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Computational crystal plasticity

Paul R. Dawson*

Sibley School of Mechanical and Aerospace Engineering, Cornell University, Upson Hall, Ithaca, NY 14853-7501, USA

Abstract

To better predict material response associated with plastic deformations, plasticity models for behaviors over an extensive range of length scales are being combined to give a more comprehensive representation of the material. The breadth of the length scales naturally enters a more complete material description through the influences that features of the structure of many sizes have on the mechanical responses. The effective inclusion of material structure in simulations is pushing applied plasticity toward more highly quantitative implementations. Computed costs are greater in many respects, but the potential rewards are simulations with much greater relevance to current engineering applications. The focus of this paper is on a number of trends and issues related to these implementations and their use. In particular, we examine the methodologies for describing material structure at multiple scales within the context of simulation and discuss techniques used to compute properties and to evolve the state based on features of the structure.

1. Introduction

Solid mechanics has long promoted a careful merger of rigorous theory and powerful solution methods to solve very complex problems. From its inception over thirty years ago, the finite element method has grown in its utility as an effective tool for solving the equations posed by comprehensive theories for the deformation of solid bodies. Much of its early development focused on improvements to the method that would guarantee more robust convergence, greater accuracy, and higher efficiency (Johnson, 1987; Zienkiewicz and Taylor, 1989; Huebner et al., 1995). Consequently, the boundary value problems treated in solid mechanics increased dramatically in size and complexity. One needs only to look at current trade journals to see the acceptance of this tool in engineering practice and the reliance on finite element analyses in design applications. This progress was accompanied by a more thorough understanding of the relationships among the character of the model equations, the discretization of the solution space, and the attributes of the solution. Examples are consistent

* Tel.: +1-607-255-3466; fax: +1-607-255-9410.
E-mail address: prd5@cornell.edu (Paul R. Dawson)

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jacobians used to solve nonlinear systems of equations (Simo and Taylor, 1984) and consistent penalty methods used to apply constraints (Engelman et al., 1982). Continued expansion to ever larger problems has been fueled by exploitation of growing computational resources: serial implementations were replaced by vector implementations, and they in turn are being succeeded by parallel implementations.

Prior to the mid 1980s, most finite element computations related to plastic deformations of metals were based on models having both isotropic and rate-independent behaviors. Creep, although recognized as rate dependent, was treated separately from what was considered to be plastic flow. As the attention to problems involving either large strains or complex loading histories grew, so did the recognition of the need for models with greater fidelity to the material. Representations of metal behavior had been under intense development in the preceding decade, and offered the capability to account for the kinetics of plastic flow both in the yield criterion and in the evolution of strength via strain hardening. Such models went under the banner of state or internal variable models, and quantified the effects of changing state via structurally-motivated model variables (Miller, 1987; Stouffer and Dames, 1996). Some of the models attempted to present a unified treatment of creep and plasticity, while others restricted attention to deformations dominated by a single deformation mechanism (Ashby, 1983). Most notable were those which prescribed the increases in strength during slip dominated deformations as being related to the increase in dislocation density (Hart, 1976; Kocks, 1976). Behaviors associated with ductile void growth (damage), evolving grain size (especially for superplastic response), and back stresses (to describe yield asymmetry) also were investigated in depth.

Since about 1990, there has been a rapid increase in the number of modeling efforts, and in their successes, that embody the material structure directly in the finite element computations (Chenot et al., 1992; Shen and Dawson, 1995; Teodosiou, 1997; Huetink and Baaijens, 1998). Two categories are mentioned: the first is the prediction of evolving structure; the second is the determination of properties from the structure. Some simulations involve only one of the two, while others couple the two together. By material structure, we mean a collection of one or more features that are known by their geometries and may be observed with microscopes of various powers of magnification. Examples include dendrites, grains, crystal lattices, dislocations and dislocation structures, precipitates, and isolated defects, such as voids or stringers. By including structure, modeling expanded in its utility and experienced greater usage in the analyses of materials processing, provided more in-depth treatments of material formability issues, and formed the basis of more numerous investigations of the fundamentals of plasticity.

Several emerging tools provide enormous opportunities for more quantitative approaches than was previously tractable and, consequently, we can expect a period of rapid progress. Parallel computing, automated data collection, and advanced visualization tools offer new possibilities in developing and applying simulations that are based on a more fundamental understanding of material behavior. There are a number of expectations for our progress. One is that we can reach more deeply into details of material structure to define properties that govern the material responses. Another is that we will bridge the transitions from manufacturing to design applications via the structure of the material much more effectively than has been done in the past. There also is the expectation, realistic or not, that simulation at a finer scale will shed light on model parameters at a coarser scale. This has been accomplished in some cases (yield surfaces, for example: Beaudoin et al., 1994; Maudlin et al., 1996), and there is hope for similar successes for other parameters that have been largely inaccessible experimentally, and for which there is little ability to make direct measurements. Examples are the surface characterizations associated with friction, heat transfer and diffusion.

While the computational horsepower to meet these challenges can be envisioned, there remains an issue that is essential to the success of the endeavor that has not been important to the prior

developments. This is the issue of communicating to each other the results, now arising from quite diverse physical scales and modeling philosophies, that are necessary to couple analyses that bridge length scales. Simulations likely will not be coupled through solution variables such as the velocity or the stress, as such variables may not convey a clear meaning across scales. Rather, we should look for the coupling to occur via observable geometric features of the material itself, as those features may be quantified mathematically and verified experimentally. However, the pathway to including richer descriptions of the material structure is not obvious, because the features are neither truly hierarchical, nor independent. A collection of samples of a material inevitably exhibit statistical variability associated with those features. Further, the significance of a given feature for different responses is not universal — the same feature may be important in one context but not in another. From practical concerns, simulations undertaken in the next few years are not likely to encompass more than a few of the features observed, nor need they in order to be useful. However, these simulations may well require that the aggregate behaviors of other features be well characterized and reduced to meaningful averages for determination of the behavior. A coherent methodology is needed just to deal with this aspect of communicating simulation data over length scales in an environment of loosely coupled simulation tools.

The geometric features that comprise the material structure of metals range from atoms to assemblies of components, and span tens of orders of magnitude in characteristic length. Here we will deal with only a very limited subset of that range: macroscale (millions of grains) to subcrystal dimensions, but generally much larger than the associated Burgers vector. This excludes the active area of simulation of dislocation dynamics, which has yet to be effectively connected with the scale of the subgrain or cell. We will categorize problems according to the relation between finite element dimensions and the crystal size. Two broad categories that arise in such a simple grouping are: elements very much larger than crystals and elements on the same size or appreciably smaller than crystals (but still much larger than a Burgers vector). This grouping is quite natural, however, when considering the manner in which the crystal lattice and its orientation are included in the models. The next section concentrates on methods to represent features of the material structure in simulation. Following that are sections devoted to applications within the two broad categories.

Briefly stated, the premise of the discussion offered in this paper is that the trend in plasticity is toward embedding enhanced structural descriptions within the constitutive models. Mechanical properties can be computed ‘on the fly’ through the interrogation of features of the material structure that control those properties. Variability in the occurrence of the features and of their interactions can enter directly through the explicit inclusion of structure in the simulations. Evolution of properties can be determined by predicting the modification to the structure. This trend forms the basis of multiscale modeling efforts in solid mechanics that have gained momentum in recent years. Such modeling holds great promise, although to date most simulations span only a single pair of characteristic lengths. For example, formability of aluminum sheet has been linked to attributes of crystallographic texture. Yet, more precise understanding may well be possible from simulations that incorporate several features and span even greater differences in characteristic size. One such case would be to link dislocations directly to the strength of a polycrystal via the structures that dislocations form. Currently, first-order correlations between strength and dislocation density are employed in many macroscopic plasticity models, and a more fundamental understanding would be quite important. To quantitatively map such associations we must consider a number of structural features simultaneously, and do so with sufficiently large populations of features to facilitate extracting meaningful trends from the simulations. In exercising this approach, we accept that the computational requirements will grow larger and larger as structural descriptions embrace greater detail. While the impetus to incorporate material structure is clear, there are many options available in the methodologies of its implementation. These are the foci of the paper.

2. Material structure

A very clear trend over the past few years has been to introduce ever greater detail of the material structure into a host of solid mechanics simulations. The material structure can be thought of as having a variety of geometric features that span a very large range in characteristic size. The intention in many cases has been to develop multiscale models, where by multiscale it is meant that features having different characteristic lengths are embedded in a single simulation or unified set of simulations. Some sort of interplay occurs among the scales, but not in a reciprocal fashion. Typically, the responses of small scale features are averaged to give a larger scale property, while the kinematics of the larger scale features are projected, not necessarily uniformly, onto the smaller scale. The multiscale modeling thrust within solid mechanics is an emerging one, and formalisms and conventions are still not mature. The concept of structure at many scales is intuitive, but greater precision in the terminology is needed to better communicate methodologies and results associated with multiscale models. Confusion can easily arise between similar but distinct concepts that employ common descriptors. For this reason, we begin with a section that attempts to draw a distinction between what we refer to as features and what we call attributes of a material. We do not mean to lay claim to any preferred terminology, but rather endeavor to increase awareness of what we regard as an issue that is critical to the success of coordinating multiscale modeling activities: the careful differentiation between state, properties, and modeling constructs.

2.1. Material features and attributes

The geometric features of material structure include the obvious ones: atoms, arrangements of atoms in lattices (crystals), grains, and phase topologies. But interestingly, the imperfections within these features have structure or patterns of their own, leading to features such as dislocations, dislocation structures, and grain clusters, for example. Further, a defect structure may overlay other geometric features, including other defect structures. Thus, features are comprised themselves of, or contain within them, one or more geometric features that are smaller in scale. Grains, for example, possess a lattice, and possibly such items as voids, precipitates, and dislocations. The dislocations appear in arrangements such as dense walls that define cells within a grain. Within the same grain could be inclusions that have comparable dimension to the dislocation arrangements. We refer to some aspects of the substructure of a feature as being attributes of that feature (Myers, 1998). We also count mechanical properties specific to a geometric feature among its attributes.

The relationship between geometric features and attributes is interesting and complex: an attribute is associated with a particular geometric feature and consists of information pertinent to that geometric feature. A geometric feature on one scale also may be associated with an attribute of a different feature on a larger scale. For example, as a geometric feature, a grain possesses its lattice as an attribute, along with its attendant slip system directions and strength. The dislocations can influence the slip system strength, but definitely are regarded as geometric features themselves. Although the precise nature and interrelationships of each can easily appear fuzzy, making a distinction between features and attributes is useful for modeling purposes. One important difference centers around physical constraints. A sample of material containing a spatial arrangement of geometric features is a body subject to balance laws for mass and momentum. In contrast to this, neither the attribute nor a probability distribution that represents its full population is a body that is subject to the complete set of balance laws, even though the evolution of the distribution may be governed by a conservation principle.

We divert briefly here to make a similar distinction in our use of the terms state and state variable. In our view, the latter is a modeling construct that typically embodies information regarding the state, but not exclusively so, and is useful for mathematical description of the material behavior. The former is an

actual measure of some material feature, herein typically a geometric measure. One may be able only to infer the value of a state variable from observed behavior, but one should always, at least in theory, be able to directly observe state. Measures of state may serve as state variables, but not necessarily vice versa, as state variables also may be dependent on the physics of plastic flow. In this way, state variables may be thought of as attributes of a particular length scale within the material.

2.2. Probability distributions of attributes

A geometric feature such as a grain appears as a distinct unit when the material is observed at an appropriate scale. An actual material sample has a specific number and position for each of its geometric features. Different samples will have different arrangements, but for materials that are regarded as having an equivalent state, the appropriate measures will be statistically identical in the sense that all could have been derived from the same probability distribution, assuming it to be known. Probability distributions thus provide a mechanism for the representation of the population of an attribute of a geometric feature. Over the volume of a body, and thus the population of grains, the variations of grain size can be described by a probability distribution. The lattice orientations taken over all of the grains define the crystallographic texture and are represented by an orientation (probability) distribution. The task then arises to adequately represent distributions, or some resultant extracted from a distribution, as required in a simulation.

It is common to represent a probability distribution approximately with a discrete set, that is: one sample that is sufficient to accurately represent any of the samples that could be drawn from the probability distribution. Other techniques (related, although not obviously) are expansions in terms of basis functions, including: harmonics, tensors, and piecewise polynomials. Probability distribution functions whose independent variables describe orientations have often been cast in spherical harmonics, with connections between pole distributions and orientation distributions. Simpler features, say ones with a single orientation axis, may be successfully described by tensors (examples including fibers in polymers). Piecewise polynomial representations have seen less use for these applications, although for the textures of metals the probability distributions for lattice orientations have been described effectively with piecewise functions over an irreducible subset of orientation space. These are finite elements having the same interpolant properties as elements employed in a host of other solid mechanics applications to discretize the volume of the solid. Initializing the nodal point values from data can be approached from the perspective of an L_2 projection. In fact, a cadre of numerical tools are available to assist with the initialization, evolution, and interrogation of distributions that are approximated with finite element discretizations.

Given a probability distribution of the attribute, one can generate a sample of material with the geometric features explicitly enumerated. Conversely, given a material sample of sufficient size (meaning that the sample contains an enumerated set of the geometric features), the statistical description of the attribute can be deduced from suitable analysis of the population. To do this unambiguously, a well-defined relationship between attributes and geometric features is crucial. Having it enables one to effectively bridge between material length scales so that properties may be derived from interrogation of those features that in fact control the behavior.

2.3. Resultant properties

Typically, a property is obtained either by averaging individual responses in accordance with the probability distribution of an attribute or by integrating the response over the volume of a sample of material. Both of these entail relating the resultant property to the individual responses via a number of modeling assumptions, assumptions that introduce uncertainty. Issues center around the sensitivity of

averages to details of the representation of structure and to the assumptions embedded in the model. Assumptions that render bounds in the behavior are particularly useful, especially if both upper and lower bounds are available, as discussed later. Care is required, in that the bound is typically on the instantaneous value of the stress, and not on the evolution of state. A lower bound computation may give higher stresses after some deformation history than an upper bound because the state evolves differently in the two models.

3. Macroscopic applications

Strong motivation for multiscale models is derived from applications at the macroscopic scale. Typical of these are problems involving a workpiece or component whose characteristic dimensions are orders of magnitude larger than that of a single crystal. For decades, strictly macroscopic theories have provided quite valuable representations of material behavior, ones that have been widely used in finite element formulations. Isotropic plasticity theory based on the von Mises yield condition with an evolving yield strength is an excellent example. But the demands on simulation have exceeded the capability of such macroscopic theories, especially in terms of some of the 'second-order' effects observed. The anisotropic yielding of a metal is one behavior in which the macroscopic theories have been inadequate to describe both the yield criterion and its changes over large strains. To a limited extent, multiscale models have already met this challenge through the introduction of crystallographic texture and its evolution in large strain applications. There are notable instances of the inclusion of other geometric features, or probability distributions describing an attribute of a feature, in computations at the macroscopic scale. This trend will continue as the benefits are great, the physical motivations are compelling, and the costs are reasonable.

3.1. Computational tasks

Regardless of the choice of the representation of material structure, certain tasks must be accomplished whenever features of the material are much smaller than the characteristic dimensions of the finite elements used in a simulation. Bridging of length scales implies the exchange of information both from smaller to larger and from larger to smaller dimensioned features. This necessitates partitioning the motion (deformation and rotation) among the individuals of a population and querying the individual behaviors to obtain effective properties of the population. The partitioning can be defined by an assumption, such as all structural units experience the same deformation, or it can be determined by applying balance laws to a sample of material with appropriate structural definition. For polycrystal behavior, for example, a number of assumed partitions (or linking rules) have been postulated and used, including: Sachs, Taylor, Relaxed Constraints, Constrained Hybrid, and Self-Consistent (with several extensions — Kocks et al., 1998). Of these, a few are particularly important as their relationships to the correct solution are well understood. Upper bounds require a kinematically admissible motion and equilibration of the internal and external rates of work. The uniform straining assumption of Taylor is the most widely applied example (Hutchinson, 1976). Lower bounds require static equilibrium plus restrict stress levels not to violate the yield condition. Lower bounds can be constructed based on a uniform stress assumption (Berveiller and Zaoui, 1978; Prantil et al., 1995). Self-consistent theory can for special circumstances give a solution that satisfies both compatibility and equilibrium. The choice of linking assumption influences the predicted behaviors in a number of ways, not just the stress level for an imposed deformation computed using the assumption. For example, texture evolves quite differently over large strains for different models, which is well documented. The linking assumption also impacts such responses as the magnitude of the yield stress asymmetry (Bauchinger effect — Barton et al., 1999)

and the relative change in stress (as measured by a Taylor factor) for different loading directions in a textured material (Miller and Barton, 1999).

3.2. Alternatives in structure representations

When representing the material structure within finite elements, it is possible to construct a sample of material having the appropriate features, or to employ a probability distribution associated with attributes of a feature. Considering again the crystallographic texture, for example, one could create a polycrystal in which each grain has an orientation specified so that the polycrystal exhibits the correct texture, or one could specify an orientation distribution without ever indicating the actual spatial arrangements of grains. The former is a sample of the material having the correct texture; the latter is a distribution function for an attribute (lattice orientation) of the crystals. The former is a body, while the latter is a characterization of one aspect of the state. On one hand, by defining a sample having smaller scale features and treating that sample as a body itself, it is possible to incorporate the effects of interactions directly. On the other hand, by representing the smaller scale features as attributes with an appropriate probability distribution together with a simple linking rule, efficiencies in the computation may be realized. The question arises: is it better to construct a sample of the material having the smaller scale features or improve on the linking assumptions so that one needs only to retain a distribution of an attribute? The former requires solution of a boundary value problem to ascertain the material response and typically will be more expensive. The latter often is very efficient, but typically does not capture the interactions between individual structural features well. Simple linking rules often are not reasonable assumptions for more complex materials (such as ones with multiple phases), but new linking assumptions are difficult to develop, especially for general loading.

To date it has been more common for simulations to be conducted using probability distributions of attributes, mainly because of computing resource limitations. However, there are a number of investigations that locally employ samples built from structural features, such as near crack tips or interfaces with particles (Cuitino and Ortiz, 1992; Ortiz, 1996). The high costs that limit the definitions of material samples with particular structural features are most likely short-lived, opening the possibility for choices to be made on the fidelity of representations, rather than their expediencies. With the continued growth of computational power and with increased recognition that the variability in properties arises from the inherent variability in structure, a persistent trend will be to bring ever greater material detail, and thus samples of the material itself, into simulations wherever properties are needed. A compromise strategy is likely to be two-fold: simple assumptions which provide bounds will constitute the majority of the simulations; simulations having samples of the structure at finer scales will augment the bounds when greater accuracy is required. The reason for this conjecture is that the simpler bounds are easy to apply, and taken together can bracket the stresses computed for the system. If a more refined answer is needed, the much greater confidence accompanying the use of a material sample will more than offset the added computational burden.

3.3. Gradients in structure

As stated in the previous section, the features that comprise a material structure do not exhibit widely separated characteristic lengths. Nor are they necessarily distributed uniformly over the material volume. This has the consequence that it may not be possible to think of the probability distribution of a given attribute as being independent from point to point. Rather, there may be significant changes in the attribute across the volume of material that is sufficiently large to define the distribution. In fact, gradients in the material structure exist in any material that has undergone plastic deformations (Hansen and Mecking, 1976; Honneff and Mecking, 1981). Element size and gradient magnitude may become

linked. Unlike the discretization of the motion, where a large gradient can be handled well (given it has simple form), strong gradients in the structure may cause large property variations, and may lead to failure of the numerical techniques to deliver answers, as is discussed later. Given that the relevant aspects of the material structure are in the form of distribution functions, then it becomes important to quantify the sensitivity of the properties to details of these distributions. Particularly important for our analyses is the extent to which the resultants are in agreement with macroscopic models, such as commonly used nonquadratic yield surfaces for the anisotropic yield surface.

3.4. Trends

A number of application areas are emerging in which simulations are playing vital roles. Metal forming simulations have been important due to the desire to predict changes in state with forming, both to produce advantageous properties and to avoid detrimental ones. A second area is in long-term behavior of components, including such topics as void migration in electronic circuitry and in fatigue initiation under cyclic loading of structural metals. A somewhat different theme in the area of forming simulations is the interpretation of mechanical tests designed to obtain material properties. Formability testing is a good example. The connections between the processing history and the mechanical performance lie with the material structure, particularly in how it varies as a consequence of forming differences. Simulation of the formability test itself can reveal or confirm the structural origins of behavioral differences, and can bracket the range in behaviors that can be attained through modification of the structure (Dawson and Beaudoin, 1997). Thinning of material in the limiting dome height test as it is affected by crystallographic texture has already been the focus of simulations. Those simulations confirm that certain features of the texture, ones which can be altered by judicious choice of rolling schedule, have strong effect on formability measures deduced from experiments. A host of other tests and properties are awaiting closer examination in this way. Another topic that is expected to draw considerable attention is the modeling of the elevation of the strength of the material with straining. Dislocations are not evenly distributed in materials that have been deformed, but congregate into features such as bands or walls. Hardening models now under development take into account more information about the distribution of dislocations than just the average density of dislocations and should provide a better basis for computing the evolution of the strength.

4. Material structure applications

The earliest examples of combining crystal plasticity with finite element analyses involved using single crystal behavior within an element instead of an isotropic yield criterion. An important application area that has been given considerable attention over the years is that of strain localization (Peirce et al., 1983; Anand and Kallidindi, 1994) with the intent of relating shear band formation to crystallographic texture. A variety of other issues are being examined currently with a similar window on the material: samples with crystals numbering in the 100's to 10,000's, resolved with just a single element or with many elements per crystal, and having two or three dimensional geometry. Many of these focus on the heterogeneous deformations that occur within a polycrystal that influence the mechanical response and evolution of state.

4.1. Crystal interactions

Early in deformations, before onset of localizations characterized by such things as shear bands, the issue of the crystal to crystal variability of straining becomes important, especially as it concerns the

evolution of texture. This has been investigated with finite element simulations (Harren and Asaro, 1989; Becker, 1991; Becker and Lalli, 1991; Kalidindi et al., 1991; Beaudoin et al., 1995a), with the intent, in part, of testing applicability of linking hypotheses for various crystal types under relatively simple loading paths, such a plane strain compression, compression with uniaxial stress, and simple shear. Results have been interesting: variability in straining has at least two important effects. First, it introduces loading path changes locally that drive the texture evolution in ways not captured by simple linking assumptions such as a Taylor hypothesis. This is evidenced by the occurrence of the brass texture component in FCC metals under plane strain compression (Beaudoin et al., 1995a) or the split of the c-axes in HCP polycrystals (Dawson and Marin, 1998), also under plane strain compression. Secondly, the heterogeneity in the deformation is dependent on the local neighborhood strongly. There is an expected correlation to orientation, but it is weak in comparison to the influence of the neighboring grains (Sarma and Dawson, 1996a). Such simulations have been repeated for a number of material types (FCC, BCC and HCP) with the similar trends computed regarding the importance of local neighborhood on the heterogeniety of deformation. Further, the trends across crystal types are consistent: higher variability with increased single crystal yield surface anisotropy.

The results can be condensed in such a way as to extract data for constructing a modified linking assumption. This has been done for the case of FCC crystals with some success (Sarma and Dawson, 1996b), but difficulties do arise that will limit this approach. In particular, there is no effective way to treat the impact of local neighborhood on the variability of the spin terms. This is critical to structure evolution, but requires an additional level of design of the simulation to extract pertinent data. The difficulty in quantifying the important contributions to the linking assumptions implies that simpler rules that are bounds, and perhaps variants of the self-consistent formulation, will be the mainstay of large scale simulations that employ representations of material attributes. More accurate linking assumptions, while highly desirable, are quite difficult to construct well. Given the gains of true multiscale models, it is unclear that any effort in developing a new linking assumption is cost effective, unless it would provide an improved bound. This is especially true for polyphase materials and mixed mode deformations (slip plus twinning, for example). Polyphase systems are extremely important as engineering alloys, and true multiscale models are expected to bring a much more complete understanding of their behaviors.

4.2. Crystal substructure

A very active and productive thrust is focused on attempts to merge the explanations of hardening and anisotropy from crystal plasticity and dislocation mechanics. Polycrystal plasticity theory and simulation have been able to describe the evolution of texture relatively well (for single phase materials) (Kocks et al., 1998). In addition to the evolving texture, these analyses give estimates of geometric hardening and yield surfaces, plus quantities that can be computed knowing the yield surface (or information adequate to construct the yield surface). The calculation of R-values is an example, although this particular case involves yield surface curvature, which is not predicted as well. On the other hand, dislocation mechanics offers excellent theory for kinetics of plastic flow (mainly averaged over structure) and explanations for material hardening (particularly the correlation of back-extrapolated yield strength with dislocation density). There is also an expanding observational data base on dislocation structure as correlated with loading and material attributes (especially stacking fault energy), although the implications of this for the strength are still largely unquantified. Herein lies a number of opportunities to develop a more fundamental understanding of strengthening in metals. There already are notable examples where modeling has been successful in reproducing features of subgrain structure associated with cells: with high resolution of mesh, cellular subgrain structure emerges (Beaudoin et al., 1995b; Panchanadeeswaran et al., 1994); with lower resolution of mesh, misorientations

are detectable (Mika and Dawson, 1999), and quite importantly match reported correlations in experimental data for the scaling relationship and the average angle versus strain (Hughes et al., 1997). A complete explanation requires the successful modeling of dislocation structures that make up geometrically necessary boundaries, including the relationship of the orientation of those boundaries to the loading and the influence of the material type on the character of the boundaries.

5. Elastoplastic issues

The elastic shear moduli for bulk samples of common engineering alloys typically are orders of magnitude larger than the strength for the corresponding material. Even when the single crystal elastic constants are considered, the point is the same: the strength is much smaller than the stiffness. As a consequence, the magnitude of elastic strains remains less than 10^{-2} (with the exception of volumetric strains associated with large temperature changes or large pressure changes). During large deformation events, such as in forming operations or crash impacts, the elastic strains are a small part of the total strain. However, the elastic response is a critical aspect of the response in a number of ways. This is due in part to the fact that the elastic deformations are a measure of the distance that the metal lies from its natural state, and thus quantifies an important driving force for change in the material. At the crystalline level, elastic strains indicate the strain energy level available to advance structural changes associated with recovery or recrystallization, and relate directly to crystal lattice spacings. Through the inclusion of material structure, a variety of issues that pertain to the elastic response can be examined in more detail. For example, the residual stresses arising from inhomogeneous deformations at the level of individual crystals can be quantified for use in studies of recrystallization. Reloading, or just changes in loading path, can be investigated in terms of transients associated with changing proportions of elastic and plastic straining, an aspect of the behavior that requires rigorous underpinnings in the simulation models.

5.1. Kinematic decompositions

Historically, macroscopic elastoplastic numerical formulations have grown out of those developed for elastic response. Early extensions were limited to motions that were geometrically linear, but increased sophistication in the formulations eliminated these restrictions. Today, the formulations for macroscopic analyses are mature, with well-documented methodologies available. The introduction of material structure has added complexity in the form of decompositions of the motion into parts associated with elastic and plastic modes of deformations, and possibly other modes that are affiliated with discontinuous motions (Lee, 1969; Teodosiou and Sidoroff, 1976; Needleman et al., 1985; Bammann and Johnson, 1987). Such decompositions are postulates of the behaviors, rather than being direct consequences of the motion alone, and are dependent on the nature of the mechanisms of deformation. As such, crystallographic slip admits a different decomposition than twinning, for example. Decompositions differ most with respect to the orientational changes of the features associated with the mechanism of deformation. The trends toward more physically based formulations, ones that explicitly embody multiple deformation mechanisms, raise the issue of meaningful or unique configurations and, in particular, where the stress-free configuration lies in relation to the current (or loaded) configuration. Here, we do not attempt to offer a general decomposition for this purpose, but rather only flag the issue as one that requires reexamination on a case-by-case basis as the scales of features becomes more numerous and disparate.

5.2. Elastoplastic transients

The domains of behavior for solids are usually simplified to only two: elastic, as characterized by the stress being inside the yield surface, and elastoplastic, with the stress being on the yield surface. A loading condition is appended to better define the situation under elastoplastic conditions: loading for increasing stress with concurrent yield surface expansion; unloading for decreasing stress with incipient change to elastic response; and neutral loading, with the stress traversing a static yield surface. Multiscale models are providing new insights into the transition from elastic to elastoplastic response, and into the nature of the short duration transients associated with the transition. For example, definitions of yielding include ones based on offset strains and ones employing back extrapolation techniques. Microstrain offset definitions have been viewed as providing the actual demarcation between elastic and elastoplastic responses. The back extrapolated definition quantifies the yield surface location following a brief structural transient. This transient often is modeled with a back stress, a quantity that evolves over the brief transient and signifies a change in the material state. However, elastoplastic models of crystal behavior involving plastic flow via slip deliver both the microstrain yield point, followed by a brief transient in the stress. By the end of the transient, the back extrapolated definition is recovered. The transient is generated through interactions among crystals, and can occur without change in crystal orientation or slip system strength. Rather, changing proportions of elastic and plastic strain rates renders a transient in the stress. One point to be made here is that the averaged behaviors of populations of material features may delete critical interactions, with the result that observed responses are captured with variables that do not reflect the same basic physical behavior as exists in the structural features themselves. In this case, the macroscopic response embodies a changing yield surface to capture the transient even though the crystal yield surfaces are unchanging. Once again, a clear distinction between state and state variables is required. Simulations offer the prospect of separating the effects of different mechanisms at a smaller length that merge in a combined behavior observed at a larger scale, and thus of more precisely attributing behavior to the proper source in the material.

6. Numerical trends

Probably to a greater extent than other disciplines, solid mechanics has made pervasive use of the finite element method as a workhorse of numerical simulations. The reason is fairly obvious: the method is well suited for applications having complicated geometries, mixed types of boundary conditions, nonlinearities in either the material behavior or the kinematics of the deformation, and temporal evolution, which are all encountered commonly in the mechanical response of solids. While commercial codes are mature at this point, for the most part they treat the entire problem at a single scale, usually the macroscopic level. New capabilities are needed, however, to assist with the demands placed by introducing an extensive description of the material structure. This trend is likely to intensify because it is a more certain course to incorporate the structure directly than to devise new macroscopic models abstracted from the computed (or measured) responses of sets of substructures. But the inclusion of structure, and the needed interrogation of it to evaluate properties, means that the cost of the material-related proportion of simulations can be substantially higher than before, necessitating greater attention to the methodologies employed. For example, there are issues associated even with convergence: variability of properties across the domain of an element and the impact of such variability on the order of integration necessary to guarantee unique answers. There are opportunities to optimize the performance of analyses in which both the geometry and the material domain are represented in discretized forms.

6.1. Hybrid formulations

Finite element implementations for elastic and elastoplastic response of solids at the macroscopic level have been dominated by displacement or velocity based formulations. Hybrid methods have been available for many years, but have played only a relatively minor role in solid mechanics simulations (Tong and Pian, 1969; Atluri, 1975; Bratianu and Atluri, 1983). Hybrid methods invoke the concept of domain decomposition, which can be a major advantage in light of the reality that materials naturally have domains, and that reflecting that reality in the computations can lead to more effective formulations. Namely, hybrid methods permit the definition of spatial domains within a body with the application of constraints between domains. An immediate example is grains, with traction equilibrium necessary at grain boundaries and continuity of motion across the grain boundaries (Beaudoin et al., 1995a). For highly heterogeneous materials, it is expected that the ability to explicitly specify the domain constraints will offer real advantages so that hybrid techniques will assume greater importance for plasticity applications.

6.2. Discretization of material parametrizations

In many instances, structural information may be represented with sufficient precision using a probability distribution to describe the likely values of a particular attribute. The parameters that depict this attribute form a space, or domain, which can be discretized for the purpose of representing the probability distribution in simulations by a variety of methods. The parameterization of the space provides a means for defining the range of the value that the attribute may assume. A common example is a three dimensional space for lattice orientations, such as given by Euler angles (Bunge, 1982) or an angle–axis pair (Altmann, 1986). A less common one is the space that describes crystal size, with the probability density giving the likelihood that crystals with particular size will exist within a particular sample. An emerging trend is to exploit the methods developed previously in solid mechanics for discretizing the volume of a body and representing field variables on this discretization for the describing the probability distribution of an attribute in a material domain. The domain of a material feature is divided into finite elements and piecewise polynomials are used to represent a variable over the elements. Such a method has already been presented for describing textures: choose an appropriate parametrization and then represent the probability distribution over that parameterization using the usual finite element interpolants (Kumar and Dawson, 1998a). Many of the same advantages are realized for the representation of the material attributes as have been realized for motion of a body in solid mechanics. In particular, it is possible to prescribe the level of continuity, to adapt the discretization to features of the probability distribution (more elements where gradients are high), and to invoke methodologies for assessing accuracy. This is quite difficult or cumbersome to accomplish with representations based on a numbered list of entities (a discrete set) that by their occurrence give a specific sample taken from the distribution.

For example, consider the specific task of initializing a distribution for simulation based on values experimentally measured. The specification of initial conditions in a manner that is consist with the discretization is a well-understood procedure for finite element analysis. Nodal point values are evaluated by an L_2 projection of initial condition data onto the discretized parameterization. This is very direct for a finite element discretization of texture: from discrete orientations one evaluates nodal point values. Of course, the level of discretization must be consistent with the density of data available and its distribution over the space. This constraint translates into levels of discretization (numbers and positions of elements) of the domain of the attribute. This is being applied to the evaluation of textures of rolled plate using data from electron back-scattered pattern measurements directly, and indirectly

from probability distributions of pole densities based on harmonic functions whose coefficients are determined from X-ray diffraction measurements (Dawson et al., 1998).

Using a governing equation stemming from conservation of geometric features (such as the volume of crystals comprising an aggregate), the probability distribution can be updated to reflect the changes that accompany deformation (such as the reorientation that accompanies slip in crystals). This has been done in detail for FCC crystals deforming by slip (Kumar and Dawson, 1998a), and recently extending to incorporate combined slip and twinning in either HCP or FCC crystals (Myagchilov, 1998). It has also become routine in other applications, such as fiber reorientation in polymer systems. This is not necessarily a simple task, even though it nominally is the same as the evolution of field quantities such as temperature changing under transient conduction. Because the spaces may be non-Euclidean, as is the case in lattice orientations, and the driving force for change is derived from the physics of plastic flow, the complexity of the formulation can be high, serving as impediment to more widespread use of the approach.

6.3. Computing environments

Implementing the models so that simulations can be conducted has been, and will continue to be, one of the factors limiting progress. Implementations that efficiently deal with multiple scales involve parallel computing both because of the long execution times and the heavy memory demands. Finite element simulations involve a number of different classes of tasks from a parallel computing perspective. Computations at crystal level to evaluate stresses or update lattice orientation are embarrassingly parallel. Other aspects involve quite complex data motion, generating the need for unique gather–scatter operations to handle data on unstructured meshes involving both locally and globally defined variables. But the software that enables parallel computing is still in a state of flux, in part because the trend in hardware has been away from systems dedicated to massively parallel computing (such as the CM machines) and toward clustering of multipurpose workstations. The 'all-encompassing' high level language has not developed much, if any, beyond CM Fortran with its advanced scientific libraries. Rather, a two part infrastructure has emerged, one part being for the computations and the other being the communications. For us, this has been a combination of a higher level language with parallel features (Fortran90) and a communication interface (MPI — Gropp et al., 1994). Code use related to multiscale analyses in the coming years will likely involve a high level of scripting, so developers might expect some percentage of use to be within an environment in which a variety of tools are combined via scripting languages. An example could be a simulation that first constructs a material sample, performs a suite of tests on its physical response, and then seeks to recognize trends from the computed fields. In this environment, the need for a fundamental replication of material, one based on observable features and attributes of the material and having a layered representation capable of a suite of interactions, plays a crucial role.

7. Summary

Metals exhibit very interesting and complex behaviors when stressed beyond the elastic limit and into the regime of plastic flow. Structural changes occur that affect the mechanical properties and continued plastic flow. A major trend in computational mechanics is to incorporate detailed representations of the material structure directly into numerical simulations. The intent is to have available features of the structure that control the mechanical behavior and that may be interrogated on the fly to obtain mechanical properties. The approach allows complex behaviors to be modeled through the interactions

of relatively simple structural features, and circumvents the need to postulate more involved macroscopic models that are adequate to capture such behaviors.

A major challenge associated with this trend is that there are many features of the structure that influence properties such as strength and ductility. Further, these features often are comprised of populations with complicated and evolving distributions. Complex interactions among individuals of the populations control the manner in which deformations are partitioned and loads are carried by a material. Multiscale modeling offers an avenue to simulate material response involving these behaviors and to permit predictions with greater fidelity to the actual material. Not only should we be able to estimate the response of a typical sample, but we also should be able to predict the variations in reponses demonstrated among nominally identical samples arising from the customary differences in processing and loading history.

The consequence of this trend is that the field of computational mechanics is moving into an era in which all aspects of plasticity simulations are more numerically intensive, but especially those dealing with the material behavior. The detailed representations of structure are augmented by more highly quantified measurements of the structure (Adams, 1997), with the result that the structure may be more accurately initialized for simulation, and the predictions can be more thoroughly verified through direct comparison to experimental data. The principal benefit is greater capability of simulation to deliver results that aid in developing engineered components having superior performance and longer life.

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