by Van der Giessen (1989c) for slip on (infinitely) many crystallographic slip systems in a polycrystal, but which is designed so as to incorporate the main features of texture development, while being simple enough to allow for a largely analytical treatment. Macroscopic plastic spin results obtained by this multiple slip model are discussed and compared with the Taylor simulations. Finally, we discuss some aspects of another, purely macroscopic, approach which uses nonsymmetric tensorial internal variables to construct the constitutive law for the plastic spin. A possible micromechanical interpretation of these nonsymmetric tensors related to single slip is presented, and new explicit results are given for the corresponding macroscopic quantities according to the above multiple slip model.

Tensors are denoted by bold-face letters; **I** is the second-order unit tensor. The tensor product is denoted by ⊗ and the following operations apply: $\mathbf{ab} = a^{ik}b_{kj}\mathbf{e}_i \otimes \mathbf{e}^j$, $\mathbf{a} \cdot \mathbf{b} = a^{ij}b_{ij}$, with proper extension to tensors of different order ($\mathbf{e}_i$ and $\mathbf{e}^i$, $i = 1, \ldots 3$, are reciprocal base vectors). Superscripts T and -1 denote the transverse and inverse of a second-order tensor, respectively, tr denotes the trace and a superposed dot denotes the material time derivative or rate.

CONSTITUTIVE FRAMEWORK FOR LARGE STRAIN PLASTICITY

Many large deformation plasticity theories use the concept of an intermediate configuration, but the precise definition and interpretation of that concept may differ. In this section we briefly recapitulate the framework we are going to adopt throughout this paper, mainly for the purpose of definition and notation, but also to emphasize the role of plastic spin in such frameworks.

Whatever the form in which the material anisotropy manifests itself to us, its origin lies in the microstructure of the material. On the basis of this observation, an important class of today's phenomenological large strain plasticity theories have explicitly endowed the continuum with a so-called *substructure* in the form of a set of three *vector directors*. This proposition is usually attributed to Mandel (1971), but completely similar ideas were put forward slightly earlier by Besseling (1968); in fact, our presentation here is a mixture of these two. The purpose of the introduction of such a substructure is to serve as a tool to monitor, at any instant, the state of the macroscopic anisotropy.

Let the director vectors associated locally with a (infinitesimal) material element in the current state be denoted by $\bar{\boldsymbol{\varepsilon}}_\alpha$ ($\alpha = 1, \ldots 3$). Upon unstressing the element elastically, so that the material element changes into the so-called intermediate state, this triad is taken to transform in an affine manner. The corresponding triad in the intermediate configuration is denoted by $\{\boldsymbol{\varepsilon}_\alpha\}$ (see Fig. 1), and we now define the director vectors such that the $\boldsymbol{\varepsilon}_\alpha$ are orthonormal vectors. The orientation of this triad $\{\boldsymbol{\varepsilon}_\alpha\}$ in reference to a spatially fixed global basis $\{\mathbf{e}_i\}$ ($i = 1, \ldots 3$) then defines the orientation of the intermediate configuration, and the so-called *isoclinic configuration* is defined as the intermediate configuration in which the triad $\{\boldsymbol{\varepsilon}_\alpha\}$ retains the same orientation throughout the deformation process. Denoting the mapping from isoclinic configuration into current configuration by $\mathbf{F}^e$, the configuration of the material element in the current state as well as that of the director vectors $\bar{\boldsymbol{\varepsilon}}_\alpha$ are linked to the corresponding quantities in the isoclinic configuration through the bijections $\mathbf{dx} = \mathbf{F}^e\mathbf{da}$, $\bar{\boldsymbol{\varepsilon}}_\alpha = \mathbf{F}^e\boldsymbol{\varepsilon}_\alpha$ (**dx** and **da** are corresponding line elements in the current and isoclinic configuration, resectively). According to the polar decomposition theorem, $\mathbf{F}^e$ can be expressed as $\mathbf{F}^e = \mathbf{R}^e\mathbf{U}^e$ with the symmetric tensor $\mathbf{U}^e$ describing the elastic stretch and with the proper orthogonal tensor $\mathbf{R}^e$ describing the orientation of the intermediate configuration relative to the current configuration. Throughout this paper, we assume that elastic strains remain negligible, i.e. $\mathbf{U}^e \approx \mathbf{I}$ so that $\mathbf{F}^e \approx \mathbf{R}^e$. Hence,

$$\mathbf{dx} = \mathbf{R}^e \mathbf{da} \ , \quad \bar{\boldsymbol{\varepsilon}}_\alpha = \mathbf{R}^e \boldsymbol{\varepsilon}_\alpha \ .$$

Plastic deformations give rise to a rate of change of the local geometry of the continuum in the intermediate configuration, which is characterized by a plastic rate of deformation tensor $\mathbf{\Lambda}^p$ such that $\dot{\overline{\mathbf{da}}} = \mathbf{\Lambda}^p \mathbf{da}$. However, by definition, the triad of directors in the isoclinic intermediate configuration remains unchanged, $\dot{\boldsymbol{\varepsilon}}_\alpha = \mathbf{0}$. Neglecting elastic strains, the continuum rate of deformation, or velocity gradient, $\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1}$ along with its strain-rate and spin parts $\mathbf{D}$ and $\mathbf{W}$, respectively, can then be decomposed as

$$\mathbf{L} = \mathbf{L}^e + \mathbf{L}^p \ ; \quad \mathbf{L}^e = \dot{\mathbf{R}}^e \mathbf{R}^{eT} \ , \quad \mathbf{L}^p = \mathbf{R}^e \mathbf{\Lambda}^p \mathbf{R}^{eT} \ ,$$

or

$$\mathbf{D} = \mathbf{D}^p \ , \tag{1}$$

$$\mathbf{W}^* \equiv \dot{\mathbf{R}}^e \mathbf{R}^{eT} = \mathbf{W} - \mathbf{W}^p \ , \tag{2}$$

where generic symbols $\mathbf{D}$ and $\mathbf{W}$ denote symmetric and skewsymmetric parts, respectively. Commonly, the tensor $\mathbf{\Lambda}^p$ is expressed in terms of the plastic part of the deformation gradient , $\mathbf{F}^p = \mathbf{F}^{e^{-1}}\mathbf{F}$, as $\mathbf{\Lambda}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p^{-1}}$. However, as discussed in detail by Van der Giessen (1989a), the introduction of $\mathbf{F}^p$ is not needed and the $\mathbf{\Lambda}^p$ itself can be regarded as the primary quantity to characterize the plastic deformation process.

The relationship (2) emphasizes the key idea behind the introduction of the director vectors, namely that the kinematics of the continuum and that of the substructure are distinct entities (see also Dafalias, 1987). The spin of the continuum is governed by $\mathbf{W}$, whereas the spin $\mathbf{W}^*$ governs the rate of change of the tensor $\mathbf{R}^e$ and hence of the orientation of the substructure/director triad, i.e.

$$\dot{\bar{\boldsymbol{\varepsilon}}}_\alpha = \mathbf{W}^* \bar{\boldsymbol{\varepsilon}}_\alpha \ .$$

This observation immediately clarifies the role of the plastic spin $\mathbf{W}^p$ as the spin of the continuum relative to the subtructure, thus providing the link between the kinematics of the continuum and that of the substructure. In addition to constitutive equations for the plastic strain-rate $\mathbf{D}^p$ like in any plasticity theory, constitutive equations must now be supplied also for the plastic spin $\mathbf{W}^p$ (Mandel, 1971).

The orthonormal triad $\{\boldsymbol{\varepsilon}_\alpha\}$ naturally serves a base of reference for the anisotropic properties of the material element in the intermediate state. Although we shall by no means give a comprehensive treatment of anisotropic constitutive properties here, we note that, for instance, the elastic strain ener-

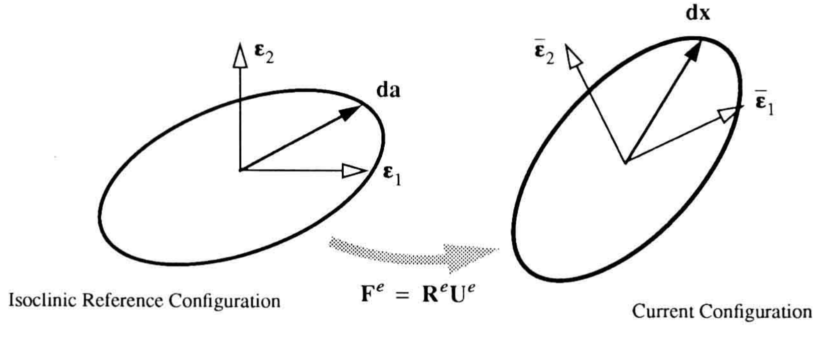

Fig. 1. Two-dimensional illustration of the current and isoclinic configurations of continuum and substructure.

gy function u (per unit mass) is formulated in a natural way in terms of the components of the elastic (Lagrangean-type) strain tensor $\mathbf{E} = (\mathbf{F}^{eT}\mathbf{F}^e - \mathbf{I})/2$ with respect to the base vectors $\boldsymbol{\varepsilon}_\alpha$ (see, e.g., Besseling, 1968; Van der Giessen, 1989a), i.e. $u = u(E_{\alpha\beta})$. The state equation for the Cauchy stress $\boldsymbol{\sigma}$ then reads,

$$\boldsymbol{\sigma} = \rho\mathbf{R}^e\frac{\partial u}{\partial \mathbf{E}}\mathbf{R}^{eT}, \quad \frac{\partial}{\partial \mathbf{E}} = \frac{\partial}{\partial E_{\alpha\beta}}(\boldsymbol{\varepsilon}_\alpha \otimes \boldsymbol{\varepsilon}_\beta), \tag{3}$$

where ρ is the mass density and where $\mathbf{F}^e \approx \mathbf{R}^e$ has been used. Similarly, the yield function φ is formulated naturally in terms of components with respect to the triad $\{\boldsymbol{\varepsilon}_\alpha\}$. Following Van der Giessen (1989a, 1989c) and considering as an example a yield function which depends only on the stress deviator $\mathbf{s} = \boldsymbol{\sigma} - (\mathrm{tr}\,\boldsymbol{\sigma}/3)\,\mathbf{I}$, the yield function is formulated in general as a function $\varphi = \varphi(\Sigma_{\alpha\beta})$ of the components on $\boldsymbol{\varepsilon}_\alpha$ of the stress tensor $\boldsymbol{\Sigma} = \mathbf{R}^{e^T}\boldsymbol{\sigma}\mathbf{R}^e$. This tensor $\boldsymbol{\Sigma}$ represents a stress tensor related to the intermediate configuration, which is dual to the rate of deformation $\boldsymbol{\Lambda}^p$. In cases where anisotropic hardening needs to be taken into account, the yield function needs to be augmented with hidden internal variables measured in the intermediate configuration, which we denote collectively by $\mathbf{A}$. Just as for the stress state dependence, non-scalar valued internal variables appear in the yield function through their components on $\{\boldsymbol{\varepsilon}_\alpha\}$, denoted collectively by $\mathbf{A}_\alpha$, i.e. $\varphi = \varphi(\Sigma_{\alpha\beta}, \mathbf{A}_\alpha)$.

The role of plastic spin in these key constitutive quantities now lies in the explicit appearance of tensor components in the triad $\{\boldsymbol{\varepsilon}_\alpha\}$: The arguments of these functions are explicitly dependent on the rotation $\mathbf{R}^e$ between the directions of anisotropy in the isoclinic and current configuration. As is obvious from the relation (2), the rate of change of $\mathbf{R}^e$ depends on the continuum spin as well as on the plastic spin. Conversely, the current value of $\mathbf{R}^e$, as needed in for instance elastic energy and yield function, is to be obtained from integrating $\dot{\mathbf{R}}^e = \mathbf{W}^*\mathbf{R}^e$ with $\mathbf{W}^*$ according to (2).

The role of plastic spin emerges even more clearly when rate equations are considered. For instance, the rate of change of Cauchy stress can be expressed as

$$\dot{\boldsymbol{\sigma}} - \mathbf{W}^*\boldsymbol{\sigma} + \boldsymbol{\sigma}\mathbf{W}^* = \mathcal{L}^e\mathbf{D}^e - \boldsymbol{\sigma}\,\mathrm{tr}\,\mathbf{D}, \quad \mathcal{L}^e = \rho R^e_{i\alpha}R^e_{j\beta}\frac{\partial^2 u}{\partial E_{\alpha\beta}\partial E_{\gamma\mu}}R^e_{k\gamma}R^e_{l\mu}(\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l)$$

by straightforward differentiation of (3) and invoking the balance of mass $\dot{\rho} + \rho\,\mathrm{tr}\,\mathbf{D} = 0$. Rewriting that in terms of the Jaumann stress rate, $\overset{\nabla}{\boldsymbol{\sigma}} = \dot{\boldsymbol{\sigma}} - \mathbf{W}\boldsymbol{\sigma} + \boldsymbol{\sigma}\mathbf{W}$, immediately shows how the plastic spin enters into the constitutive equations. Of course, this discussion is by no means exhaustive; its sole purpose was to give an indication of where and how the concept of plastic spin appears in constitutive relations for large strain plasticity. For more details one is referred to the specialized literature. It may be noted that in the case of an isotropic material, the elastic energy function and the yield function can be expressed in terms of the invariants of the tensors involved, so that the orientation of the triad $\{\boldsymbol{\varepsilon}_\alpha\}$ is irrelevant. Therefore, the plastic spin is a redundant quantity and can be arbitrarily set equal to zero for isotropic materials, as was already deduced by Mandel (1971).

In the above, we have incorporated the anisotropy in the formulation of, for instance, the yield function $\varphi = \varphi(\Sigma_{\alpha\beta})$ by expressing it directly in terms of components in $\{\boldsymbol{\varepsilon}_\alpha\}$. An alternative approach would be to express it as an isotropic tensor function of the tensor $\boldsymbol{\Sigma}$ along with the base vectors $\boldsymbol{\varepsilon}_\alpha$, so that $\varphi = \phi(\boldsymbol{\Sigma}, \boldsymbol{\varepsilon}_\alpha)$ $(\alpha = 1, \ldots 3)$. The use of such an approach together with the representation theorems for isotropic tensor functions (Wang, 1970) for specific types of anisotropy, such as orthotropy or transverse isotropy, can be quite fruitful (see e.g. Loret, 1983). However, for general anisotropy, all that these representation theorems tell is that $\varphi = \phi(\boldsymbol{\Sigma}, \boldsymbol{\varepsilon}_\alpha)$ is fully equivalent to $\varphi = \varphi(\Sigma_{\alpha\beta})$.

Finally, it is noted though that the relevance of the plastic spin concept and the necessity for its constitutive description are still being debated in the recent literature (see, e.g., Nemat-Nasser, 1990). However, this seems to be solely due to the fact that some authors do not explicitly define a substructure (or a director triad) embedded in the material, so that in fact their concept of plastic spin is sweepingly different from that appearing in Mandel's and related works as discussed above. Instead of such an explicit substructure, other implicit concepts are employed to monitor or define directions of anisotropy, such as the principal directions of the plastic stretch tensor (Nemat-Nasser, 1990), and the spin of these directions is used explicitly in the pertinent rate constitutive equations. So, this latter approach is in many respects really an alternative to substructure based theories; with such alternative implementations of the concept of spinning of anisotropy directions, many of the aspects to be discussed presently are equally relevant.

PLASTIC SPIN ACCORDING TO CRYSTAL PLASTICITY

For polycrystalline metals, the prime source of anisotropy on a macroscopic scale is texture development during large strain deformation processes. In this paper, we confine attention to *crystallographic texture* which is due to the formation of a preferred lattice orientation of the crystallites; morphological texture will be neglected. In order to describe the macroscopic material response in terms of the constitutive framework of the previous section, one must first identify the substructure that is relevant to this kind of anisotropy, followed by identifying the associated plastic spin; this will be briefly discussed first. In the subsequent subsection we will summarize the Taylor polycrystal theory that is used then to actually determine the plastic spin during a number of deformation processes by numerical simulation.

Substructure and Plastic Spin for a Polycrystal

Crystallographic texture development is due to lattice rotations accompanying crystallographic slip. We therefore start our considerations here with single slip. The kinematics can be conveniently described employing the above-mentioned framework (cf. e.g. Rice, 1971; Asaro, 1983; Aifantis, 1987). Consider a slip system $(\mathbf{n}_0, \mathbf{b}_0)$ in the isoclinic reference configuration, with $\mathbf{n}_0$ denoting the unit normal to the slip plane and $\mathbf{b}_0$ the unit vector in the slip direction. The identification of the substructure for such a slip system is straightforward: choose $\boldsymbol{\varepsilon}_1 = \mathbf{b}_0$ and $\boldsymbol{\varepsilon}_2 = \mathbf{n}_0$, so that $\boldsymbol{\varepsilon}_3 = \mathbf{b}_0 \times \mathbf{n}_0$. When $\dot{\gamma}^p$ is the slip rate on this slip system, the plastic shear flow determines the plastic rate of deformation in the isoclinic configuration as

$$\boldsymbol{\Lambda}^p = \dot{\gamma}^p \mathbf{b}_0 \otimes \mathbf{n}_0$$

Since, the slip system $(\mathbf{n}_0, \mathbf{b}_0)$ remains unchanged in the isoclinic configuration, $\boldsymbol{\Lambda}^p$ depends only on the slip rate $\dot{\gamma}^p$. Neglecting elastic strains again, so that $\mathbf{F}^e = \mathbf{R}^e$, the slip system vectors in the current configuration can be obtained by a rigid rotation, i.e. $\mathbf{b} = \mathbf{R}^e \mathbf{b}_0$, $\mathbf{n} = \mathbf{R}^e \mathbf{n}_0$. Hence,

$$\mathbf{L}^p = \dot{\gamma}^p \mathbf{b} \otimes \mathbf{n} \tag{4}$$

so that the plastic strain-rate $\mathbf{D}^p$ and the plastic spin $\mathbf{W}^p$ are determined immediately by the slip rate and the current slip system geometry. In general, the slip induced plastic spin $\mathbf{W}^p$ is not equal to the applied spin $\mathbf{W}$. With the above interpretation of the substructure, it follows that the tensor $\mathbf{W}^*$ according to (2) determines the spin of the slip system, i.e. $\dot{\mathbf{b}} = \mathbf{W}^* \mathbf{b}$, $\dot{\mathbf{n}} = \mathbf{W}^* \mathbf{n}$.

For future reference, we note here that with the above identification of the $\boldsymbol{\varepsilon}_\alpha$, the components of $\boldsymbol{\Lambda}^p$ with respect to the $\boldsymbol{\varepsilon}_\alpha$, $\boldsymbol{\Lambda}^p = \Lambda^p_{\alpha\beta} \boldsymbol{\varepsilon}_\alpha \otimes \boldsymbol{\varepsilon}_\beta$, read $\Lambda^p_{12} = \dot{\gamma}^p$ and $\Lambda^p_{\alpha\beta} = 0$ otherwise. The fact that

$$\Lambda^p_{21} = \boldsymbol{\Lambda}^p \cdot (\mathbf{n}_0 \otimes \mathbf{b}_0) = \mathbf{L}^p \cdot (\mathbf{n} \otimes \mathbf{b}) \equiv 0 \tag{5}$$

has been put forward by Van der Giessen (1990) as a key property of plastic deformations caused by single slip. Moreover, it was suggested to use (5) as a kinematic constraint on $\boldsymbol{\Lambda}^p$ imposed by the fact that single slip occurs on the $(\mathbf{n}_0, \mathbf{b}_0)$ slip system.

Each crystallite in a polycrystalline metal contains $n > 1$ possible slip systems. Here, we consider only cubic crystallites, for which $n = 12$ corresponding to the $\{111\}\langle 110\rangle$ type slip systems for FCC crystallites and $n = 24$ for the $\{110\}\langle 111\rangle + \{112\}\langle 111\rangle$ slip systems for BCC crystallites. Also for such a crystallite the identification of the substructure is obvious: choose the director vectors $\boldsymbol{\varepsilon}_\alpha$ to coincide with the principal lattice directions (cf. Mandel, 1971). The contributions of each of the n slip systems to the rate of deformation $\boldsymbol{\Lambda}^p$ or $\mathbf{L}^p$ for a single crystallite are additive, so that after taking symmetric and skewsymmetric parts,

$$\mathbf{D}^p = \sum_{s=1}^{n} \dot{\gamma}_s^p \mathbf{M}_s , \quad \mathbf{M}_s = \frac{1}{2}(\mathbf{b}_s \otimes \mathbf{n}_s + \mathbf{n}_s \otimes \mathbf{b}_s) ; \tag{6}$$

$$\mathbf{W}^p = \sum_{s=1}^{n} \dot{\gamma}_s^p \boldsymbol{\Omega}_s , \quad \boldsymbol{\Omega}_s = \frac{1}{2}(\mathbf{b}_s \otimes \mathbf{n}_s - \mathbf{n}_s \otimes \mathbf{b}_s) \tag{7}$$

where a subscript s is used to denote a particular slip system. Postponing the actual determination of the slip rates $\dot{\gamma}_s^p$ to the next subsection, let us assume that they are known in a given state. With the orientation g of the crystallite being given in that state as well, the rotation tensor $\mathbf{R}^e$ is known instantaneously and $\mathbf{W}^*$ is determined immediately by (2) again. $\mathbf{W}^*$ is interpreted now as the lattice spin.

The last step now is from a single crystallite to a polycrystal comprising a large number m of differently oriented crystallites. As pointed out by Mandel (1982), the choice of a substructure corresponding to a polycrystalline aggregate is not trivial. The seemingly obvious extension of the identification for a single crystal, by trying to define some kind of 'average lattice' on the basis of the current crystal orientations, involves major complications. Instead, Mandel (1982) suggested to define the substructure in a kinematic way: the substructure for a polycrystal is a triad of vectors that rotates with a spin equal to the volume average of the spin of the individual lattice orientations. Formally, this definition can be written as

$$\dot{\bar{\boldsymbol{\varepsilon}}}_\alpha = \overline{\mathbf{W}}^* \bar{\boldsymbol{\varepsilon}}_\alpha , \quad \overline{\mathbf{W}}^* \equiv \langle \mathbf{W}^* \rangle = \frac{1}{V}\int_V \mathbf{W}^*(\mathbf{x}) dV$$

where $\mathbf{W}^*(\mathbf{x})$ is the lattice spin at location $\mathbf{x}$ in the polycrystal and V is the volume of the aggregate considered.

Having defined the substructure for a textured polycrystal in that way, the corresponding plastic spin associated with texture development is immediately found from (2) as

$$\overline{\mathbf{W}}^p = \mathbf{W} - \overline{\mathbf{W}}^* \tag{8}$$

Note that this *macroscopic plastic spin* $\overline{\mathbf{W}}^p$ is in general not equal to the volume average $\langle \mathbf{W}^p \rangle$ of the plastic spin within each crystallite according to (7).

It is of importance to note here that the macroscopic plastic spin thus defined, can — in principle — be determined from experiments. Suppose that the lattice orientations within a polycrystalline sample can be measured (e.g. by X-ray techniques) with sufficient accuracy at two nearby instants during a deformation process. This information can then be used to compute (an average value of) the spin $\langle \mathbf{W}^* \rangle$, and the macroscopic plastic spin follows from (8). This means that constitutive equations for this plastic spin can be verified directly with experimental values. It should be realized though that this hinges on the fact that this plastic spin is associated with crystallographic texture development only, which in itself is a phenomenon that can be observed on a sample more or less directly.

Obviously, the theoretical evaluation of the volume average $\langle \mathbf{W}^* \rangle$ over a polycrystalline aggregate is a formidable task. An approximation is obtained by the Taylor model.

Taylor-Bishop-Hill Polycrystal Theory

Within the framework of crystal plasticity, as discussed above, the Taylor-Bishop-Hill theory provides a practically applicable model for the plastic deformation of a polycrystalline aggregate. The first, basic assumption made in the Taylor model is that the velocity gradient **L** is homogeneous within each crystallite. It varies only with a long wavelength, much larger than the grain size; for most practical calculations, it is assumed to be equal in all m crystallites. This means that the volume average of the lattice spin, $\langle \mathbf{W}^* \rangle$, simply reduces to a weighted average of the lattice spin $\mathbf{W}_k^*$ for the (entire) kth crystallite, so that also the macroscopic plastic spin defined through (8) is identical to the average plastic spin:

$$\overline{\mathbf{W}}^* = \frac{1}{V}\sum_{k=1}^{m} V_k \mathbf{W}_k^* \ , \quad \overline{\mathbf{W}}^p = \frac{1}{V}\sum_{k=1}^{m} V_k \mathbf{W}_k^p \ ; \quad V = \sum_{k=1}^{m} V_k \ , \tag{9}$$

as suggested already by Mandel (1982). Here, $\mathbf{W}_k^*$ is obtained from (2) after substitution of the crystallite's plastic spin $\mathbf{W}_k^p$ according to (7), and V_k is the weight factor for crystal k.

The macroscopic plastic spin can be evaluated once the slip rates within all crystallites are known. Given the fact that cubic crystals possess a relatively large number of possible slip systems, the determination of the slip rates poses a well-known problem in crystal plasticity. Among the various solutions proposed, the Taylor-Bishop-Hill approach is one of the simplest. For details on this theory and the particular implementation used for our simulations, we refer to the paper by Van Houtte (1988). Suffice it to note here that the critical resolved shear stress for slip according to Schmid's law is taken to be a material constant on each slip system; slip system hardening and latent hardening are being neglected, and slip is also asssumed to be rate-independent.

Once the slip rates are known, the plastic spin of each crystallite can be calculated from (7). For a particular applied velocity gradient **L**, the lattice spin $\mathbf{W}^*$ and the plastic spin $\mathbf{W}^p$ depend on the crystal orientation. After a large strain, most crystallites will rotate to orientations for which the crystal lattice spin $\mathbf{W}_k^* = \mathbf{0}$. This means that the crystal lattices do not rotate any more at ongoing deformation. For such so-called final orientations, the crystallite's plastic spin equals the applied spin **W**.

Results

In this section we present some results for the macroscopic, average plastic spin for a polycrystalline aggregate consisting of $m = 294$ crystallites. The initial crystal orientations constitute a uniform coverage of Eulerian orientation space so that the aggregate represents an initially isotropic material. The critical resolved shear stress is taken to be the same for all slip systems. The numerical analysis is based on a time step Δt such that $\Delta\varepsilon_e \equiv \dot{\varepsilon}_e \Delta t = 0.05/\sqrt{3}$, where $\dot{\varepsilon}_e$ is the applied effective strain-rate defined through $\dot{\varepsilon}_e^2 = (2/3)\,\mathrm{tr}\,\mathbf{D}^2$. A class of homogeneous 2D plane strain deformation processes in the x_1–x_2 plane are considered, which correspond to stationary flow as characterized by constant components of the velocity gradient **L** with respect to the global Cartesian basis $\{\mathbf{e}_i\}$. For these deformations we consider here only the $\overline{W}_{12}^p$ component of the macroscopic plastic spin according to (9). The velocity gradient given in the insert of Fig. 2 corresponds to a deformation process which can be envisaged by first deforming a block in simple shear along the x_1–direction to a shear strain γ and then deforming it by planar isochoric stretching ("rolling") to a stretch λ in the x_2–direction. The parameter κ is a measure of the amount of rolling relative to the amount of shearing. Pure rolling corresponds to $\kappa \to \pm\infty$ while $\kappa = 0$ corresponds to pure simple shear.

Van der Giessen and Van Houtte (1991) presented some preliminary results for exactly the same conditions. First, they showed the development of plastic spin during pure simple shear up to shears of $\gamma = 10$, for either FCC or BCC polycrystals (these results are reproduced later in Fig. 6). It was found that initially, at $\gamma = 0$, the plastic spin vanishes because of the initial isotropy, while the plastic spin increases quickly due to texture development. In the early stages of the process, say $\gamma < 1.5$, the plastic spin is observed to be virtually identical for FCC and BCC polycrystals, but for larger shears the