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Modeling and experiments in plasticity

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Abstract

We focus on challenges in advancing the modeling of plastic flow processes to incorporate distinct characteristics of various length scales within materials and structures. The motivation is twofold. First, the goal of tailoring the material microstructure to control plastic deformation and related failure processes is of great economic importance. Product development cycles have become so short that traditional empirical approaches to alloy modification are noncompetitive in the global marketplace. Second, materials selection and design for durability, which rests upon our understanding of phenomena occurring at microstructural scales as well as at the scale of structural components, is of critical importance as we head into an era where an extensive infrastructure must be maintained. Cost constraints on new systems dictate much more quantitative design and analysis procedures than in the past. Research needs are discussed in a number of key areas involving experiments and modeling, including: experiments conducted at multiple length scales of resolution; principles for multiscale modeling and scale effects in plasticity; coupling of plasticity-induced damage with texture and phase transformations; progressive cyclic deformation and failure; microstructure-scale plasticity of cast alloys and low symmetry polycrystals; and employment of massively parallel computing to determine model parameters and forms of evolution equations for internal structure variables. © 1999 Elsevier Science Ltd. All rights reserved.

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1. Introduction

In terms of importance to the infrastructure of power generation, transportation vehicles and engineering structures, now and into the foreseeable future, metals and their alloys represent the most economically significant class of engineered materials, in the U.S. and abroad. Inelastic deformation of metals at temperatures less than about 40% to 50% of the melting point is governed primarily by the generation and crystallographic glide of dislocations. Prior to the 1930s, foundational concepts of

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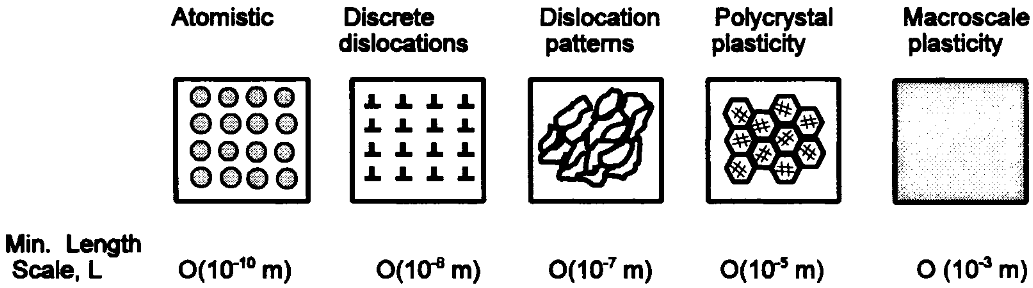

Fig. 1. Window of resolution for dislocation plasticity/viscoplasticity, including the typical minimum explicit length scale of resolution at each scale.

plasticity were introduced to model the observation of yielding and plastic flow in metals based on distortion energy and maximum shear criteria. Since the identification of dislocations and the atomic origins of slip in the 1930s, enormous advances have been made in understanding the underlying physics of plastic deformation. This has advanced theories of plasticity, including the description of evolution of polycrystal texture, dislocation interactions and hardening laws. Much has been learned about the physics of strain hardening, dislocation interactions, and effects of second phases and high angle boundaries.

The richness of the history of investigation of elastic–plastic behavior of metals imparts a sense of venerate maturity to the subject. In view of the complexity of observed behavior, much of this maturity underlies the engineering theory of plasticity. It is of undisputed utility. Yet, we are in a rather primitive stage of developing models for plastic deformation of metals that are true to the physics of real material systems. There are ranges of applications for which we have no acceptable models. Existing theory is best described as a calibration of experiment, with little predictive capability.

There is good reason for this. Plasticity is a phenomenon that is affected by kinetics and processes of dislocation generation and interactions occurring across a wide range of length scales. The fact that quasi-stable, nonequilibrium configurations of lattice defects exist at multiple scales, combined with the long range nature of interaction forces between atoms and clusters of multiple phases, renders the assessment of internal stress fields supremely challenging, let alone the evolution of these configurations (e.g., plastic flow and its resistance). Long range order presents complications to the theory in terms of scale effects. Here, there are few parallels to the analyses of turbulent flows of Newtonian fluids, where short range molecular interactions predominate and the long range order appears only in the nature of transport processes. No first principles analyses have ever been performed for quasi-static deformation at larger microstructural scales of heterogeneity, due to severe computational restrictions on atomistic calculations. At the atomistic scale, the problem is inherently nonlocal, with contributions to the forces and deformations of individual atoms deriving from a large ensemble of atoms, as expressed in the theories of quantum mechanics or various approximations found in molecular dynamics. Continuum theories often take the liberty to cut off nonlocal action to facilitate a local treatment, largely irrespective of the gradients of long range forces that may occur at a particular scale of homogenization. There are at least five length scales at which plasticity may be addressed, as shown in Fig. 1 below. From left to right, the salient scales are atomistic (molecular dynamics), collections of dislocations (discrete dislocation theory), sub-grain dislocation substructures (continuously distributed dislocation theory), grain (crystal plasticity theory) and macroscale (classical kinematic–isotropic hardening theory with a macroscopic flow potential). Solid solution or precipitate strengthened metallic alloys, multiphase alloys and whisker, particulate or fiber-reinforced metal matrix composites each exhibit additional length scales intermediate to those depicted in Fig. 1 which affect the hardening and flow behavior, as well as the interaction and growth of defects such as microvoids. Of course, we omit time from explicit consideration here, but note that dynamical atomistic approaches are severely limited to short time scales, whilst the others are amenable to quasi-static cases. Moving from left to right in Fig. 1, we may roughly describe the state variables for a representative window as decreasing in number in accordance with a shift from characterizing the full dynamical state to the thermodynamical state of the system.

Indeed, plasticity must be considered as a subject whose veracity depends on the eye of the beholder. The basic engineering theory builds on the concept of a yield surface in either stress space or strain space that serves as a plastic flow potential subject to certain stability or dissipation arguments, leading to convexity of the yield surface and normality of the plastic strain rate to it. There are sound physical bases for the first order theory when one assumes dislocation glide to be uniquely driven by associated slip system shear stresses within each grain (Rice, 1971), averaged over a polycrystalline structure. The basic theory, of local nature and expressed at the macroscale (far right in Fig. 1), enables estimation of required forces and plastic flow in important technological applications such as stamping, drawing, rolling, forging, extrusion, impact, high speed machining of metals, collapse of structures, indentation, elastic–plastic fracture and fatigue at notches. It a is robust and proven tool for approximation of the inelastic behavior of structures.

However, the intense interest in moving down through the length scales is evidenced by the many international conferences dedicated to the subject (e.g., Plasticity '91, Plasticity '93, Plasticity '95) and inclusion of sessions on this subject in nearly every major conference in solid mechanics. What is the practical significance of these current trends? Presently, we cannot 'close the loop' on material structure–property relations. If we have a material that has been well-characterized for a *specific* heat treatment, composition (and gradients), process history and loading path, the engineering theory at the macroscale can provide reasonable estimates of flow stress and plastic strain. However, even in this case it will be difficult to predict material ductility due to void nucleation and growth for various applications beyond those used to fit constants, or to predict fatigue or fracture characteristics.

In what follows, we will focus mainly on the issue of various scales of processes that occur during plastic deformation and experiments and models that address collective behaviors at these scales. The discussion of discrete dislocations pertinent to thin films or other nanostructures is left to another Chapter, as are considerations of thermally activated motion, dynamic plasticity, a more focused discussion of scale effects, and nuances of computational crystal plasticity. After providing an overview, we discuss the practical benefits of pursuing plasticity experiments and modeling at various length scales, and then discuss specific areas of research need.

2. A brief overview of the field

The 1940s–1950s witnessed the origins of the modern theory of incremental plasticity which addressed the existence of a flow potential for plasticity of metals, along with related issues of material stability, convexity and normality to the yield surface in stress space (Drucker, 1959) or strain space (Il'iushin, 1961). We omit many of the significant theoretical developments concerning the structure of the macroscopic theory for sake of brevity here. The kinematics of crystalline slip had been established earlier in the century by Taylor (1938) and co-workers, following the independent postulation of dislocations in 1934 by Taylor and Orowan. The principle of maximum plastic dissipation proposed in the 1920s served as a pre-cursor to developments by Taylor (1947), Hill (1948) and Bishop and Hill (1951) that have laid a foundation for the general theory of plastic flow of crystalline metals.

As test control capabilities improved in the 1970s, experiments became more sophisticated, examining effects of loading path direction changes and yield surface probing schemes addressing distortion of the yield surface as a nearly continuous function of the loading path (cf. Hecker, 1976; Phillips and Lee, 1979; Shiratori et al., 1979a, 1979b) for both large strain and relatively small strain histories. Verification of the yield surface as the plastic potential was undertaken rather aggressively, with support for associative flow arising from most conditions examined. Without devoting the space deserving of these many investigations, suffice it to say that these studies revealed the full complexity of the problem of the behavior of metallic polycrystals under general loading paths. From the macroscopic viewpoint, the deformation of the yield surface is highly complex, requiring a fairly substantial tensorial framework with numerous constants to model the distortion and rotation in stress space for each point in a deformation history.

The notion of elastic deformation with respect to the underlying undeformed lattice (isoclinic configuration) had been firmly adopted by the early 1970s (cf. Mandel, 1973). By the late 1970s, the viability of crystal plasticity as a descriptive computational tool for overshooting behavior, hardening and polycrystalline texture development had been established (cf. Asaro and Rice, 1977; Asaro, 1983; Kocks, 1970, 1987). This continuum theory (cf. Havner, 1992; Yang and Lee, 1993), emerged as an extension of the early work of Taylor (1938), offering a vehicle to enhance description of plastic anisotropy that emerges naturally from the discrete nature of crystallographic slip, as well as the development of crystallographic texture (lattice rotations to accommodate kinematical constraints), as depicted in the box second from the right in Fig. 1. Indeed, this theory provides a significant step forward for realistic modeling of the kinematics of plastic deformation due to dislocation glide, while leaving some of the other aspects necessary to ‘close the loop’ on structure–property relations for further development.

A considerable body of research developed concerning various self-consistent models of polycrystalline behavior based on the crystal plasticity construct applied at the level of individual grains (cf. Kröner, 1961; Budiansky and Wu, 1962; Hill, 1965; Hutchinson, 1970; Havner, 1973; Iwakuma and Nemat-Nasser, 1984; Nemat-Nasser and Obata, 1986; Molinari et al., 1987; Harren et al., 1989; Harren and Asaro, 1989). More recent work has focused on finite element calculations involving large numbers of grains (cf. Mathur and Dawson, 1989; Anand and Kalidindi, 1994). Key issues include the modeling of the collective stress–strain behavior, the proper rate of texture evolution, shear localization as affected by crystallographic anisotropy and the development of hardening laws at the slip system level that account for self hardening and interactions among slip systems (latent hardening). Much of the work in the 1970s through 1980s focused on hardening laws (cf. Havner, 1992), predominately of intragranular nature. Measured yield loci related to very small offset definitions or deviation from linearity exhibit marked translation away from the origin, necessitating additional considerations in the hardening laws (cf. Weng, 1987; Bassani, 1990).

The 1980s witnessed a restatement of the need to consider rotation of material microstructure in establishing physically based incremental macroscale theories of finite deformation plasticity (cf. Drucker, 1984), and the advent of attempts to imbue macroscale plasticity theories with representation of plastic rotation of substructure during finite straining of materials with oriented internal structure. This internal orientation of substructure then plays the role as the reference configuration for hyperelasticity, essentially reflecting the role of the lattice. Various formulations for the anti-symmetric part of the plastic velocity gradient, the plastic spin, were proposed based on physical arguments or representation theorems for antisymmetric isotropic tensor functions (Dafalias, 1985) or micromechanical arguments for substructure spin (Aravas, 1994).

2.1. Microstructure and continuum plasticity theory

Further refinements are necessary within the theory of crystal plasticity to address some common experimental observations. These fall principally into three categories: formation of low energy, non-equilibrium arrangements of dislocations into organized patterns such as ladders, veins, cells and microbands well below the scale of the initial grain size; generation of geometrically necessary dislocations that serve to accommodate lattice misorientation or polyphase strengthening in polycrystals; and identification and modeling of non-Schmid and nonassociative behaviors that arise from averaging over various micro-frictional processes such as shear of microvoid or excess vacancy sheets along heterogeneous shear bands within the crystal (slip is rarely homogeneous), and from the microscopic plastic rotation fields associated with the first two categories above.

There have been a few attempts to cast the effects of dislocation substructures directly into hardening laws. This requires the recognition of hard (cell walls or ladder & veins) structures interspersed among soft (dislocation free) material, as in a two phase composite. Kratochvil (1990) presented an explanation for the driving force for heterogeneous substructures as a consequence of instability of a uniform dislocation density in deformed metals. Muller et al. (1994) introduced a nonlocal constitutive law obtained by application of Green's functions representing the effects of dislocation substructures on kinematic hardening behavior of the 'composite' structure. Similarly, Freed et al. (1992) applied composite micromechanics to the calculation of the strengthening effect of dislocation cell structure.

Hughes and Hansen (1995) and Hughes et al. (1997) have recently discovered a scaling principle that describes the manner in which dense dislocation walls composed of geometrically necessary dislocations form and refine their spacing during finite straining of high symmetry cubic crystals. They find that these boundaries separate domains comprised chiefly of dislocation cells which are substantially disoriented relative to neighboring domains, leading to microtextures. After strains on the order of 1.5–2.0, the orientation distribution of these cell blocks over traverse of only a few microns effectively spreads over the standard stereographic triangle of orientations. This negates the notion of the original grain as the fundamental unit of orientation following substantial plastic flow. Implications for the diffusion of texture and complexity of workhardening processes within grains are evident. Various workers (Teodosiu, 1991; Leffers and Hansen, 1992; Rollett et al., 1992) have developed embryonic descriptions of the influence of these subdivision processes.

Under cyclic loading at small strains, the powerful influence of dislocation substructure is readily observed. About two decades ago it was first reported (Lamba and Sidebottom, 1978; Kanazawa et al., 1979; McDowell, 1983, 1985; Krempl and Lu, 1984) that cyclic hardening for certain metals and alloys subjected to nonproportional combined tension–compression and torsion greatly exceeded the level of flow stress observed under pure uniaxial or torsional (proportional) loading. Such experiments debunk the concept of a so-called 'universal' cyclic stress–strain curve even at small strains assumed in earlier theories of plasticity. This was attributed to enhanced dislocation–substructure interactions as the strain rate vector rotates relative to the material.

Recent developments have generalized nonlinear kinematic hardening relations to multiple components (cf. Chaboche, 1989; Moosbrugger and McDowell, 1990; Ohno, 1990), with association of each component to hardening processes at a different length scale, ranging from cell walls, for example, to grain boundaries or clusters of microtexture. Recognizing the basic deficiency of simple linear dynamic recovery models to capture cyclic plastic strain accumulation (ratchetting) in the presence of mean stress, also present in two surface models of cyclic plasticity (cf. Dafalias and Popov, 1975; Krieg, 1975) without elaborate and somewhat ad hoc subloading surface constructions, nonlinear dynamic recovery terms have been introduced to model ratchetting (Ohno and Wang, 1992).

It is fair to say the unified treatment of both small and large strain behavior represents an outstanding problem in the plasticity of polycrystalline metallics. The retention of short range kinematic hardening effects necessary for reverse yielding or abrupt strain path direction changes represents a challenge for a theory valid to arbitrarily large strain; further, the proper coupling of deformation-induced anisotropy due to large strains with subsequent cyclic behavior (cyclic deformation and fatigue) remains largely speculative. Practical applications include components subjected to primary deformation processing prior to service.

2.2. Heterogeneous plastic flow

It should be clear from the foregoing that metals are anything but homogeneous and monolithic. They are composite materials with some stationary and some evolving scales of heterogeneity. The problem of modeling shear localization in plasticity is often addressed as a principal concern in connection with heterogeneity. This is but one of many important issues pertaining to heterogeneity of plastic flow and hardening.

Discussion of heterogeneity naturally leads into consideration of polar and nonlocal theories of plasticity. Following on the heels of propositions of couple stresses (or torque stresses in unconstrained flows) in granular heterogeneous media by the Cosserat brothers (Cosserat and Cosserat, 1909) and subsequent related developments in micropolar and couple stress theories in elasticity and plasticity (Truesdell and Toupin, 1960; Kröner, 1963; Green and Rivlin, 1964; Eringen, 1972), a strong interest has emerged more recently in development of nonlocal, nonequilibrium theories to represent patterning or organization of defect structures and scale effects in hardening and flow (cf. Walgraef and Aifantis, 1985; Aifantis, 1987; Kubin and Canova, 1992; Gulluoglu and Hartley, 1992; van der Giessen and Needleman, 1995; Aifantis, 1995). Work by Dillon (1977) on the incorporation of strain gradients in plasticity was followed by contributions (cf. Bammann, 1984; Walgraef and Aifantis, 1985; Bammann and Aifantis, 1987; Aifantis, 1987; Zbib and Aifantis, 1992; Sluys et al., 1995) related to the influence of the gradients of dislocation density (diffusional terms in dislocation force–flux relations), and to approaches which admit material length scales to normalize the influence of strain gradients on the material workhardening behavior. Such length scales have eluded definitive characterization. Fleck et al. (1994) revisited dislocation–lattice curvature relations (Nye, 1953; Kröner, 1963) to explain scale effects in plasticity; they proposed that the development of constrained modes of plastic deformation (gradients of plastic rotation) due to dislocation glide in crystals is accommodated by generation of geometrically necessary dislocations (GNDs), providing additional strengthening beyond that of statistically trapped dislocations. It stands to reason that the GND density depends on geometrical characteristics such as grain size and the scale of the applied strain gradient relative to microstucture. The self-organization of GNDs into periodic low energy structures reported by Hughes et al. (1997) casts further complication into the role of dislocation substructures, consistent with the evolutionary theory of low energy, stress-screened dislocation structures (cf. Kuhlmann-Wilsdorf, 1989). Self-organization of dislocation substructures in plasticity is decidedly nonlinear and nonequilibrium and cannot be modeled using the standard tools of linearized irreversible thermodynamics (Glazov et al., 1995) or notion of a sequence of constrained equilibrium states (cf. Rice, 1971).

Some authors have proposed theories of plasticity in which microvorticity plays a dominant role. The scale of this vorticity is on the level of heterogeneities in the material, for example the spacing between inclusions, grain size, or other dominant features that enhance localization of plastic flow (cf. Panin, 1992). Constitutive treatment of couple stress effects associated with flow of granular materials goes back to the turn of the century (cf. Cosserat and Cosserat, 1909) and has been revitalized periodically since the 1950s. Techniques for modeling fields of microvorticity in granular materials (cf. Bardet and Huang, 1992) may be fruitful to pursue in conjunction with formation of material substructure instabilities such as shear or kink bands and microvoid sheets. A unified treatment of microvorticity is lacking in terms of conjugate thermodynamic couple–rotation relations. There presently exists some lack of uniformity of the treatment of plastic flow and concurrent material damage processes across the gamut of length scales, reflected by the very simplistic models of coupling of damage and deformation that form the present state-of-the-art. The relevant distinction of length scales associated with micropolar effects and/or nonlocal action has not received much attention.

Hence, the manifestation of macroscopic shear bands triggered by heterogeneity which has received so much attention in the literature is only indicative of a much deeper, richer set of physical phenomena that span the scales of length and time. Indeed, associative plastic flow in monolithic metallics is a fortuitous consequence of the intimate and relatively unique relation of glide dislocation velocity on each system to its conjugate resolved shear stress (cf. Rice, 1971) and statistically homogeneous averaging of the plastic deformation over suitably large volumes compared to characteristic lengths of heterogeneity. The nucleation of cavities into the flow field (separation and sliding of material surfaces and gradients of microvorticity) may destroy this associativity, for example, as may an highly heterogeneous field of local yielding as is typical of metal matrix composites (Dvorak, 1993).

2.3. Plastic compressibility effects

Drucker (1984) points to important issues regarding plastic compressibility and material stability at extreme pressures that yet remain to be fully resolved. Up to moderate pressure, plastic flow is relatively pressure insensitive apart from coupling with porosity (cavities). Experiments have long revealed the importance of modeling both nucleation and growth of voids in ductile metals. Rice and Tracey (1969) produced an early formulation for void growth and plastic compressibility effects. Subsequent development of yield surfaces and plastic potentials for the void growth problem represents one of the major advances of the macroscale continuum theory of plasticity in the last 20 years (cf. Gurson, 1977), enabling the modeling of bulk porosity effects on localized plastic flow and fracture (cf. Tvergaard, 1981, 1982; Mear and Hutchinson, 1985; Becker and Needleman, 1986; Needleman and Tvergaard, 1987). Such flow potentials have made significant impact on modeling, including porosity limitations in metal forming, constraint effects on porosity and shear localization in metal matrix composites and heterogeneous metallics, and constraint effects in elastic–plastic fracture process zone mechanics, to name but a few examples. The theory is yet incomplete with respect to several phenomena, including void aspect ratio effects on void growth in work hardening materials, effects of microstructure constraints on growth of small voids, effects of nonuniform void distribution on void growth and coalescence, and scale effects (nano-voids versus micro-voids) on collective void nucleation and growth. It is more correlative than predictive.

Modeling is still in relatively nascent stages but as pointed out by Ortiz (1996), there have been significant recent advances in computational micromechanics of crystals to bring to bear on this issue. Several advances are necessary to better quantify void nucleation processes, including heterogeneity of nucleation sites, describing continuous nucleation, and nucleation in shear and in the presence of hydrostatic compression. Strength differential effects in tension and compression associated with heterogeneity of slip and plastic compressibility have implications for nonassociativity with the yield surface at both the macroscopic and mesoscopic scales (cf. Rudnicki and Rice, 1975; Nemat-Nasser et al., 1981). Promising tools in the micromechanical study of nucleation include the interface decohesion models which approximate the work of separation and sliding (Needleman, 1987, 1990). With such models, along with supporting atomistic calculations as appropriate, the processes of void nucleation and growth in heterogeneous microstuctures may be better understood. Further, their role in inducing nonassociative plastic flow and localization at higher scales is of considerable practical interest.

2.4. The emergence of high resolution characterization tools

Experimental studies of large strain plasticity increasingly make use of characterization tools such as high resolution Transmission Electron Microscopy (TEM) to discern features at length scales on the order of fractions of nanometers to microns. This is critical in furthering our understanding of formation of dislocation structures at various scales — how they order and presumably locally minimize the collective free energy of the system. As this is fundamentally a self-organizational phenomenon, the search for experimentally-derived scaling laws to describe the organization process (e.g. feature wavelength, dislocation density gradients, etc.) may prove extraordinarily fruitful, along with increasing capabilities to conduct three-dimensional simulations of dislocation multiplication and interaction (cf. Kubin and Canova, 1992; van der Giessen and Needleman, 1995; Zbib et al., 1997). Molecular dynamics may prove to be useful as well to study embryonic stages of self-organization of dislocation structures, starting from a low defect lattice; it is not out of the question in the foreseeable future to analyze material volumes containing on the order of a billion atoms on teraflop computing platforms. Molecular statics can shed light on quasi-equilibrium structures and patterning of defects, possibly enabling Monte Carlo simulations of coupled plastic deformation and evolution of dislocation substructure patterning.

Orientation imaging microscopy has been introduced (cf. Adams, 1997) to provide high resolution information on the orientation distribution of grains to support deformation and fracture studies at a level of detail at which nearest neighbor orientation statistics can be considered; applications include deformation, fatigue and fracture of polycrystals, ranging from conventional metals such as steels to transformation-induced plasticity (Fischer and Werner, 1997).

Atomic Force Microscopy (AFM) and nano-indentation offer means to interrogate the elastic–plastic behavior of subvolumes of material at scales far below the bulk, leading the way to new understanding of the role of grain boundaries, nanoscale interfaces, surface topologies, and so on.

3. Practical benefits of multiscale plasticity

The need for engineering models of plasticity for large scale structural calculations will be sustained into the foreseeable future. It is likely, however, that the era of arduous experimental study and associated empirical construction of yield surfaces and flow potentials will be largely supplanted by a combined approach of variable resolution experimental measurements and computational micromechanics which afford much more robust study of the *sources* of anisotropy and its evolution. Of course no model can fully capture reality. Engineering models will likely embrace elements of lower length scales, such as the orientation distribution of grains or other microstructure attributes, in future structural calculations. One can argue that crystal plasticity itself is on the verge of being a practical tool for engineering analysis, but it is still too computationally demanding for large scale analyses. However, it is available today as a tool for substructure analysis of selected regions of stress concentration within a structure or as a means to conduct forming analyses on simple parts.

There are two very compelling reasons to understand and model plasticity over a range of length scales:

(i) to design materials to exploit plastic deformation and
(ii) to develop a consistent, unified theory of the formation and evolution of defects during plastic flow.

Materials design is an inexorable technology ‘pull’ which is gaining momentum as we head into the next century. The classical empirical approach of alloy development is giving way to engineering or tailoring metals, alloys and their composites for specific properties to serve specific functions. In view of the enormous fraction of the U.S. GNP that is linked to metals technology, this design approach merits considerable attention. It will serve as an enabling technology for new product lines, such as lightweight automotive frames, constructed from cast Al or Mg alloys. Existing staple alloys such as steels can realize dramatic improvements in strength and toughness by application of emerging simulation tools that deal more quantitatively with phase equilibria, quantum/molecular simulations and multi-phase computational micromechanics. Materials design calls for a greater quantitative understanding of microstructure–property relations, principally achieved through simulations of representative (realistic) microstructures. This challenge lies squarely at the interface of constitutive theory, experimental mechanics, materials science and engineering, and materials physics and chemistry. Principles of concurrent engineering which have become a mainstay of manufacturing practice will become equally important in fabrication of metals. Specialty metal suppliers in the future will compete on the basis of their tailoring expertise, and entirely new markets will be born. The competitive advantage to be gained by this technology is also potentially enormous in traditional structural materials when one considers the sheer volume of production. In contrast, many academic studies of the last 20 years have focused on rather high-end, specialty alloys for defense applications.

At present, calculations are typically performed to rather crudely approximate mechanisms of fracture and fatigue of metallics. These estimates are based on idealizations such as continuum void growth laws, fracture mechanics and stress–life or strain–life curves which most often lack an intimate link to the dislocations and separation processes that create and multiply defects within the structure, and contribute to plastic deformation. Where do microvoids and microcracks come from, for example? If we modify a material through composition or process history, even modestly, how can we provide guidelines on assessment of its durability without costly and time-consuming testing and characterization programs that have been typical of our existing 'storehouse' of conventional alloys? Further, can we modify it with the intent to achieve specific service improvements, rather than face a trial-and-error development cycle?

There has been substantial progress on understanding ductile–brittle failure transition in metals by consideration of dislocation emission from the crack tip, but it appears that we are still far from a structure of plasticity theory that unifies deformation and fracture processes to the extent possible. It is almost inevitable that such a theory will explicitly consider microstructure, in contrast to the macroscale engineering plasticity models or even state-of-the-art crystal plasticity models of today. In some cases, such as thin films, optoelectronic devices or MEMS devices, the need for explicit models of dislocations or even quantum level analysis is obvious. In other cases, such as tailoring structural materials to resist certain failure modes or succumb to others, the need for multi-resolution models with nanometer or micron scale resolution may likewise be essential, although not as easily recognized at first glance.

The theory of engineering plasticity will undoubtedly benefit in the coming era. The lines of distinction between plasticity and failure processes will blur, and modeling of processing will become more intimately linked to specific applications. As a result, consumer goods will benefit from both financial and functional perspectives.

4. Research needs

Some of the open avenues for further exploration of physically based theories of plastic flow should be apparent from the preceding discussion. We close this Chapter by first summarizing some areas with high potential for significant advances in understanding and modeling plastic flow, intentionally avoiding separation into categories involving either experiments or modeling. It is precisely the synergy of the combination that is necessary to advance the subject.

4.1. Multiscale resolution experiments and modeling

Optical characterization methods have progressed to the point where evolution of microstructures and dislocation substructures can be observed. High resolution TEM is capable of sub-nanometer resolution and can be employed as a tool to support discrete dislocation analyses in thin films and their interfaces, surface effects in MEMS devices, dislocation core fields and vacancy migration. Lower resolution TEM can be used to construct montages of dislocation substructures with significantly large fields of view to scales on the order of microns to support understanding of self-organizational principles and related scaling laws. Computational micromechanics results can be compared with results of experiments conducted at various length scales to form a bridge between model and reality. Advances in digital signal processing can assist in the evaluation and interpretation of spatial images or temporal data. For example, wavelet technology offers a means to compress and store data from a time–frequency spectrum that may be associated with various physical phenomena occurring at different time and length scales.

The evolution of plastic strain, hardening and evolution of damage in actual metallic systems is invariably influenced strongly by heterogeneity. Ordinary self-consistent micromechanics approaches are often of little avail in dual phase microstructures obtained by thermomechanical processing or to model plastic flow in complex alloys. Quantitative analysis of images has progressed to the point where various forms of correlation functions for positions of heterogeneities (e.g. radial distribution functions or K-functions, nearest neighbor distributions, pair correlation functions for multiple geometric attributes, higher order nearest neighbor distribution functions, and Dirichlet tesselation) are available to embed into theories of elasto–plasticity for real microstructures (Ripley, 1981; Spitzig et al., 1983; Stoyan and Wiencek, 1991; Yang et al., 1996). Similarly, contiguity and cluster parameters (cf. Fischer and Werner, 1997) may be employed together for real microstructures to sort out nearest neighbor and clustering effects on plastic flow. These statistics may be incorporated into higher order theories of plastic flow, providing natural material length scales for normalization of scale effects and coupling of plastic deformation and fracture processes with microstructure. They may also be used for purposes of reconstruction of microstructures for purposes of solving microscale boundary value problems. Direct computation of plastic flow in material microstructures using meshing procedures based on veronoi tesselation (Ghosh et al., 1997) or other means (cf. Brockenbrough et al., 1992; Fischer and Werner, 1997) permits more realistic simulation of behavior and moves a step closer to alloy design for functionality. A re-examination of plasticity and elastic–plastic fatigue and fracture of complex alloys using computational micromechanics is a fruitful area to be pursued in the coming decade. Full field measurements of displacement fields and changes of internal structure for heterogeneous media will deepen the connection to computation and close the gap on understanding and modeling of phenomena. Strategic design of experiments carried out from initially constant structure along different trajectories in load space will be most helpful to understand deformation heterogeneity and self-organized substructures that can be quantified with image analysis.

4.2. Coupling of plasticity-induced damage with texture

The modeling of the evolution and influence of texture during finite straining of metals has come a long way in past two decades. However, little attention has been devoted to the effects of texture on subsequent cyclic deformation and fatigue. One of the most costly and least-well quantified failure mechanisms, fatigue is associated with cyclic microplasticity. The distribution of slip among grains, the nature of cyclic plastic deformation ahead of and in the wake of cracks with length on the order of repeating microstructure are subjects of enormous potential for emerging computational cyclic plasticity theories. The role of texture on the deformation and failure of metallic components in structures is of extreme importance and has received surprisingly little quantitative treatment. It is well known that texture affects virtually all mechanical properties to first order, but very few practical analysis tools have been brought to bear on this problem. Effects of texture on dislocation substructures caused by cycling deserves attention. The coupling of plastic deformation-induced anisotropy with micromechanical analyses of fatigue and fracture is an area that begs for fundamental research. The question of how general multiaxial kinematic hardening behavior is affected by finite prestrain is also of considerable practical interest from the perspective of subsequent cyclic behavior or for modeling of multi-pass forming operations. The influence of texture and heterogeneity on process zone mechanics in elastic–

plastic fracture is also an important practical consideration for rolled or stretch-formed sheets, for example.

4.3. Progressive cyclic deformation and failure

Most models for cyclic plastic strain accumulation in the presence of mean stress have been framed at the macroscopic level. The precise origins of cumulative plastic strain due to microstructural scale ratchet mechanisms (leading to slip accumulation in the large) has not been examined in detail. The roles of high angle boundaries and distribution of nearest neighbor grain misorientation have not been clarified, nor have comparisons been made between single and polycrystals with nominally the same composition. There is need to pursue shakedown limit solutions for cyclic plastic flow in representative microstructures. Fatigue limits may be related to shakedown, for example, especially for complex microstructures. For multiphase metallics such as steels, Ti and many other structural alloys, the role of mismatch of elastic properties of the phases and heterogeneity of flow in the vicinity of phase boundaries on void nucleation and growth is of concern in cyclic loading, coupled with the issue of cyclic plastic strain accumulation.

4.4. Scale effects in plasticity

Recognizing the various distinct length scales of organization of microstructure below scales of typical grain size in conventionally processed metals ranging from atomic to tens of nanometers to micron-scale clustering (cf. Fig. 1), it is unlikely that analysis at a single window of resolution will suffice to describe all potential applications. For example, point and line defects in thin films for electronic applications warrant detailed study using molecular dynamics or discrete dislocations because they affect functional performance. Similarly, fundamental studies of interface fracture, decohesion (work of separation and sliding) and plastic deformation at atomistic scales are necessary to support modeling concepts at higher length scales. More fundamental understanding of friction laws for real surfaces in contact is possible with future molecular dynamical calculations that seek to deconvolute the influence of true surface area of contact from the interface shear strength, an objective not yet fully accomplished in laboratory experiments.

MEMS devices are being fabricated at length scales where edge effects due to discreteness and scale effects are primary considerations. Owing to the nonlocal nature of atomistic or molecular dynamics simulations, a deeper understanding of scale effects in the elastic–plastic behavior of small devices and interfaces is a natural outcome. Molecular dynamics also offers the opportunity to examine many of the fundamental solutions of dislocation mechanics and interactions, for example the size and shape of dislocation cores, effects of interstitial atomic atmospheres and the like. Ideal applications of atomistics already addressed in the literature include the ductile to brittle transition in fracture and nano-indentation (cf. Ortiz, 1996).

Dynamical atomistics or molecular dynamics is limited by practical considerations (picosecond time scales and submicron length scales) in its capability to examine quasi-static generation and organization of line defects in metallics with initial disorder at practical length scales of interest for short and long range hardening and flow mechanisms. To this end, simplified treatments of 2-D (Gulluoglu and Hartley, 1992; van der Giessen and Needleman, 1995) and 3-D dislocation simulations within substantial representative volumes (cf. Canova et al., 1992; Zbib et al., 1997) show substantial promise to provide understanding of quasi-equilibrium dislocation substructures, self-organization and stress-shielding, and improved descriptions of 3-D crack tip plastic deformation and fracture processes.

By working upwards in scale of solution from molecular dynamics to discrete dislocations to continuously distributed dislocations, it may be possible to develop scaling laws which describe aggregate dislocation behavior and strengthening effects at higher length and time scales of interest. Improved models for static and dynamic recrystallization, which are governed by heterogeneity of stored energy in the microstructure, represents another fertile area of application of discrete dislocation models and crystal plasticity.

Problems of shear localization in metals are of considerable practical importance in metal forming, high speed machining, and high strain rate impact problems. We list localization within the context of scale issues only to emphasize that the multiscale nature of the progression of shear banding, for example, is among the more challenging problems in computational plasticity, let alone properly capturing the physics. A key problem is that the extent of the localization behavior at some point is statistically inhomogeneous at the scale of the representative volume of material used in finite element analysis, leading to strong mesh dependencies in the solution and a great deal of uncertainty and non-uniqueness in post-bifurcation and failure predictions. While the problem has received much attention in terms of adaptive numerical approaches, general principles for localized versus distributed shear banding are elusive, as are general models for post-bifurcation behavior. The influences of material rate sensitivity and temperature dependence in moderating the process are now rather well established, as is its triggering by heterogeneity. However, patterning of localization events (energy release) and nonlocal constitutive models that additionally serve to limit localization are still very much on the frontier.

4.5. Coupling of plasticity with phase transformations and material damage

Plastic deformation induced by phase transformation is a key mechanism of toughening in certain alloy systems (cf. Fischer and Werner, 1997). Although phenomenological models have been developed, the driving forces for heterogeneous plastic flow in the presence of phase transformation are incompletely understood. Coupling of twinning with plasticity is a problem that very likely must be resolved at fine scales and then scaled upwards for meaningful polycrystal description; initial in-roads have been made. New kinds of metallic systems may be developed for actuation and damping that exploit combinations of transformation and plastic flow to accommodate deformation, for example metal matrix composites with shape memory alloys as second phase. The emergence of damage at various length scales associated with slip, decohesion, cleavage, and constraints of high angle boundaries or phase boundaries is an area rich in potential for study using, for example, more realistic computational crystal plasticity models (cf. Ortiz, 1996; Zikry and Kao, 1996). Nonlocal and micropolar approaches for coupling of plastic deformation and damage will receive increasing attention in the coming years, especially in terms of physical connections.

4.6. Microplastic behavior of cast alloys and low symmetry polycrystals

Cast metals with low ductility due to brittle inclusions and shrinkage or gas porosity offer a different set of challenges than wrought, ductile polycrystals. Composite micromechanics is applicable, but only with recognition of the highly nonuniform distribution of particles and voids within the casting. Mean field mechanics is of little value in plasticity and damage evolution of these materials. Interdendritic regions of high inclusion content are preferred regions for localization of plastic strain and fracture. Acknowledgment of the dominance of extremal characteristics of microstructure distribution along with computational modeling of realistic microstructures are necessary to make headway. Similarly, plastic incompatibility at grain boundaries associated with slip in low symmetry crystals promotes high intergranular stresses and motivates special treatment (cf. Parks and Ahzi, 1990). Nano-indentation and AFM studies of gradients of plastic deformation within individual grains in low symmetry polycrystals may deepen understanding of the behavior and lead to improved models.

4.7. Massively parallel computing

Most of the advances in computational plasticity have been realized within a serial processing environment. Future advances in tackling large degree-of-freedom plasticity analyses will benefit from developing algorithms for parallel processing, with applications ranging from detailed elasto–plastic analysis of large structures to sets of nested multiscale analyses. Because of the short time scales and explicit integration techniques, dynamic plasticity is quite amenable to parallelization, as are MD simulations. There is potentially much to be gained in computational micromechanics analyses of plasticity, even in the quasi-static regime, by decomposing the behavior of microconstituents among processors using reasoned approximations. For example, polycrystal plasticity based on the Taylor model of uniform deformation among grains permits assignment of analysis of individual grains at each strain increment to individual microprocessors, with communications at the end of the increment for purposes of volume averaging, all within the constitutive update routine (cf. Kalidindi and Anand, 1991). Indeed, massively parallel algorithms for microscale plasticity analyses may prove to be the most viable route for practical support of the design of materials and process routes.

4.8. Principles for multiscale modeling

An issue related to high performance computing is how to interpret the results of elasto–plastic analyses conducted at different scales of resolution. For example, in one case fine details of microstructure may be considered while in a larger scale analysis these effects must be properly averaged or matched. In some cases, fundamentally different theoretical frameworks may be used at different length (and time) scales. Several possible schema have emerged. For example, substructuring can be performed by adopting an effective medium in larger scale analyses, with heterogeneity manifested in a finer scale analysis, a sort of homogenization approach. But the selection of the effective medium and the boundary conditions are nontrivial if the problem involves statistical inhomogeneity at the scale of averaging (e.g. heterogeneity on the scale of averaging or element size). For some problems, domain decomposition or overlapping matching of solutions with successive iteration on boundary conditions may be more appropriate. Tadmor et al. (1996) recently introduced the concept of quasi-continuum analysis, in which interatomic potentials can be used to compute the material response with atoms embedded within the prescribed displacement fields of finite elements. At higher length scales, the evidence of multiple scales of inelastic rearrangement should be evident in the formulation.

For problems involving significant plastic strains and evolution of structure, adaptive re-meshing is often essential. The general problem of continuation and matching of elasto–plastic behavior over multiple length scales will undoubtedly witness considerable activity in the coming decade. The importance of consistency of the thermodynamical treatment across length scales cannot be overstated.

4.9. Determination of parameters & evolutionary forms

In view of the highly nonlinear models that arise in modeling of plastic flow and internal structure rearrangement, difficulties in parameter estimation often limit the practical utility of models. Of course, lack of uniqueness is a hallmark of nonequilibrium irreversible processes. Another problem is that in multiscale plasticity models, each scale or mechanism may have its own set of parameters, perhaps physically distinct but not necessarily amenable to decoupling by experiment. Scale-specific measurements of in-situ properties is one means of sorting this out. Some models involve a number of assumed constitutive equations over a range of scales, e.g. polycrystal plasticity. A wide range of other tools for computing evolutionary processes may benefit the treatment of self-organizing dislocation substructures and damage at various scales. Using artificial intelligence algorithms to extract the mathematical forms for evolution of internal structure from experimental data or results of intensive computation is an exciting future direction to pursue as well.

5. Closure

We close this Chapter by recognizing that heterogeneity at various length scales has pervaded our discussion of future research directions in plasticity. These directions will support improved deformation processing of metals, development of new materials of hybrid nature, and more predictive relations for in-service material failure. From an experimental standpoint, we now have access to relatively inexpensive image acquisition and analysis capabilities that dwarf those of a decade ago due to advances of computing technology. Laser-based interferometric systems can provide in-situ measurements of displacement fields of heterogeneous microstructures. Unobtrusive thin film sensors based on MEMS technology are now being fabricated with multi-function capability of acoustic emission detection, microaccelerometry, and other local signals. With such tools, the scale of the measurement can often be selected so as not to obscure or average over heterogeneities of interest. From a modeling perspective, we may embrace emerging concepts regarding *evolution* of structure, the defining characteristic of plasticity. Plastic deformation is a manifestation of rearrangement of microstructure. While at each stage the dislocated system may be analyzed as elastic (cf. dislocation theory), the evolution process is nonequilibrium in nature and is highly nonunique as well. From the physics literature we may draw on emerging understanding of self-organizing systems, percolation, scaling laws and re-normalization techniques. Application of artificial neural networks and pattern recognition algorithms for emergent behaviors that arise from large scale computation (i.e., massively parallel computing or high resolution experiments) may prove useful in interpreting outcomes (distributions really) of computations with numbers of degrees of freedom that boggle the mind. Genetic algorithms may offer a means of selecting paths for microstructure evolution during plastic flow among a multitude of conceivable trajectories. Multiscale statistical design of experiments approaches for assessing the relative significance of various model features for heterogeneous systems (cf. Horstemeyer, 1995) may help sort out which elements of models deserve further refinement within a highly nonlinear system of constitutive equations, and what level of detail or scale of resolution is necessary for modeling practical problems at higher length scales.

We must always bear in mind Drucker's 1984 admonition that "the appropriately idealized stress–strain relation for the solution of a problem of continuum mechanics is the simplest one that contains the essence of the physical behaviour of importance of the problem to be solved". However, it is not simply a matter of preference, but also of scale.

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