MULTI-SCALE STOCHASTIC ANALYSIS OF HETEROGENEOUS MATERIALS

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The current increase in computational power allows us to completely rethink the modeling of inelastic behavior of engineering materials and the corresponding testing procedure [1-6]. In particular, the traditional phenomenological models are more and more giving way to multi-scale modeling procedures, where one goes down to much smaller scales in order to be able to properly interpret the particular mechanisms of inelastic behavior. One such model, which is built upon the ideas inherited from structural mechanics, is presented in this lecture. The predictive capabilities of this model are illustrated for a couple of challenging problems of dynamic fracture and crack propagation. In the second part of this lecture we address related topics pertinent to problems of material design and testing, as well as the construction of probability bounds for computed results. Moreover, a novel approach to structural optimization that pertains to tailoring the material to best suit the given use is presented, where optimality conditions and equilibrium equations are placed to the same level. Several important points are addressed in detail regarding the models proposed herein:

i) In this work we consider a strongly coupled multi-scale problem in the context of inelastic structural mechanics. We assume that a finite ratio of scales exists such that we can replace the more standard phenomenological and analytical homogenization approaches by a lower level numerical description of the micro-structural behavior. More specifically, we use continuum damage and plasticity based finite element method (FEM) models to describe the matrix-inclusion type of micro-structure (e.g., for a porous or hard inclusion composite). The micro-scale FEM model is then coupled to the macro-scale FEM model through a localized Lagrange multiplier approach. This multi-scale strategy is very well adapted to a parallel computing algorithm using a component template library. The efficiency of the implementation

is shown on large scale numerical examples. A more elaborated description of the parallelization procedure is also presented in our paper [1,2].

ii) In our recent work [3] we propose a methodology for dealing with the problem of designing a material microstructure the best suitable for a given goal. The chosen model problem for the design is a two-phase material, with one phase related to plasticity and another to damage. The design problem is set in terms of shape optimization of the interface between two phases. The solution procedure proposed herein is compatible with the multi-scale interpretation of the inelastic mechanisms characterizing the chosen two-phase material and it is thus capable of providing the optimal form of the material microstructure. One can thus achieve the optimal design of the nonlinear behavior of a given two-phase material with respect to the goal specified by a cost function, by computing the optimal form of the shape interface between the phases. The original approach based upon a simultaneous/sequential solution procedure for the coupled mechanics-optimization problem is proposed. Several numerical examples show a very satisfying performance of the proposed methodology. The latter can easily be adapted to other choices of design variables.

iii) Our goal in recent paper [4] is to present how to use a part of Stochastic Finite Element Method in mechanical problems. We will focus on the Karhunen-Lo\`eve Expansion coupled with Monte Carlo Simulations and its application to describe the size effect encountered in structure involving quasi-brittle materials such as geomaterials.

iv) In recent work [5] we discus the finite element model using the embedded discontinuity of strain and displacement field, for dealing with a problem of localized failure in heterogeneous materials by using the structured finite element mesh. On the chosen 1D model problem we develop all the pertinent details of such finite element approximation. We demonstrate the presented model capabilities for representing not only failure states typical of a slender structure, with generalizing linear fracture mechanics crack induced failure in an elastic structure, but also the failure state of a massive structure, with combined diffuse (process zone) and localized cracking. A robust operator split solution procedure is developed for the present model taking into account the subtle difference between the types of discontinuities, where the strain

discontinuity iteration is handled within global loop for computing the nodal displacement, while the displacement discontinuity iteration is carried out within a local, element-wise computation, carried out in parallel with the Gauss-point computations of the plastic strains and hardening variables. The robust performance of the proposed solution procedure is illustrated by a couple of numerical examples. Concluding remarks are stated regarding the class of problems where ED-FEM or X-FEM should be a favorite choice.

v) In our recent work [6] we set to develop a model reduction procedure based on statistical modes, which is applicable to nonlinear system under dynamic loads. The system can be characterized by nonlinear inelastic behavior, and contain initially a refined mesh representation which is needed to represent inelastic behavior mechanisms. The reduced model should be capable of achieving the main goal of providing the sufficiently accurate representation of the chosen quantities.

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MULTISCALE MODELING OF ALLOY SOLIDIFICATION

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A multiscale model based on a database approach is presented to investigate alloy solidification. Appropriate assumptions are introduced to describe the behavior of macroscopic temperature, macroscopic concentration, liquid volume fraction and microstructural features. These assumptions lead to a macro-scale model with two unknown functions: liquid volume fraction and microstructure features. These functions are computed using information from the solution of selected micro-scale problems. This work addresses the selection of the sample problems relevant to the interested problem and the utilization of data from the micro-scale solution of the selected sample problems. A computationally efficient model, which is different from both the micro-scale model and macro-scale model, is utilized to find relevant sample problems. In this work, the computationally efficient model is a sharp interface model that does not account for nucleation and treats the solidification material as a pure material. Similarities between the sample problems and the interested problems are explored by assuming that the liquid volume fraction and microstructure features are functions of solution features extracted from the solution of the computationally efficient model. The solution features of the computationally efficient model are defined as the interface velocity and thermal gradient in the liquid at the time the sharp interface passes through. An analytical solution of the computationally efficient model is utilized to select sample problems relevant to solution features obtained at any location of the interested problem domain. The microscopic solution of selected sample problems is then utilized to evaluate the two unknown functions (liquid volume fraction and microstructure features) in the macro-scale model. Interpolation is utilized in the feature space to greatly reduce the number of sample problems needed and to make the database approach a computationally efficient one. The efficiency of the proposed multi-scale framework is demonstrated with numerical examples that consider a large number of solidifying crystals. A computationally intensive fully-resolved micro-scale analysis is also performed to evaluate the accuracy of the multiscale framework.

MODELING AND SIMULATION OF SHEAR BANDS IN METALS AND IMPACT DAMAGE OF STEEL PLATES BY DEFORMABLE PROJECTILES

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Conventional continuum mechanics models of inelastic deformation processes are size scale independent. In contrast, there is considerable experimental evidence that inelastic flow in crystalline materials is size-dependent. At present there is no generally accepted framework for analyzing the size-dependent response of an inelastically deforming material. This is due to the fact that very limited quantitative numerical comparisons with experimental results were conducted, particularly, in localization problems. As soon as material failure dominates a deformation process, the material increasingly displays strain softening and the finite element computation is considerably affected by the mesh resolution. Several localization limiters that incorporate length scale measures in the constitutive relations have been successfully used in the literature to remove the inherent mesh sensitivity of the numerical failure predictions and to solve size scale dependency. A gradient-enhanced elastic-viscoinelastic material model that possesses explicit and implicit material intrinsic length scales is used to study the effect of including these material lengths on the localization of plastic flow in shear bands. It is shown that the inherent material length scale predictions agree well with the width of the shear bands in ductile metals as compared to the experimental results.

The effective use of existing Finite Element Codes in the direct simulation of hypervelocity impacts by blunt projectiles is limited by the dependence of the size of localized failure regions on the mesh size and alignment. This gives rise to a non-physical description of the penetration and perforation processes. A micromechanical constitutive model that couple anisotropic thermo-viscodamage mechanism with thermo-hypoelastoviscoplastic deformation is presented as a remedy to this situation. Explicit and implicit microstructural length scale measures, which preserve the well-posedness of the differential equations, are introduced through the use of the

viscosity and gradient localization limiters. Simple and robust numerical algorithms for the integration of the constitutive equations are also presented. The proposed unified integration algorithms are extensions of the classical rate-independent return mapping algorithms to the rate-dependent problems. A simple and direct computational algorithm is also used for implementing the gradient-dependent equations. This algorithm can be implemented in the existing finite element codes without numerous modifications as compared to the current numerical approaches for integrating gradient-dependent models. Model capabilities are preliminarily illustrated for the dynamic localization of inelastic flow in adiabatic shear bands and the perforation of a 12mm thick Weldox 460E steel plates by deformable blunt projectiles at various impact speeds.

MESOSCALE MODELING OF THE RECRYSTALLIZATION OF SUPERALLOYS

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The aerospace industry has a great need for models of microstructure evolution during the processing of superalloys, in particular the kinetics of recrystallization and grain growth. Two forces are driving this need. First, the mechanical properties of forged components depend strongly on the microstructure obtained through thermomechanical processing. Second, superalloy manufacturing has become a mature business for which most improvements in terms of productivity and reliability are expected to come primarily from the precise optimization of processing itself, rather than from the development of new alloys per se.

The most common method used in industry to model recrystallization is based on the semi-empirical JMAK, or Avrami, formulation. This method requires minimal computer resources but lacks a firm physical basis, thus preventing extensions of the approach outside the realm of measurements let alone to other (even similar) alloys. Conversely, academic approaches have focused on techniques such as Monte-Carlo and cellular automata, but their large computing requirements pose issues regarding coupling with finite-element-method (FEM) analysis. An alternate method combining the advantages of both (viz., the ease of use of the first and the physical basis of the second) was thus developed. This new formalism aims at representing grains in a statistical, rather than discrete, manner by focusing on grain populations composed of so-called meso-scale units (MSUs). MSUs describe the grains they contain through average values such as grain size, dislocation density, etc. Hence, each MSU represents a specific family of grains that are expected to exhibit similar evolution due to similar characteristics that arose from their previous history. Furthermore, one of the key issues posed by recrystallization concerns conservation of volume, for the growth of some grains has to be compensated by the loss of volume of others. This requirement is handled through a geometric framework that functions as an internally-consistent part of the model. Its inputs (grain-boundary velocities for each pair of MSUs and nucleation rates) are provided by a set of equations that evaluate the driving forces for each MSU. Additional efforts are now underway to improve the physical basis of expressions used for mechanisms such as nucleation. The connection of this microstructure description with the macroscopic flow stress is another challenge that must be resolved to enable the coupling of microstructure evolution with FEM calculations for future full-scale process simulations.

MODELING OF ELASTOPLASTIC DAMAGE IN COHESIVE GEOMATERIAL USING NON LINEAR HOMOGENIZATION TECHNIQUE

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Most geomaterials are heterogeneous media and their macroscopic mechanical behavior depends on mineralogical composition, local mechanical behavior of each constituent and microstructure. In the case of cohesive geomaterials, plastic deformation and damage are the two principal inelastic mechanisms. So far, various phenomenological models have been developed for the description of coupled plastic damage behavior in these materials. Being based on extensive experimental data, these models can actually capture the main features observed at the macroscopic scale. However, the phenomenological models are not able to link macroscopic behavior to physical mechanisms involved at microscale; for instance, these models can not properly take into account the influence of mineralogical composition on the macroscopic response of rock materials.

In order to develop an alternative but more physically-based approach, the purpose of the present work is to formulate and validate a micromechanical model for the description of elastoplastic and damage behavior of cohesive geomaterials. The typical material chosen is the Callovo-Oxfordian hard clay; this is motivated by the feasibility study for geological storage of nuclear waste in France. Extensive experimental studies have shown that the mechanical behavior of this material is clearly dependent on the mineralogical composition, varying with depth and water saturation degree. Therefore, the purpose of micromechanical modeling is to provide a rigorous approach able to account for such dependency.

The hard clay is considered as a heterogeneous composite composed of an elastoplastic matrix and of linear elastic or elastic damage inclusions. The macroscopic constitutive law is obtained by adapting the incremental method introduced by Hill; it consists to build the macroscopic tangent matrix of the material from the non linear local behavior of each phase. Due to the matrix/inclusion morphology of the microstructure of the hard clay, a Mori-Tanaka homogenization scheme is used. After the numerical validation of the model through the comparison with the unit cell analysis using finite element method, the proposed

micromechanical model is applied to the analysis of stress strain response of hard clay. The main contributions of the present work can be summarized in three aspects. An original formulation is proposed for the local behavior of hard clay constituents, including a physically-based and mathematically coherent elastic damage model for quartz grains. We have extended the applicability of the Hill-type incremental method for non- linear homogenization. More specifically, the use of a non associated plastic model for clay matrix allowing plastic volumetric compressibility and dilation constitutes a novel advance on the application of the incremental method. Another new feature of the proposed developments is the combination of the plastic and damage behaviors, which are typical for geomaterials. Finally, it is shown that by considering a modified version of the original Hill method based on the use of a randomization/isotropization procedure of the local tangent matrix, the model predictions are in good agreement either with FEM analysis on the unit cell and with experimental data. In particular, the micromechanical model can correctly take into account the influence of mineralogical composition.

Some possible extensions of the present work will also be presented, including the description of time dependent behavior and comparison with the non uniform transform field analysis (NTFA) in order to take into account non uniform distribution of local plastic strain fields.

GRAVITY FLOW OF A MODEL GRANULAR MATERIAL

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We present experimental results concerning the flow of a densely packed grain collection down a two-dimensional inclined channel with rough boundary conditions at the bottom. For the range of inclinations corresponding to a steady regime and to nonsliding conditions at the bottom ($21° < \theta < 28°$), we obtain quasi-linear velocity profiles, that in contradiction with the predictions of the kinetic theory. We attribute this discrepancy to the inadequacy of the binary collision picture to describe the case of dense packings, characterized by the existence of continuous paths of long-lasting contacts through the bulk. We also show that the various velocity profiles obtained for different flow rates and slopes merge on a single master curve, according to the following scaling law: $v_x/\sqrt{gd} \propto [\sin(\theta-\theta_c)/\cos(\theta_c)]^{1/2} y/d$ (d being the grain diameter and θ_c the maximal angle of repose).

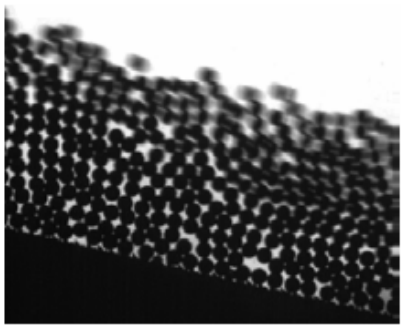

Figure 1. Flow of a collection of monodisperse aluminum spheres (restitution coefficient e=0.6, flow rate 1100 grains/sec, exposure time of the photograph : 1/125 sec). .

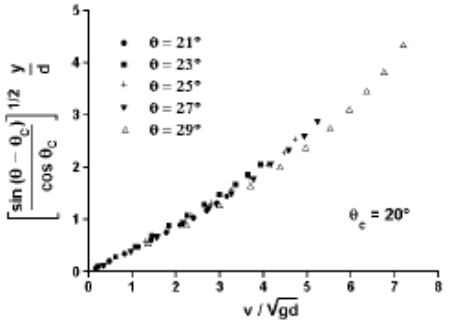

Figure 2.Adimensioned velocity profiles corresponding to various slopes, as a function of the adimensioned velocity (the flow obtained for $\theta = 29°$ is non-uniform) . Note that the shear rate is nonzero at the vicinity of the free surface..

Emphasizing the role played by multicontact collisions and by the fast and damped propagation of momentum and energy through the continuous paths of transient contacts, we propose an explanation relying on the following basis. We consider that all the kinetic energy

gained by a grain during its chute (i.e. during a time $\dot{\gamma}^{-1}$, where $\dot{\gamma}$ is the shear rate) is totally dissipated through the bulk (by means of acoustic waves) in a very short time compared to $\dot{\gamma}^{-1}$

Considering in parallel Coulombian friction, we obtain then for the steady regime shear rate $\dot{\gamma} \propto [\sin(\theta-\theta_c)/\cos(\theta_c)]^{1/2}\sqrt{gd}$ that in qualitative and quantitative agreement with the experimental data. Note that this scheme accounts successfully for the paradoxical nonzero value of the shear rate at the vicinity of the free surface. We also demonstrate that for dense particulate flows, the main part of the dissipation is due to frictional sliding.

LENGTH SCALES IN MECHANICS OF GRANULAR SOLIDS FROM DEM SIMULATIONS

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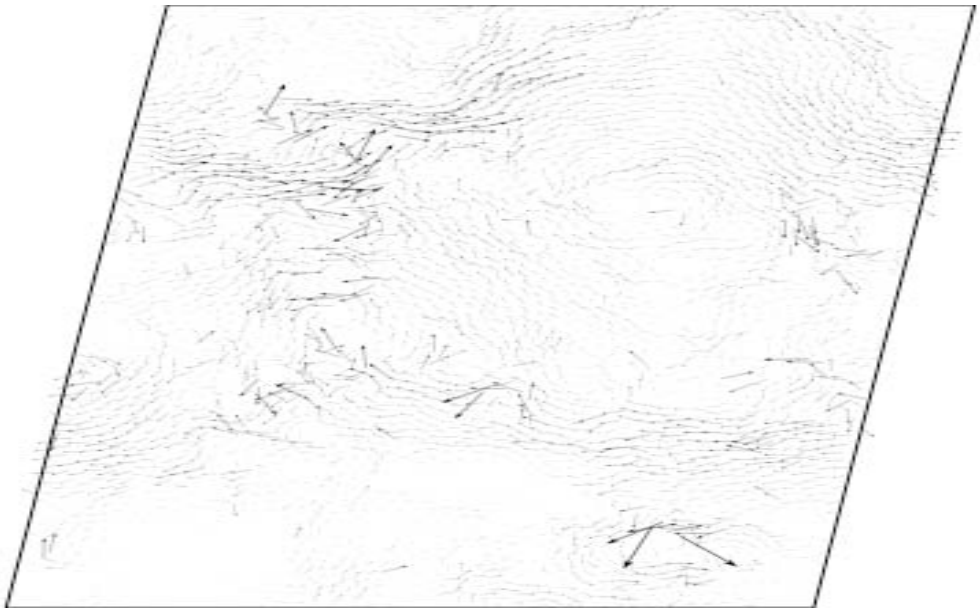
Granular media are described at two scales: 1) The contact scale for elastic, frictional and cohesive interactions between two particles; 2) The particle scale for the integration of the equations of motion. We first briefly compare two fundamentally different discrete elements methods (DEM), namely contact dynamics (CD) and molecular dynamics (MD), in dealing with these scales for the simulation of granular media. Then, we show that intrinsic force inhomogeneities (force chains) occur but they integrate out over a few particle diameters so that a representative elementary volume (REV) of rather small size can be defined as far as static Cauchy stresses are concerned. However, as a result of steric exclusions among particles, we observe large-scale (system size) inhomogeneities in friction mobilization and particle displacements. Mobilized and sliding contacts form clusters whose average size diverges as the limit of plastic deformation is approached. On the other hand, the nonaffine components of particle displacements occur in large eddy-like structures with a power spectrum analogous to fluid turbulence scaling. Finally, we discuss the relevance of various length scales to the plastic behavior of granular materials, in particular with respect to flow rule and evolution of internal variables.



Snapshot of particle displacements in a homogeneously sheared granular packing; from F. Radjai and S. Roux, Phys. Rev. Lett. 89, 064302 (2002)

INITIAL YIELDING AND ANISOTROPIC HARDENING OF HEXAGONAL METALS

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Because of twinning and texture evolution, the yield surface for hexagonal closed packed (hcp) metals displays asymmetry between the yield stresses in tension and compression, and significantly changes its shape with accumulated plastic deformation. Traditional yield criteria and hardening laws cannot accurately model these phenomena. In this work, initial yielding is described using a yield criterion capable of capturing both anisotropy and strength differential effects initially proposed by Cazacu, et al., (2006) and recently generalized to incorporate additional linear transformations for increased accuracy (Plunkett, et al., 2007). The evolution laws for the strength differential parameters and anisotropy coefficients can be determined using a combination of experimental data and the results of numerical tests performed with a crystal plasticity model.

Application of the model to the simulation of the three-dimensional deformation of a pure zirconium beam subjected to four-point bend tests along different directions is presented. Comparison between predicted and measured macroscopic strain fields and beam sections shows that the proposed model describes very well the difference in response between the tensile and compressive fibers and the shift of the neutral axis.

FAILURE AND PLASTIC STRAINS IN GRANULAR MATERIALS: A MULTISCALE APPROACH

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This lecture deals with two basic features of granular materials. First, a certain type of failure, described as a loss of sustainability, is investigated. For non-associated materials such as granular assemblies a broad domain exists, strictly within the plastic limit, where different failure modes can coexist. The notion of loss of sustainability was recently shown to be a proper mode of bifurcation. Given a mechanical rate-independent system in equilibrium under prescribed control parameters, the mechanical state is reputed unsustainable if and only if the system can reach spontaneously another mechanical state. It was established in a very general manner that such bifurcation modes, characterized by a development of kinetic energy, are detected by the vanishing of the second-order work. Afterward, by specializing the investigation to granular materials, both macroscopic (on the specimen scale) and microscopic (on contact scale) second-order works are shown to be related through a fundamental multiscale relation. This relation, at the basis of our microstructural investigation, indicates that a material cause (related to the plastic behavior of some contacts) together with a geometrical cause (related to the deletion of contacts) are responsible for the vanishing of the macroscopic second-order work. Then, the existence of a regular or a singular flow rule for the plastic strains is queried from a multiscale approach. By considering our micro-directional model, it is shown that a regular flow rule exists only in two-dimensional conditions, and disappears as soon as more general three-dimensional loading conditions are considered. The microstructural origin of this basic feature is discussed, and the strong influence of the loading history on the nature of the plastic flow rule is clearly pointed out.

KEYWORDS:
Granular material, Flow rule, Loss of sustainability, Bifurcation, Homogenization, Discrete element method, Micro-structure, Second-order work.

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A MULTISCALE MODELLING OF DYNAMIC DAMAGE BY MICRO-VOIDING WITH APPLICATION TO SPALLING

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When subjected to tensile pressure a metallic material undergoes an internal damage by void nucleation and growth. The final stage of damage is characterized by void coalescence and material failure by the onset and propagation of macroscopic cracks. Plastic and viscoplastic theories have been developed to account for micro-void damage, most of them being based on the GTN (Gurson-Tvergaard-Needlemean) model of ductile damage. These models must be revisited when extreme loading conditions are encountered as during impacts and shocks. For instance, in plate impact experiments the rate of pressurisation can be of the order of several Gpa per nanoseconds in the spall plane and the level of the shock pressure can be of the order of some ten Gpa. When subjected to solicitations of that level, micro-voids undergo a rapid growth producing an important acceleration of the material particles in the vicinity of voids. The subsequent micro-inertia effects (which can significantly refrain void growth, Ortiz and Molinari (1992)) cannot be ignored in the modelling of dynamic damage. Approaches based on damage models which do not account for these micro-inertia effects (e.g. the GTN model) cannot be used when intense dynamic loadings are considered.

The scope of the presentation is to develop a multiscale model of damage where micro-inertia effects are accounted for, see Czarnota *et al* (2006). Void nucleation is supposed to be pressure controlled. A void is nucleated when the local pressure becomes higher than a critical nucleation pressure. To account for the dispersion due to the heterogeneous microstructure and to internal residual stresses, a statistical information on the distribution of potential nucleation pressures in introduced in the model in terms of a Weibul law, Molinari and Wright (2005). To each nucleated void is associated a hollow sphere constituted by the void surrounded by an external shell made up of matrix material. The void growth-kinetic is obtained from the dynamic evolution of the hollow sphere models. Two levels can be distinguished in the present homogenization scheme. The first step of homogenisation is developed at the level of a composite sphere by the analysis of the dynamic response of this local element. The viscoplastic response of the matrix and micro-inertia effects are

introduced at that level. The second step consists in defining a transition law from the local level of composite spheres (each of them having a different response) to the macroscopic level. Here we explore two simple schemes, the first based on the assumption of uniform pressure, the second on the assumption of uniform volumetric deformation.

Applications are made on plate impact experiments for tantalum, Roy (2003). During impact, two compressive waves are generated respectively in the target and projectile. By reflection at the free boundaries two release waves are generated which interact in the spall plane and generate a very high pressure loading. The particle velocity has been measured at the free surface of the target, providing information about the evolution of the internal damage. All the experimental results obtained at different impact velocities and for different values of the plate thickness are reproduced by the present model with excellent accuracy. Moreover, the modelling allows understanding the evolution of the dynamic damage within the material which cannot be directly accessible by in situ measurements.

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SOME GENERAL PROPERTIES OF ESHELBY'S TENSOR FIELDS IN CONDUCTION AND ANTI-PLANE ELASTICITY

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Determination of the macroscopic (or effective) transport properties of a heterogeneous material in terms of its microstructure and the properties of its microscopic constituents is a lastingly standing issue in mechanics and physics. The thermal conduction problem is mathematically analogous to that of electrical conductivity, permittivity, permeability or diffusivity. Under certain conditions, it is also mathematically similar to the problem of anti-plane elasticity. To estimate the thermal conductivity of heterogeneous materials, analytical and computational homogenization methods have been developed. In the case of random heterogeneous materials, these methods are often based on the thermal counterpart of the well-known Eshelby's elastic result: the temperature gradient or heat flux field inside an ellipsoidal inclusion undergoing a prescribed uniform temperature gradient and embedded in an infinite medium is uniform. In other words, Eshelby's thermal second-order tensor relating the final temperature gradient to the prescribed one inside the ellipsoidal inclusion is a uniform field. The present work studies the general properties of Eshelby's thermal tensor field for an arbitrarily shaped inclusion in infinite isotropic and anisotropic media, which is no longer uniform. In particular, we show that the isotropic part of Eshelby's thermal tensor field is always uniform inside the inclusion and null outside the inclusion independently of the shape and connectivity of the inclusion and of the anisotropy of the medium surrounding the inclusion. The recent results on Eshelby's elastic tensor fields for a non-ellipsoidal inclusion are all concerned with isotropic media. By contrast, the results derived in the present work on Eshelby's thermal tensor fields for a non-ellipsoidal inclusion are on both isotropic and anisotropic media. They are expected to be useful for estimating the effective transport properties of heterogeneous materials.

COALESCENCE OF VOIDS AND FORMATION OF SHEAR BANDS IN POROUS DUCTILE SOLIDS – THEORETICAL MODELS AND NUMERICAL STUDIES

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It is well known that propagation of cracks in ductile materials occurs through two distinct mechanisms: coalescence of cavities and formation of shear bands (« void sheet mechanism »). The first mechanism dominates for mode I loadings and the second one for mode II loadings. In mixed-mode situations, both can occur, with a possible coupling between the two.

Gurson's [1] famous « homogenized » model for plastic porous materials, as improved by Tvergaard and Needleman [2], does incorporate some phenomenological modelling of coalescence, but not of formation of shear bands. As a result, it fails in some instances where this mechanism is important. It is for example incapable of reproducing the experimentally known fact (Kyeonglak [3]) that kink angles of cracks propagating under mixed-mode conditions are always much smaller (typically, less than 20°) in ductile materials than in brittle ones. Explaining such a phenomenon seems to necessitate the development of a theoretical description of formation of shear bands in porous ductile materials. In order to be applicable to mixed-mode situations, the theory should also include coalescence and possible interactions between the two phenomena.

The theoretical study of coalescence has been the topic of several papers in recent years. In one of these, Gologanu *et al.* [4] proposed to schematize a representative volume element (RVE) in some plastic porous medium, in which coalescence was taking place, as a superposition of alternately sound and porous planar layers perpendicular to the direction of the major principal stress. The mechanical fields were schematized as homogeneous in each layer. The sound layers were considered to obey the standard von Mises model and the porous one Gurson's model. The onset of coalescence corresponded in this approach to the brutal concentration of the strain rate in the porous layer, the sound ones becoming suddenly rigid. The deformation mode of the RVE then became a pure uniaxial extension in the direction of the major principal stress, without any lateral necking. The simplifying hypothesis of homogeneity of the strain rate and stresses in each layer made it possible to obtain the solution almost entirely analytically.

The theoretical study of formation of shear bands in plastic porous materials was investigated in an old but seminal paper due to Drucker [5]. This author showed that if a RVE in some plastic porous *periodic* material is subjected to some shear loading, the strain rate tends to concentrate in thin planar layers connecting the voids, rather than to spread over the whole RVE. This effect is intimately tied to the presence of some porosity, in spite of the fact that void growth under shear is nil or very limited.

This paper presents a unified theoretical framework for the description of coalescence of cavities and formation of shear bands in porous ductile materials. The approach proposed encompasses both Gologanu *et al.*'s [4] treatment of coalescence and Drucker's [5] argument on shear bands, and also covers situations of mixed mode where both phenomena are present and interact. Its principle consists of extending the former authors' analysis, which was limited to axisymmetric stress states, to arbitrary 3D loadings incorporating shear components. Again, the onset of coalescence and/or formation of a shear band corresponds in this approach to the sudden concentration of the strain rate in the porous layer. However the deformation mode of the RVE is no longer a simple uniaxial extension but now incorporates some shear component(s). Again, the solution can be obtained almost completely analytically, thanks to the simplifying hypothesis of homogeneity of the strain rate and stresses in each layer.

The validity of the theory developed is then assessed by comparing its predictions to the results of some 3D micromechanical finite element computations. The simulations consider a typical voided RVE subjected to some proportionally varying loading. They are similar in principle to Koplik and Needleman's [6] well-known simulations of cylindrical RVEs subjected to axisymmetric stress states, but consider more general loadings involving some shear component. This makes it necessary to use more complex, periodic boundary conditions. The initial shapes of the RVE and the enclosed void are assumed to be cubic and spherical, respectively. The numerical results do confirm the simple analytical model developed.

The theory is finally applied to the prediction of kink angles of cracks propagating in ductile solids under mixed-mode conditions. This is done in a first step without really coupling this theory to finite element computations, but using it instead as a kind of « post-processor » of such computations. The principle consists of performing a numerical simulation prior to propagation of the crack using Gurson's model, and then applying the theory in the elements around the crack tip to determine the most « favorably oriented » porous band. The « most

favorable » orientation is heuristically defined as that corresponding to the lowest possible value of the « ductility » (equivalent strain at the onset of localization). The kink angles thus predicted theoretically are in good agreement with those actually measured by Kyeonglak [3]. The next step will consist of no longer using the model as a mere post-processor, but incorporating it into some finite element code and using it to simulate the development in time of cracks propagating in ductile solids under mixed-mode conditions.

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MODELLING SUBGRAIN TEXTURE EVOLUTION WITH EXPERIMENTAL VALIDATION USING DIRECT INPUT FROM MICROSTRUCTURE IMAGES

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We present a numerical formulation based on Fast Fourier Transforms to obtain the micromechanical fields in plastically deformed 3-D polycrystals. This formulation, developed in the last decade [1] as a fast algorithm to compute the elastic and elastoplastic response of composites using as input a digital image of their microstructures, has been in turn adapted to deal with 3-D polycrystals deforming by dislocation glide [2]. The FFT-based formulation provides an exact solution of the governing equations in a periodic unit cell, has better performance than a Finite Element calculation for the same purpose and resolution, and can use voxelized microstructure data as direct input. To illustrate the capabilities of this model, we first discuss the construction of a 3-D unit cell using: a) 2-D orientation maps, b) Voronoi tessellation to build a 3-D substrate, and c) a buffer zone with infinite compliance to simulate stress-free surface boundary conditions. Next, we show FFT-based predictions, together with comparisons with experimental results obtained with Orientation Imaging Microscopy (OIM), on local texture development (i.e. evolution of average orientations and average misorientations) in a recrystallized Cu polycrystal deformed in unixial tension. The rotations of the average orientations and the orientation-dependent magnitudes of the average misorientations are well reproduced by the FFT-based model.

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SOME ASPECTS OF THE NONLINEAR BEHAVIOR OF MICROCRACKED MATERIALS

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In this communication are presented some recent studies of the nonlinear behavior of microcracked materials. Two complementary aspects are investigated.

The first part of the study is devoted to anisotropic damage of quasi brittle materials due to progressive microcracking. We first present the basic principles of Eshelby-based homogenization methods and their applications to microcracked materials including the so called unilateral effects due to micro-cracks closure. This homogenization framework is then used to develop a complete micromechanical damage model. For this purpose, a damage surface and a damage evolution law based on an energy release concept are proposed. Furthermore, we extend the model by coupling the anisotropic damage with friction phenomena including dilatancy due to closed microcracks. A wide validation of the model is proposed either for concrete and for rocks materials under complex multiaxial loading paths. Finally, after implementing the micromechanical model in the Finite Element software ABAQUS (Subroutine UMAT), we present some applications which deal with civil engineering or geomechanical strutures; a good agreement is observed between the numerical results and in situ data (Excavation Disturbed Zone (EDZ)).

In the second part, we investigate a 3D micromechanical modelling of ductile porous materials composed of a rigid perfectly plastic matrix containing penny-shaped cracks. For this purpose, we consider an Eshelby-like trial velocity field in the standard limit analysis of porous materials (Gurson, 1977) as well as in its extensions to the case where voids are non spherical. The obtained pressure-sensitive macroscopic criterion is valid for arbitrary loadings and gives good predictions for low stress triaxility (in particular purely deviatoric loadings). It is shown that these results agree with the existing (nonlinear) Hashin-Shtrikman bound. Moreover, significant new improvements of the existing Gurson-type criteria are shown for the plastic matrix weakened by penny-shaped microcracks.

NUMERICAL MODELING OF MICROSTRUCTURAL PHENOMENA IN POLYCRYSTALLINE METALS

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It is well known that the localization of plastic flow is strongly influenced by deformation-induced textures and anisotropy. In turn, this localization can affect, to some degree, the texture development in a polycrystal. This suggests that polycrystal deformation models are required to properly stimulate plastic stability and localization phenomena. It is thus expected that polycrystal models can provide an improved understanding of the relation of localization to the microstructure of the material, and can consequently be more successful in prediction strain localization than can macroscopic, numerical modeling of large strain plasticity phenomena are considered. In particular, instabilities and localized deformation phenomena for FCC, HCP and BCC polycrystals subjected to various deformation modes are investigated. In-house finite element analyses based on a rate-dependent crystal plasticity model have been developed to stimulate the large strain behaviour of polycrystalline metals. Simulations are performed using two approaches. In the first approach, each material point in the finite element analysis is considered to be a polycrystalline aggregate having a large number of grains and the Taylor theory of crystal plasticity is adopted to model the behaviour of the polycrystal. In the second approach, each grain is represented individually using on or more finite elements, and the constitutive response within each element is given by the single crystal constitutive model. Both approaches account for initial textures, as well as texture evolution during large plastic deformations. The numerical analyses incorporate high performance parallel computing features. The results of simulations for various deformation modes are discussed, and in certain cases comparisons are made with

experimental results. The effects of various parameters such as initial texture, strain hardening, material strain-rate sensitivity, geometric imperfections, strain paths and boundary conditions on the formation of localized shear band are discussed. The importance of modeling texture evolution to properly predict localized deformation and instability initiation is emphasized.

A CONSTITUTIVE MODEL FOR GRNULAR MATERIALS WITH SURFACE ENERGY FORCES

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Microstructural models for stress-strain behavior of granular material can be derived from properties of inter-particle contacts. Considering the mean behavior of all contacts in each orientation, the overall stress strain behavior can be obtained as an average of the contact behavior for all orientations. The basic idea is to view the packing as represented by a set of micro systems. The inelastic behavior of each micro-system is characterized and the overall stress-strain relationship of the packing is obtained from an average of the behaviors of micro-systems. In this paper, the micro-systems are regarded as inter-particle planes, or mobilized planes, which requires to describe only a simple relation between the vectors of forces and relative displacements on a contact plane. The stress and strain tensors are obtained by integration over all spatial orientations. In the model, a simple elastic-plastic behavior is assumed on each contact plane. The elastic part is based on the Hertz-Mindlin's contact formulation, while the plastic part is based on a Mohr-Coulomb friction law with an isotropic hardening assumption and a non associated flow rule. For the whole packing, a critical state behavior is assumed at large deformations and the friction angle on each plane is related to the actual void ratio compared to the critical void ratio at the same state of stress.

The ability of the model to reproduce the main features of sand behavior has been demonstrated. Model simulations were compared with drained triaxial tests results at different initial void ratios and different confining stresses leading to contractant or dilatant behavior of the sand specimens. A comparison between numerical simulations and experimental results demonstrated that the model is capable of reproducing the general trend for both loose and dense sands.

It is then extended to introduce surface energy forces at the particle contacts. All materials, with or without a net surface charge, exhibit surface energy forces, which act at a very short range. But whereas these forces are negligible for usual sand or silty sand on Earth, they are significantly important under tiny atmospheric pressure, such as on the Moon. As a matter of

fact, observations made during Moon's explorations have shown that lunar soil has an additional component of shear strength described by a cohesion, *c*, of several kPa higher than the one which could be found under Earth's environmental conditions. Before any construction on Moon and Mars can be envisaged, a proper understanding of soil properties and its mechanical behavior in these different environmental conditions is essential.

The surface forces between two solid grains result from the addition of electrostatic and Van der Waals energy fields. The electrostatic component in lunar soil is assumed to be negligeable. Therefore, in this paper, the surface energy forces are calculated from Van der Waals energy fields. It is noted that when the distance *D* between two neighboing particles is greater than 2 nm, the effect of the Van der Waals forces is practically negligible. This distance *D* is a function of the amount of molecules which can be adsorbed on the solid surface. Molecule adsorption on a solid surface is conditioned by temperature, gas pressure and atmospheric composition. On Earth, adsorption conditions are easily fulfilled due to the presence of a high atmospheric pressure. Therefore the distance *D* can easily exceed several nms and the effect of the Van der Waals force are negligible. Under lunar atmospheric condition, the thickness of the adsorbed molecule layer is likely to be very thin. Under these conditions and in accordance with the observations made on the Moon's surface, the model shows that the shear strength for lunar soils appears to be 12 to 15% higher than that of earth soil. The stiffness of the lunar soil is also higher. Differences in Earth soil shear strength measured at atmospheric pressure and at ultrahigh vacuum indeed tend to compare well with estimates based on the model.

DISLOCATION DYNAMICS AND SIZE EFFECTS IN THE TORSION OF ICE SINGLE CRYSTALS

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Single crystals of ice subjected to primary creep in torsion exhibit a softening behavior: the plastic strain rate increases with time. In a cylindrical sample, the size of the radius has effects on this response. The smaller the radius of the sample becomes, the softer the response at constant average shear stress across a section. This effect of size on mechanical response is addressed by using a recent theory for the coupled dynamics of statistically distributed dislocations and excess dislocations [1, 2]. In this theory, excess dislocations are defined as a continuous manifestation of lattice incompatibility. They induce elastic internal stresses, to which statistical dislocations make no contribution. Both dislocation species contribute to plastic flow however, and their dynamics are coupled in the sense that gradients in the plastic distortion field from statistical dislocations generate excess dislocations. Reverse coupling occurs when excess dislocations contribute to forest hardening. The underlying dislocation dynamics suggested by simulations based on the above model is as follows. Under stress gradients obtained from a positive torque, positive excess screw dislocations nucleate close to the exterior of the sample. These dislocations glide in basal planes (normal to the torsion axis) towards the center of the sample and eventually form pile-ups, inducing directional (kinematic) hardening and internal back-stress. Statistical dislocations are scarce, and forest hardening is virtually non existent in the simulations. Cross-slip through prismatic planes is induced by long-range internal stresses. By coupling neighboring basal planes, it regulates the distribution of dislocation glide along the axis direction. When reverse torsion follows forward torsion by sequentially applying a negative torque, negative screw dislocations are nucleated. Driven by both the applied stress and the existing back-stress, the latter annihilate with the positive pile-ups obtained from forward

torsion. They may eventually form negative pile-ups depending on initial dislocation density levels. The simulations do retrieve the softening behavior and the size effects observed in the forward creep response. Dispersion of the results due to initial dislocation microstructure and sample height effects is discussed. Continuous hardening of the response to reverse torsion is predicted in association with the resilience of positive pile-ups, whereas a sequence of hardening-softening behavior is seen to result from the formation of negative pile-ups. Both types of response are actually observed in reverse torsion experiments.

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A MICROSTRUCTURE-BASED PLASTIC POTENTIAL FOR POLYCRYSTALLINE METALLIC AGGREGATES

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The elastic-plastic behaviour of metallic polycrystals is described from a global regularization, over all grains, of the crystal Schmid flow criterion, previously introduced as the “regularized Schmid law” (RSL) by Arminjon (1991). So doing, the polycrystal is considered through a Homogeneous Equivalent super-crystal. According to the selected homogenization procedure, different estimates of the polycrystal effective behaviour result. They have in common to derive from a microstructure-based single plastic potential that can simultaneously account for texture, hardening and morphology evolutions in a physically realistic manner.

A practical advantage of such a regularization of the plastic flow criterion at the poly-crystal scale is its consistency with standard formulations of finite element codes, what formally makes it of easy use in numerical simulations (Berbenni and Franciosi, 2004).

However, the resulting global scheme remains complex for routine manipulations, especially owing to the non linearity of the material constitutive phases and to the large number of crystallographic phases in metallic materials.

When specializing to the homogenization procedure of the affine type (Masson et al, 2000), here applying to the self-consistent scheme for aggregates, a particular description for the crystallographic slip on all the slip planes of the polycrystal is shown to allow the use of the Transformation Field Analysis method (TFA) developed by Dvorak (1992). This description for multi-planar slip is of hierarchical multi-laminate (HML) nature and takes benefit of an orthogonality property between the modified Green operator integral of laminate layers and the Schmid tensors for slip systems gliding in the laminate planes (Franciosi and Berbenni 2006, 2007). Stress and strain fields being homogeneous in laminate layers, the TFA applies quite safely.

The presented lecture will describe the general features and discuss the particular characteristics of the so called RSL-TFA-HML modelling for polycrystals. It will illustrate and comment on

simple examples the effective behaviour that results from considering realistic crystal hardening law forms.

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WHAT HAVE WE LEARNED FROM DISCRETE DISLOCATION DYNAMICS ? A REVIEW OF THE RECENT STUDIES

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Three dimensional discrete dislocation dynamics (DDD) simulations have been imagined by L. Kubin, G. Canova and Y. Bréchet in the early nineties in order to fill the gap between the atomistic simulations and the continuum mechanics. The idea was to develop a numerical tool which could handle large populations of dislocations in interaction through their elastic stress fields. In such a code, the dislocation lines can be viewed as elastic inclusions embedded in an elastic matrix. Then, the effective stress at a dislocation is obtained using the superposition principle, as the summation of the stress field coming from the dislocations as if they were in an infinite medium and a second elastic stress tensor enforcing the boundary conditions. With the years, many improvements have been made to the first version of the so-called *edge/screw* model. Nowadays, more complex *nodal codes* have been developed and complex boundary conditions have been introduced usually by coupling DDD with the finite element method. This new type of numerical modeling is now well developed and the last few years have seen the first applications where DDD is used as a predicting tool to understand the physics at the origin of a typical behavior. As an example, DDD simulations have been used to compute the values to give to parameters of constitutive equations used in dislocation density based model of crystal plasticity. More recently, numerical simulations of the fatigue behaviour of 316L stainless steel have been performed (see Figure 1a). In these simulations, the DDD code gave all the details for the formation of the dislocation microstructure in persistent slip bands [1]. Thanks to a large campaign of simulations, it was even possible to derive the number of cycle needed for a crack to initiate [2].

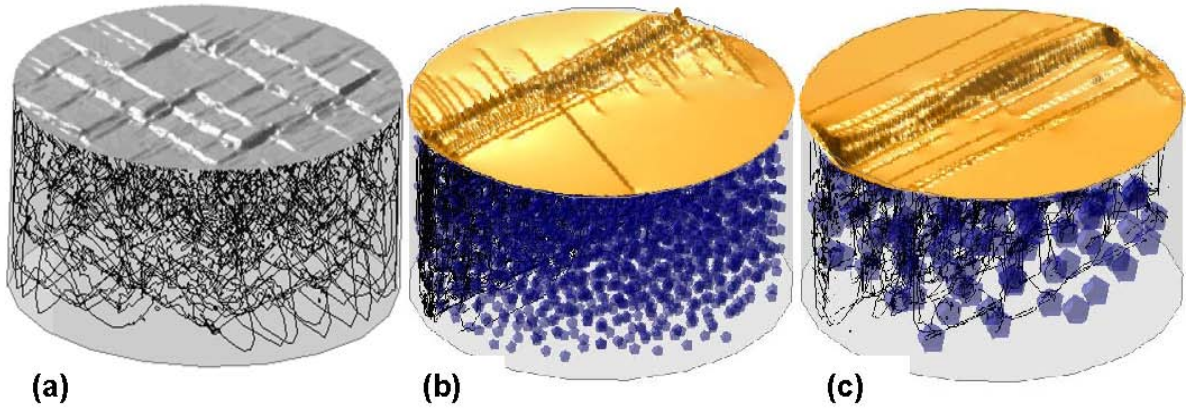

Figure 1: Fatigue simulation of **a-** 316L stainless steel and precipitate hardened material with **b-** shearable and **c-** non-shearable particles.

The interaction of dislocations and precipitates has also been studied with DDD and fatigue simulations of precipitate hardened materials have been performed with different particle sizes (Figure 1b-c)[3]. It was found that size distribution for the particles is an important parameter for fatigue life. The presentation will first explain the basic ingredients of the edge-screw DDD model developed in Grenoble and a detailed study of the mechanisms at the origin of crack initiation in fatigued 316L surface grains will be given.

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DIRECT SCALE TRANSITION APPROACH FOR VISOHYPERELASTIC PARTICULATE COMPOSITES

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This work is issued from a research program concerning the vulnerability of energetic composites, i.e. highly-filled particulate aggregates such as propellant-like materials. A multiscale modelling is being developed in order to predict the global (macroscopic) response of the composite starting from its constituents' behaviour and accounting for microstructural interactions and morphology. Further requisite is to provide reasonable and accessible estimates of local fields. The modelling at stake represents a non-classical averaging approach based on the concept put forward by Christoffersen (J. Mech. Phys. Solids, 1983, 31, 55-83) in the context of linear elastic behaviour of constituents, namely grains and matrix, the latter formed by an assemblage of thin layers. This initial concept was extended and codified by some of the present authors to include dissipative phenomena, notably small strain viscoelasticity (Nadot-Martin et al., Eur. J. Mech. A, 2003, 22, 89-106), and large deformations in the context of (visco-)hyperelasticity (Guiot et al., Mech. Res. Comm., 2006, 33, 441-449 ; Comp. Sci. Techn., 2006, 66, 2726-2735).

It is known that viscoelastic response of constituents is a strong challenge for scale transition as it involves space/time interactions on the local level and leads to the global inference identified as a "long-range memory effect" (see f. ex. Beurthey and Zaoui, Eur. J. Mech. A., 2000, 19, 1-16). The multiscale modelling in question deals successfully with this problem, as shown by Nadot-Martin et al. (2003) op. cit. Its notable specificity –which goes back to the very formulation by Christoffersen– lies in an upstream schematization of the morphology and of internal arrangement of constituents (grains + layers) associated with a series of assumptions regarding local kinematics. In such a manner, the approach, which can be called a morphology-based one (MA), offers a way to take into account some intraphase heterogeneity (local field fluctuations) which is another challenge for contemporary nonlinear micromechanics. Moreover, most of existing nonlinear scale transition schemes are referring to the notion of equivalent linear composite and need prior linearization of the constitutive laws. This procedure and the choice of the linearized moduli have serious consequences for the global estimates. It is to be stressed that the viscoelastic scale transition MA considered and the corresponding solving procedure regard directly the time domain and do not need any prior transformation like the Laplace-Carson one. It thus represents, as it is also the case of the recent work by Lahellec and Suquet (Int. J. Solids Struct., 2007, 44, 507-529), a direct approach to the viscoelastic homogenization problem. This crucial aspect is pointed out here by double computational analysis for a composite with hyperelastic grains and a viscohyperelastic matrix arranged in a periodic manner. The two computational procedures for the composite, by the Finite Element Method and by the morphology-based approach (MA), are compared on the local as well as the global scale level. It is shown that the direct scale transition (MA) gives satisfactory results at both scales in this context. The aptitude of the MA-methodology to deal with current challenges of nonlinear scale transition and notably its ability to treat a viscoelastic homogenization problem in a direct manner is being emphasized. Prospective studies dealing with random microstructures are outlined.

MESOSCOPIC SIZE-EFFECTS IN ATHERMAL MICROCRYSTAL DEFORMATION

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New challenges emerge for property prediction as volume-element sizes approach those of the material structure and mechanistic processes. Thus, an important frontier in both metallurgy and mechanics is the development of a modeling framework that accurately represents length-scale effects and dislocation structure. Emerging mechanics formulations incorporate a length scale tied to distortion gradients aimed at modeling the effects from geometrically necessary dislocations (GND). However, recent experimental studies show important intrinsic size effects exist separately from an evolving GND structure at a mesoscopic scale. Further, the relationships between the new mechanics formulations and actual GND structures remain unresolved. Recently, some of the present authors introduced methods for preparing micron-scale samples via focused ion beam machining and, compression testing at room temperature using a commercially-available nanoindenter. These new methods provide a tool for probing aspects of mesoscale mechanics. The present studies experimentally examined a number of materials at sizes that approach those for the physical micromechanisms of deformation, but remain accessible to discrete dislocation modeling. Typically, the tests evaluated single-slip orientations for microcrystals having diameters ranging from 0.5-40 microns and several strain rates and testing modes. The stress-strain responses of these materials varied with specimen diameter, loading rate, dislocation mechanisms and the nature of the internal structure. Uniaxial compression tests of single crystals of LiF, pure Ni, Ni_3Al alloys, Ni superalloys and fine grained

polycrystalline Ni showed material-unique size dependent responses. The LiF and Ni microcrystals exhibited a strongly size-dependent flow stress over the whole range of specimen sizes tested. This presentation discusses that response. For several materials, including the LiF and Ni microcrystals, an intermittent deformation response was observed. By analysis of that intermittency, the deformation response of the Ni microcrystals was shown to exhibit the characteristic attributes of self-organized criticality. Some of the materials responses were represented within 3-D discrete dislocation kinetics simulations which revealed important new micromechanisms for strengthening. One such mechanism, source-truncation hardening, is especially potent in microcrystals. Other mechanisms, termed 'exhaustion hardening,' result from junction or debris formation just as for dislocation forest hardening but, these occur within an altered size-affected sampling of the dislocation processes. Completely mechanistically self-consistent simulation of such results, by either discrete dislocation or continuum methods, stands as a challenge for emerging materials modeling approaches. The results suggest that a better understanding of dislocation nucleation, percolation, substructure evolution and SOC phenomena are need for understanding size-affected mesoscopic plasticity.

BIFURCATIONS AND INSTABILITIES IN GRANULAR MEDIA: FROM MICRO TO MACRO SCALES

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It is now well recognized that granular media exhibit failure states strictly inside Mohr-Coulomb plastic limit condition (see for example undrained triaxial loadings or "q constant" drained paths on loose sands). Some of these failure modes can be described by the second order work criterion and correspond to diffuse failures (i.e. without shear band patterns). These failure states have been extensively studied by considering phenomenological constitutive relations. Bifurcation domains and cones of unstable stress directions have been obtained numerically and analytically from various elasto-plastic relations. These results will be briefly recalled in the introduction.

In a second part, a discrete element method is used and the behaviour of cubical specimens of 10000 spheres is directly simulated. The second order work is computed from the stress-strain states at the boundaries of the specimen at various stress-strain states and for different stress directions. From this direct simulation, a bifurcation domain and cones of unstable stress directions are exhibited and compared with the ones given by the incrementally non-linear relation, calibrated on the same medium. Diffuse failure modes are indeed simulated for the conditions given by the theory.

Finally, in a third part, a micromechanical model is considered which is based on an elastic-plastic force-displacement relation between two grains, some homogenisation/localisation techniques and a statistical description of the spatial distribution of contacts. From this model a bifurcation domain and cones of unstable stress directions are also obtained. Moreover, based on the fine description of the contact mechanics, it is possible to give a micromechanical interpretation of the macroscopic instabilities noticed experimentally and numerically.

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MICROMECHANICAL MODELLING OF THE VISCOPLASTIC BEHAVIOUR OF EARTH MANTLE OLIVINE

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Olivine, which constitutes the main (polycrystalline) mineral of the Earth's upper mantle, is submitted in situ to extreme thermo-mechanical conditions. Large scale convection cells in the mantle make the material deform plastically at large strain with complex deformation paths, and high pressures and temperatures can induce dynamic recrystallization and partial melting. A better understanding of the Earth's inner structure requires an improved knowledge of the flow in-situ and of microstructures possibly encountered deep in the Earth, which should be strongly affected by the behavior of olivine. In situ plastic deformation is most likely due to dislocation creep, so that pronounced crystallographic textures are produced at large strain. However, at the grain scale, olivine exhibits a highly anisotropic viscoplastic behaviour, with a lack of slip systems and only three independent systems available. Pronounced textures and melt fraction thus strongly affect the effective viscosity, and its anisotropy. Earlier published works, based on the application of the "tangent extension" of the Self-Consistent scheme (VPSC), suggest that a material can deform with three systems only. However, significant improvements have been obtained during the last decade for the modelling of the effective behavior of non-linear composites and polycrystals by means of homogenization techniques. In particular, the so-called Second Order theory (SO) of Ponte-Castañeda (2002) has been shown to improve significantly on earlier theories, as has been demonstrated for several model composites and polycrystals. This work is concerned with the application of SO theory to melt-free and partially melted olivine. The effect of the crystallographic texture on the effective behavior, but also stress and strain rate distribution in the different crystallographic orientation, will be shown and compared to full-field computation based on Fourier Transform techniques.

DAMAGE AND PERMEABILITY IN QUASI-BRITTLE MATERIALS: FROM DIFFUSE TO LOCALIZED PROPERTIES

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This contribution presents a review of the works carried out at R&DO in Nantes, in collaboration with Electricité de France. The aim is the study of sensitive structures like containment vessels of nuclear power plants, and the evaluation of their gas tightness more specifically. The objective is the computation of the leakage rate of vessels subjected to internal pressure (typically during integrity tests). It requires the evaluation of the material permeability, as a function of the moisture content in concrete and of the amount of damage. We focus mainly on the relationship between gas permeability, material damage and cracking. Experimental tests prove strong interaction between mechanical state and transport properties of concrete (see e.g. Choinska et al. 2007) and there exist at least two asymptotic cases where some theoretical modelling exists:

- In the case of diffuse damage, analysis of discrete lattices show that the material permeability should be controlled by the decrease of average stiffness due to micro-cracking (Chatzigeorgiou et al. 2005). Such a relationship has been checked experimentally by Picandet et al. (2001).

- In the case of localised damage, and after a macro-crack has formed, permeability is controlled by a power function of the crack opening (Poiseuille flow). The exponent of the power law depends on the geometry of the problem.

For quasi-brittle materials with evolving microstructure due to mechanical loads, a transition regime should be observed between the two above asymptotic cases, from diffuse micro-cracking to discrete macro-cracking. In this contribution, we define a matching law between existing relations of permeability evolution with damage and with crack opening that is

consistent with these two asymptotic cases. The key issue is to relate the crack opening to the variables in the continuum approach so that the two asymptotic cases are expressed in the same variable system and can be matched. A simplified averaging approach is used for this purpose. The permeability law is then derived using a simple mixing formula that weights each asymptotic regime with damage. In order to emphasize influence of the matching law on structural response, we run finite element simulations of a Brazilian splitting test and comment some size effect results obtained in the mechanical and hydraulic problems.

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SHOCK COMPRESSION IN CONCRETE UNDER 20 GPa – EXPERIMENTAL AND MODELING INVESTIGATIONS

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The frame of this work is the modeling of shock response of concrete structures submitted to the effects of projectile penetration or contact detonation, in a range of pressure levels from 0 to 20 GPa.

Though concrete is currently the most widely used construction material, the knowledge concerning its response under shock loading response remains rather modest. An exhaustive review of the research effort in this field illustrates this fact. The origin of the important dispersion that affects the limited available data is analyzed and discussed. The main factors appear to be related to the composition and the heterogeneity characteristics.

Concerning the composition factor, the authors propose a simple method to predict the shock Hugoniot of concrete based on a mixture theory, considering concrete as a mix of cement hydrates, free water, rock and voids. The potential of this approach is illustrated by comparisons to the available data.

Then, the heterogeneity factor is investigated. Experimental results recently obtained on special concrete compositions are presented. Those results allow to relate the wave structure to the size of the aggregates, and so, to the level of heterogeneity of the composition. Complementary numerical simulations illustrate the ability of a mesoscopic model to describe this phenomenon, and the failure of the homogenized approach to do so.

Finally, the rate sensitivity of concrete is discussed through a numerical analysis of the experimental results.

MULTISCALE METHODS FOR THE FAILURE OF HETEROGENEOUS MATERIALS

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Methods for treating unit cells which lose positive definiteness of the tangent stiffness, i.e. are associated with a material that loses strong ellipticity, are described. These methods can also be used when the material response predicted by the unit cell loses rank one stability. Its notable feature is the decomposition of the unit cell response into a discontinuity and a smooth response. The methods are combined with the extended finite element method so that arbitrary discontinuities at the macroscale can be treated. The adherence of this method to the energetic theorems of Hill is explored. The examples that are studied include a composite with circular inclusions and a microcracking solid with an emerging macrocrack. Potential applications to shear band modeling are described.

A PARALLEL CODE FOR PHENOMENOLOGICAL MESOSCALE FIELD DISLOCATION MECHANICS

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Phenomenological Mesoscopic Field Dislocation Mechanics PMFDM (Acharya and Roy, 2006) is a model of plasticity that forges a precise link between the classical theories of **elasto-viscoplasticity** and **continuously distributed dislocations,** based on averaging the latter to obtain an augmentation of the former. The two classical approaches have been pursued (historically) by separate groups of researchers with different research objectives; more importantly, while there has been strong appreciation amongst researchers of the fact that the two classical theories must somehow be related, a sound mathematical model with physically rigorous underpinnings eluded the community for thirty-odd years. PMFDM offers a tractable link.

PMFDM finds its best expression in (mesoscale) applications at a length scale spanning μm to mm and when non-uniformity of deformation is a consequence of both boundary conditions and material heterogeneity. Accommodation of a realistic boundary value problem while resolving mesoscale features is computationally challenging. To this end, a parallel code has been developed to solve the 1) stress problem, 2) hardening and 3) transport associated with the excess dislocation density. Several examples will be presented that highlight the interplay between the boundary value problem and mesoscale evolution.

CONSTITUTIVE MODELING AND FORMING SIMULATIONS FROM AN INDUSTRIAL PERSPECTIVE

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This presentation is concerned with the numerical simulation of the forming of aluminum alloy sheet metals. In order to design a process for a specific material, it is necessary to account for the attributes of the material in the simulations. Although the numerical methods are generic and can be applied to any material, constitutive models, that is, the mathematical descriptions of material behavior, are material-specific. Therefore, macroscopic and microscopic aspects of the plastic behavior of aluminum alloys are reviewed first.

This presentation also illustrates the importance of material and process interactions. In principle, modeling of forming and microstructure evolution should be a concurrent process. However, in view of the size of forming simulations and the complexity of materials and physical phenomena occurring during plastic deformation, it seems more efficient to use macroscopic constitutive models with one or more internal variables to account for the microstructure. Constitutive models at lower scale are, of course, very important for the understanding of the microstructure evolution and to provide a basis for the development of more advanced macroscopic material models. Possible ways to transfer information from micro- to macro-structure based models are emphasized in the different approaches presented in this work.

The following are then discussed to cover theoretical and implementation aspects of sheet metal forming simulation:

1) Constitutive equations suitable for the description of aluminum alloy sheets
2) Testing procedures and analysis methods used to measure the relevant data needed to identify the material coefficients
3) Tensile and compressive instabilities in sheet forming. For tensile instability, both strain- and stress-based forming-limit curves are discussed.
4) Springback analysis
5) Finite Element (FE) formulation
6) Stress-integration procedures for both continuum and crystal-plasticity mechanics
7) Finite element design

Finally, various examples of the simulation of aluminum sheet forming are presented. These examples include earing in cup drawing, wrinkling, automotive stamping, hemming, hydroforming, and clam-shell-resistant design via FE analysis and the Taguchi optimization method.

INVESTIGATION OF THREE-DIMENSIONAL STRESS FIELDS AND SLIP SYSTEMS FOR FCC SINGLE CRYSTAL SUPERALLOY NOTCHED SPECIMENS

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Metals and their alloys, except for a few intermetallics, are inherently ductile, i.e. plastic deformation precedes fracture in these materials. Therefore, resistance to fracture is directly related to the development of the plastic zone at the crack tip. Recent studies indicate that the fracture toughness of single crystals depends on the crystallographic orientation of the notch as well as the loading direction. In general, the dependence of crack propagation resistance on crystallographic orientation arises from the anisotropy of (i) elastic constants, (ii) plastic deformation (or slip), and (iii) the weakest fracture planes (e.g. cleavage planes). Because of the triaxial stress state at the notch tips, many slip systems that otherwise would not be activated during uniaxial testing, become operational. The plastic zone formation in single crystals has been tackled theoretically by Rice and his co-workers and only limited experimental work has been conducted in this area. The study of the stresses and strains in the vicinity of a FCC single crystal notch tip is of relatively recent origin. We present experimental and numerical investigation of 3D stress fields and evolution of slip sector boundaries near notches in FCC single crystal PWA1480 tension test specimens ([001] load orientation and $[\bar{1}10]$ notch direction), and demonstrate that a 3D linear elastic finite element model that includes the effect of material anisotropy is shown to predict active slip planes and sectors accurately. The slip sector boundaries are shown to have complex curved shapes with several slip systems active simultaneously near the notch. Results are presented for surface and mid-plane of the specimens. The stress distribution and slip fields are a strong function of axial location through the thickness. Effect of temperature on slip field evolution is also investigated. The results demonstrate that accounting for 3D elastic anisotropy is very important for accurate prediction of slip activation near FCC single crystal notches loaded in tension. Results from the study will help establish guidelines for fatigue damage near single crystal notches.