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POLYCRYSTALLINE PLASTICITY: CONSTITUTIVE EQUATIONS AND APPLICATION TO DEFORMATION PROCESSING

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In polycrystalline metals the major cause of anisotropic plastic response is crystallographic texture resulting from the reorientation of the crystal lattices of grains during deformation. We have developed an elastic-plastic, rate-dependent polycrystalline model for low homologous temperatures in which plastic deformation within individual crystals is taken to be by crystallographic slip alone. To predict the global response of the polycrystal, the transition from the micro-response of the individual grains to the macro-response of the polycrystalline aggregate, we follow the pioneering work of G. I. Taylor and assume that the deformation gradient within each grain has a uniform value throughout the aggregate, and that all grains have equal volume. In this approximate model, compatibility is satisfied and equilibrium holds in each grain, but equilibrium is usually violated between grains. We have developed a new fully implicit time-integration procedure for the constitutive model and implemented it in a finite element program. The new computational procedures can be used in two types of finite element calculations: (a) where an integration point represents a material point in a single crystal, and the constitutive response is given by the single crystal model, and (b) where an integration point represents a material point in a polycrystalline sample and the constitutive response is given through a Taylor-type polycrystal model.

We have carried out a detailed evaluation of our elastic-plastic Taylor-type polycrystalline model. Specifically, the model has been evaluated by comparing the predictions for the evolution of crystallographic texture and the stress-strain response in simple compression and tension, plane strain compression, and simple shear of initially isotropic face centered cubic (fcc) copper against: (i) corresponding experiments, and (ii) finite element simulations of these experiments using a multitude of single crystals with accounting for the satisfaction of both compatibility and equilibrium in the weak/finite-element sense. Our experiments and calculations have shown that the Taylor-type model is in reasonable first-order agreement with the experiments for the evolution of texture and the overall stress-strain response of single-phase polycrystalline copper.

The good predictive capabilities of our physically based anisotropic constitutive model for polycrystalline materials, together with our new computational procedures for simulating the stress-strain behavior and the evolution of texture under non-homogeneous deformation conditions have also been demonstrated by comparing numerical simulations against experimental measurements on micro-forgings of *initially isotropic* and *initially pretextured* copper.

CRACK-DISLOCATION MODELS OF YIELD AND FRACTURE IN MULTILAYERED MATERIALS

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Multilayer morphologies frequently prevail in the design of electronic devices and coatings for high temperature or wear applications. They represent one of the most carefully produced classes of materials to date, in which layer thickness, stochiometry of elements within a layer, impurity content, and interfacial structure are atttempted to be controlled. As such, these materials offer an unprecendented opportunity to study fundamental phenomena. Recent efforts have attempted to address whether, in principle. microlaminates may be designed to offer a superior combination of high flow stress and fracture toughness. This work suggests that substantial modifications to the classic trade-off between fracture toughness and flow stress may be possible, particularly if the amplitude and period of dislocation resistance provided by the multilayer are controlled through selection of component materials, interfacial structure, and layer thickness.

PROBLEMS IN CRYSTAL PLASTICITY AND STRAIN LOCALIZATION

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The theory of crystal plasticity is one of the hallmarks in continuum mechanics. Within a thermodynamic framework where crystallographic slips are regarded as internal (state) variables, one can study a wide range of problems. Nevertheless, two central issues remain open, one concerns constitutive equations for multislip hardening and the other the widely-observed phenomena of highly inhomogeneous flow. Recently we have developed a new theory of hardening under multiple slip conditions that underlies some of the most fundamental plastic flow behaviors found in single crystals. These include the transition from easy glide to rapid (stage II) hardening, the orientation dependence of hardening, and strain localization.

In the early stages of plastic flow of single crystals for many, if not most, metals, slip ceases to be homogeneous and a microstructure develops through the formation of coarse slip bands. This involves a very regular laminate-like patterning. Similar phenomena occur in bicrystals and polycrystals. Based upon a new understanding and theory of single crystal hardening we have shown that fine secondary slips play an important role in the nucleation and saturation of such localized modes of deformation.

A completely open issue is the evolution of microstructures resulting from localized plastic deformation (pattern formation) and its effect on overall properties and failure mechanisms in ductile materials, and very few features can be explained theoretically or computationally. Fine secondary slips may also be key to the issue of patterning, e.g. thickness and spacing of coarse slip bands particularly in single-phase materials, through the effects of geometrically necessary dislocations on hardening.

CRYSTAL PLASTICITY AND ITS EFFECTS ON LOCAL DEFORMATION IN POLYCRYSTALS

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Plastic deformation in metals occurs by dislocation glide along well defined crystallographic directions within the grains of a polycrystal. A preferred distribution of the crystallographic orientations of these grains produces material anisotropy which can lead to difficulties in manufacturing or degradation of product performance. Models which predict the evolution of the crystallite orientation distribution have been used for more than fifty years, but the need for more accurate predictions continues to drive model development.

A crystal plasticity model which allows finite strains and accounts for crystal lattice rotation with deformation is reviewed, and an extension of the method to crystals deforming by pencil glide is given. Implementation of the model into a finite element program is discussed. Results from model validation studies will be presented which show that predictions of crystal lattice rotations during deformation are in good agreement with experiments for single crystals. A detailed model of a two dimensional section of a polycrystal does not show favorable agreement. This model illustrates the profound effects of grain interactions on lattice reorientation, and the failure of the model is attributed to neglecting grain interactions in the third direction. These results have significant implications for simplified models for orientation evolution which ignore specific grain interactions.

A DETAILED LABORATORY STUDY OF THE ANALYTICAL FOUNDATIONS OF A GENERAL THEORY OF FINITE PLASTICITY IN ORDERED SOLIDS

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From laboratory measurements extending back to the early 1960's a frame indifferent general continuum theory for large finite plastic strain in ordered solids has been developed. Its foundations are based on a stress $\sigma = RT_R$, a work function $W = \text{trace } \sigma V = \text{trace SE} = T\Gamma$, a laboratory based internal constraint on the left Cauchy-Green stretch tensor V, trace V = 3, compatible with the measured decrease in volume during deformation, and, as also shown in the laboratory, a rigid body rotation $R^{-1} = R^T$ that is minuscule even when measured just prior to catastrophic collapse. This lecture presents laboratory experimental results revealing that the Cauchy stress $\sigma^* = [III_V]^{-1} FT_R^T$, the stress $\sigma = RT_R^T$ that replaces it in the present theory, and the left Cauchy-Green stretch tensor $V = I + E$ are all coaxial and symmetric, and that for R = I, the second invariant T of the deviatoric stress S and the second invariant Γ of the finite strain $E = V - I$ provide a universal parabolic rule that applies for stress paths of arbitrary composition and direction.

This general nonlinear theory of finite strain plasticity is shown here to square with a recently published nonlinear theory of finite strain elasticity by BEATTY and HAYES. Introducing the above laboratory discovered internal constraint trace V = 3 , they derived their general theory from an examination of inequalities in the analytical foundations of rational mechanics.

PLASTICITY: STEPS TOWARD A PHYSICAL THEORY

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Development of a physical theory of plasticity that would allow the prediction of the mechanical response of crystalline solids on the basis of their composition and microstructure has long been the goal of research in plasticity. Recent developments on theoretical, experimental and computational fronts have given renewed hope that significant progress towards this goal is being made. As an indication of this progress, recent results by the author's colleagues and their collaborators at Brown are described.

Understanding of the dislocation core region in aluminum has been advanced on several fronts through an interactive effort involving (i) high resolution transmission electron microscope (HRTEM) images of atom positions in the core region (Paine and Schwartzman); (ii) atomistic calculation of these positions based on an embedded atom method (EAM) (Phillips); (iii) finite element method (FEM) calculations of the atom positions based on use of the EAM potentials to evaluate the stresses by assuming that atom positions within an element correspond to those of an affine deformation of the element (Ortiz); and (iv) experimental determination of the interplanar potential for relative sliding of the two sides of the slip plane, by means of Computational Fourier Transofrm Moire (CFTM) (Kim). For a Lomer dislocation the calculations (ii) and (iii) agree remarkably well at distances greater than only two atomic distances from the center of the dislocation. This result provides encouragement that the so-called quasi-continuum approach (iii) can be used seamlessly over a range of size scales ranging from nearly atomistic to macroscopic. The interplanar potentials obtained from (iv) appear to be reasonable for relative sliding up to one-fourth of the Burgers vector. Availability of this experimental method offers exciting possibilities for relatively direct cross-checking with the atomistic simulations (ii).

Dislocation mobility measurements are reviewed with emphasis on the high velocity regime investigated in plate impact experiments (Clifton). These experiments, combined with atomistic simulations based on the Lennard-Jones potential (Weiner and Clifton), suggest that the intrinsic resistance of the lattice provides approximately a linearly viscous drag on the motion of dislocations and the drag coefficient is approximately proportional to temperature at ambient temperatures. This relatively simple description of the mobility of dislocations is in sharp contrast to the complexity that arises due to dislocation/dislocation interactions. Dislocation patterns obtained in high strain rate pressure-shear experiments on high purity copper specimens are reviewed briefly as an indication of the dislocation patterns that develop.

ADAPTIVE METHODS FOR PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS WITH APPLICATION TO SHEAR BAND FORMATION

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As problems increase in complexity, there is corresponding need to automate a greater portion of the solution process. Adaptive methods utilize preliminary solutions computed with a coarse discretization and a low-order technique to automatically identify and improve solutions where needed. We review the basic enrichment schemes of (h-type) mesh refinement/coarsening, (p-type) local variation of order, and (r-type) mesh motion and their use singly or in combination. We describe methods of estimating discretization errors and strategies for using them to control adaptive enrichment. Concentrating on adaptive hp-refinement because of its high convergence rate, we describe algorithms for solving parabolic systems that utilize one-step and multi-step temporal integration. Adaptive strategies for time-dependent systems require techniques to balance space and time errors. We describe a simple approach to this issue that maintains the local temporal error at a fraction of the spatial error.

The adaptive software has been applied to physical problems arising in diverse disciplines and we consider solutions to problems involving shear band formation and propagation. The enrichment strategies are capable of locating shear bands as they evolve and accurately resolving solutions within layers. Techniques for performing multi-scale analyses, where models are varied in proportion to accuracy, will also be described.

ASPECTS OF FINITE DEFORMATION OF CRYSTALS AND POLYCRYSTALS

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Theoretical, and for the most part analytical, investigations of significant but relatively simple experimental configurations corresponding to the atomic lattice structure and crystallographic slip systems of f.c.c. and b.c.c. metals are reviewed. Primary emphasis is given to the f.c.c. crystal class. The following topics are addressed: double-slip geometric analysis, including derivation of the cone of unextended directions in non-symmetric double slip and reinterpretation of the classic single-crystal experiments of G. I. Taylor (from the 1920's); latent hardening experiments, the overshooting phenomenon, and associated hardening theories; and finite crystal shearing, plastic spin (i.e. the relative rotation of gross material and underlying lattice), and lattice rotation in four and six-fold multiple slip in channel die compression. Lastly, new theoretical predictions of the formation of subgrains and microshear bands in polycrystals are given through exact solution of the governing pairs of hyperbolic partial differential equations for stress and velocity fields in symmetric bycrystals under (110) compressive loading in the channel die.

DYNAMIC SIMULATION OF DISLOCATION MICROSTRUCTURES

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The nature of dislocation microstructure formation and evolution remains cloudy, yet such knowledge is essential to a fundamental understanding of the deformation mechanisms of crystalline materials. Over the past few years, a number of direct simulations of dislocation microstructures have been performed. We will review the earlier simulations and will review their successes and failures. We will present the results of our current work, which has been focused on developing accurate, yet computationally fast, algorithms for eventual porting to massively-parallel platforms.

CONSERVATIVE METHODS FOR COMPUTATIONAL PLASTICITY

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The continuum equations governing the dynamics of an elasto-plastic material can be formulated as a system of conservation laws. These laws represent not only the balance of mass, momentum, and energy, but also the continuity of the material and the convection of the internal plastic state.

We present two applications of the conservative formulation. First is an Eulerian numerical algorithm based on a second-order Godunov method and material interface tracking; this algorithm is applied to impact problems. Second is an algorithm for tracking a fully-developed shear band, which is modeled as a discontinuity imbedded in a thermal layer.

IMPLICATIONS OF INHOMOGENEITY AND ANISOTROPY FOR CLASSICAL PLASTICITY MODELS

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A variational procedure is proposed for estimating the effective behavior of nonlinear composite materials. It is assumed that the local constitutive behavior of the composite material is characterized by a potential function, in such a way that the effective behavior of the composite may also be described in terms of an effective potential function. This class of material models includes, for example, deformation theory of plasticity, which is appropriate for infinitesimal, nearly proportional deformations of metals at low temperatures, and nonlinearly viscous models, which are appropriate for large deformations at high temperatures. The procedure is based on a new variational principle which expresses the effective potential of a given nonlinear composite in terms of the effective potentials of an appropriate class of linear comparison composites. This result allows the conversion of a large number of results, in the form of either bounds or various types of estimates, for linear composites into corresponding results for nonlinear composites.

In this presentation, we will explore the coupled effects of nonlinearity and anisotropy. In particular, we will apply the procedure to determine estimates for the effective yield surfaces and post-yielding behavior of fiber-reinforced metal-matrix and other types of two-phase composites. The results show strong nonlinear effects, specially for anisotropic composites with continuous reinforcement, such as laminated and fiber-reinforced composites. In addition, we determine a new bound for the class of isotropic (no texture) FCC polycrystals in the context of power-law creep. The results are found to be somewhat stronger than the classical bound of Taylor, but remarkably close to Hutchinson's self-consistent estimates.

Finally, based on the observation that the microstrucuture of a composite material may change significantly under the effect of large deformations, we propose a new model for the effective behavior of porous composites. This model is capable of accounting for the evolution of the anisotropy in the material due to the change in shape of the pores. It is shown that the predictions of the model may be quite different from those of the classical model of Gurson, particularly, under low-triaxiality loading conditions.

THE RIEMANN PROBLEM AND A GENERALIZED RIEMANN PROBLEM IN DYNAMIC PLASTICITY

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Although the assumption of rate-independent elastic-plastic materials is unrealistic for certain materials and for high strain-rate loading, it provides a reasonable and useful approximation in many situations. In the past the Riemann problem for wave propagation in fluids or gases has been investigated mainly by researchers in fluid dynamics and applied mathematics while the Riemann problem for solids has been studied mostly by engineers and the mechanics community. While the basic mathematical tools employed are the same, there have been very little dialogues between the two groups until recently. A distinct feature of the Riemann problem for elastic-plastic solids is that there are two different sets of differential equations for the elastic region and the plastic region. As a result there are two sets of stress paths)a term used by engineers) or wave curves (a term employed by applied mathematicians). The governing differential equations for the plastic region are not a system of conservation laws. Consequently there is no Hugoniot equation for the plastic region, and hence no plastic shock waves. Any attempt to generate a plastic shock inevitably leads to an elastic unloading. Some interesting and unexpected results will be presented. A generalized Riemann problem has been considered recently for a system of conservation laws. For wave propagation in elastic-plastic solid a generalized Riemann problem has been studied. Here again one finds interesting and unexpected results.