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Abstracts

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Contents

TOPIC 1

Thermodynamics, transport theory and statistical mechanics in the context of continuum modeling discrete systems

General Lecture

Duality and phase diagram of one dimensional transport

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Models involving transport of particles from one end to other along a one dimensional lattice or a track obeying some form of mutual exclusion are typical nonequilibrium problems which have found current relevance among others in molecular motors carrying cargo on a track in biological systems, or traffic jam. Occurrences of more than one type of steady state phase, especially under open boundary conditions, have made these models important because of the possibility of nonequilibrium phase transitions even in one dimension.
The phases observed are, generally, of the following types. (i) Injection or withdrawal rate dominated, (ii) a shock phase consisting of piecewise continuous densities, and (iii) special phases, e.g., a phase where the current through the system is maximum. The phases are separated by first-order or continuous transitions. Special critical points have also been observed.
We use a continuum approach to this discrete problem to introduce the idea of duality between a phase transition to the shock phase and a boundary transition. With the help of this duality, the generic features of the phase diagram are shown to be determined by the nature of a set of coarse-grained functions, without any explicit need of details of the microscopic dynamics. However one microscopic parameter of the discrete problem, namely, a small distance cutoff (e. g., lattice spacing or size of hardcore particles) remains crucial and it cannot blindly be set to zero when the continuum limit is taken. Questions like relevance of any change in the microscopic rules in making qualitative changes in the phase diagram can now be answered by our approach.
This approach is used to study a Katz-Lebowitz-Sphon type interacting system. We show the existence of a nonequilibrium tricritical point in an extended phase diagram and discuss the scaling behaviour in and around the novel tricritical point.

The self-consistent effective medium approximation (SEMA): New types of critical points in a composite medium

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The fact that the self-consistent effective medium approximation (SEMA) leads to incorrect values for the percolation threshold, as well as for the critical exponents which characterize that threshold, has led to a decline in using that approximation. I will show that SEMA has the unique capability, which is lacking in other approximation schemes for macroscopic response of composite media, of leading to the discovery or prediction of new critical points. This is due to the fact that SEMA can often lead to explicit equations for the macroscopic response of a composite medium, even when that medium has a rather complicated character. In such cases, the SEMA equations are usually coupled and nonlinear, often even transcendental in,character. Thus there is no question of finding exact solutions. Nevertheless, a useful ansatz, leading to a closed form asymptotic solution, can often be made. In this way, singularities in the macroscopic response can be identified from a theoretical or mathematical treatment of the physical problem. This is demonstrated for some problems of magneto-transport in a composite medium, where the SEMA equations are solved using asymptotic analysis, leading to new types of critical points and critical behavior.

A theory of mixture for heterogeneous solids and its application to spinodal decomposition and coarsening

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A theory of mixture for heterogeneous solids is presented based on a novel, straightforward method for the exploitation of the second law of thermodynamics. In particular, the constitutive equations for the entropy flux, the heat flux density, the stress tensor, and the diffusion flux are formulated as a consequence of the non-negative entropy production. Furthermore, we derive the established Gibbs equation as well as the Gibbs Duhem relation which also follow from the formalism. Moreover, it is illustrated, how local mechanical strains due to thermal misfits or external loadings, modify the free energy and, consequently, the chemical potentials of the components. All consecutive steps are illustrated, first, for a simple mixture and, second, for a multiphase system. Here so-called higher gradients of the concentrations are considered regarding the different phases. However, it becomes clear that more/other variables of modified/different physical problems beyound the illustrated ones can easily be treated within the presented framework. As a potential application of the theory we will specialize and numerically examine the resulting equations to the case of the binary solder alloy AgCu where spinodal decomposition and coarsening has experimentally been observed.

TOPIC 2

Continuum mechanics of complex fluids and deformable solids with microstructure

General Lecture

On modifications of Newton's second law and linear continuum elastodynamics*

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Newton's law, F=ma, has withstood centuries but applied to a body's motion in principle requires tracking trillions of electrons and nuclei. Instead one "averages things out" and applies Newton's law macroscopically. However, building upon previous work of Sheng et.al.(2003), Liu et.al.(2005) and Avila et.al.(2005), we show that if one doesn't keep track of vibrations of all constituents, Newton's law takes a different form in which force depends on acceleration not just at the present time but also at previous times. We provide simple models with a direction dependent mass at a given frequency. For elastic bodies the continuum mechanics equations are also modified. The modified versions of these equations, are a generalization of the equations proposed by Willis to describe elastodynamics in composite materials. It is argued that these new sets of equations may apply to all physical materials, not just composites. The Willis equations govern the behaviour of the average displacement field whereas one set of new equations governs the behaviour of the average weighted displacement field, where the weighted displacement field may attach zero weight to ``hidden" areas in the material where the displacement may be unobservable or not defined. Two other sets of new equations govern the behaviour when the microstructure has microinertia, i.e. where there are internal spinning masses below the chosen scale of continuum modelling. In the first set the average displacement field is assumed to be observable, while in the second set an average weighted displacement field is assumed to be observable.

*joint work with John Willis.

On conservation and balance laws in micromorphic elastodynamics

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Keywords: conservation laws, balance laws, Noether symmetries, micromorphic elasticity, path-independent integrals.

In this talk, following Noether's theorem we investigate the Lie point symmetries of linear micromorphic elastodynamics (linear elastodynamics with microstructure). Conservation and balance laws of linear, micromorphic elastodynamics are derived. We generalize the J, L and M integrals for this theory. In addition, we give the Eshelby stress tensor, pseudomomentum tensor, field intensity vector, Hamiltonian, angular momentum tensor and scaling flux generalized to micromorphic elastodynamics.

Instability and energy minimization in solids with microstructure

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In elastic or pseudo-elastic solids with fully reversible microstructural changes, the energy minimization is a standard approach based on the concept of stability of equilibrium in a dynamic or thermodynamic sense. The well-known notions of ellipticity, rank-one convexity and quasi-convexity of a nonlinear elastic energy function are related to material stability aspects. When the evolution of microstructure is associated with intrinsic dissipation, the stability analysis becomes more complex. It is shown that the classical condition of thermodynamic stability of equilibrium does not comply with the concept of rate-independent dissipation. Therefore, an extended condition of thermodynamic stability is developed which in general is less restrictive than the classical one on account of a rate-independent dissipation term in the respective Lyapunov functional. The incremental dissipation is incorporated here either directly in the internal state variable formalism or indirectly in the expression for the deformation work. As an example, a stability condition is derived that prevents spontaneous formation of deformation bands in an inelastic continuum at fixed external conditions.

Due to path dependence of dissipation, distinction must be made between instability of equilibrium addressed above and instability of a deformation path under varying loading. To examine the latter, the total incremental energy is considered that is supplied to the system consisting of the deformed body and loading device to produce quasi-statically a small increment of deformation. Under a symmetry restriction imposed on the constitutive law, it is shown that the incremental energy minimization up to the first and second-order terms yields an exact solution to the boundary value problem posed in velocities. In the case of a non-convex incremental energy functional related to non-unique solutions, the justification of selecting the energy minimizer follows from the analysis of stability of deformation paths. The energy approach, standard in elasticity, is extended in this way to rate-independent inelastic phenomena in a broad class of solids.

The problem of material instability is addressed for a class of solids whose microstructural rearrangements are due to activity of discrete mechanisms. This includes plasticity of crystals and polycrystals, damage, micro-cracking, phase transformation, etc., incorporated in a unified theoretical framework. Of special interest is the case when instability of a uniform deformation path leads to the formation of a microstructure in an initially homogeneous continuum. This is illustrated by numerical simulation of the formation of initially one and later two families of shear bands in an incrementally nonlinear elastoplastic material.

It is concluded that the incremental energy minimization, with accuracy to the second-order terms, provides a unified approach to a wide class of evolution problems in time-independent inelastic solids, including also evolving microstructures. If the response is not unique then, according to the energy criterion of path stability, the solutions that correspond to unstable paths are automatically rejected. Applicability of this approach is limited by the requirement imposed on the incremental constitutive laws which implies symmetry of the tangent stiffness matrix in discretized problems.

Periodic homogenization of Hamilton-Jacobi-Bellman equations

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This talk is concerned with periodic homogenization of Hamilton-Jacobi-Bellman equations arising in some stochastic control problem with rapidly oscillating periodic structure. We prove homogenization results by using probabilistic arguments based on stochastic differential equations. We also discuss the rate of convergence of solutions as well as the limiting stochastic control problem.

Homogenization-based constitutive models for porous, viscoplastic materials

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The modeling of void growth and ductile damage of viscoplastic composites has been the subject of numerous works over the past forty years. Various models have been proposed for the estimation of the effective behavior of isotropic porous composites with the Gurson model [1] (GUR) being the most used in the literature. The current work is concerned with the application of the ``second-order'' nonlinear homogenization procedure of Ponte Castaneda [3] (SOM), to generate estimates for the effective behavior of viscoplastic, isotropic, porous composites. This method is a generalization of the earlier variational method of Ponte Castaneda [2] (VAR), which has been rigorously shown to be an upper bound. Although the Gurson model is known to violate the variational bound at low stress triaxialities, it still remains a very powerful and simple tool for estimating the macroscopic behavior of isotropic porous composites, when these are subjected to high triaxial loads. The reason lies in that it recovers the exact result of a cylindrical cavity (shell), which is subjected to hydrostatic loading. Unfortunately, the variational bound is not very accurate in that case. In this work, we propose a modification of the originally proposed ``second-order'' method, so that the exact solution of the shell problem is recovered. The SOM is applied to porous composites consisting of cylindrical voids with circular cross-section in the $x-y$ plane, and aligned in the $z-$ direction, which are subjected to plane-strain loading conditions. The microstructure

is assumed to be such that the overall response of the composite is isotropic in the $x-y$ plane, while the effective behavior of such a composite depends in general on the two isotropic invariants I_1 and I_2 .
The behavior of the non-vacuous phase is assumed to be of a power-law form such that the stress potential is given by

$$U(\boldsymbol{\sigma}) = \frac{\sigma_o}{n+1}\left(\frac{\sigma_{eq}}{\sigma_o}\right)^{n+1}, \quad n = \frac{1}{m},$$

where $\sigma_{eq} = \sqrt{\frac{3}{2}\boldsymbol{\sigma}_d \boldsymbol{\sigma}_d}$ is the equivalent stress and $\boldsymbol{\sigma}_d$ is the deviatoric part of the stress tensor attained from the relation, $\boldsymbol{\sigma}_d = \boldsymbol{\sigma} - \sigma_m \mathbf{I}$, with $\sigma_m = \frac{1}{2}\sigma_{kk}$ being the hydrostatic stress. In addition, σ_o denotes the flow stress of the non-vacuous phase, and m is the strain-rate sensitivity parameter, which takes values between, $0 \le m \le 1$. The value of $m = 1$ corresponds to a linear material, while for $m < 1$ the medium becomes nonlinear, with $m = 0$ being the extreme case of perfectly plastic behavior. Furthermore, the volume fraction of the vacuous phase, namely the porosity, is denoted as f .
In what follows, we present estimates for the effective, stress flow potentials and the macroscopic strains delivered by the *SOM* , for a porous composite with cylindrical microstructure. The results predicted by the *SOM* are compared with recent results from high-rank, nonlinear laminated composites (*LAM*), introduced by deBotton and Hariton [4]. Fig. 1 shows stress flow potentials delivered by the models that have been introduced before for several values of the porosity f and the nonlinearity of the non-vacuous phase m . In these plots, $\overline{\Sigma}_m$ and $\overline{\Sigma}_{eq}$ denote the macroscopic hydrostatic and equivalent stress, respectively. For $m > 0$, the *SOM* is in very good agreement with the *LAM* , while the *VAR* overestimates the strength of the porous composite, at high triaxial loadings (i.e $\overline{\Sigma}_m >> \overline{\Sigma}_{eq}$). For the case of $m = 0$, the *SOM* and the *GUR* are both designed to recover the exact point for $\overline{\Sigma}_{eq} = 0$, but they deliver different estimates for the rest of the loadings. Moreover, the *GUR* model violates the variational bound at low triaxialities (i.e $\overline{\Sigma}_{eq} >> \overline{\Sigma}_m$) .

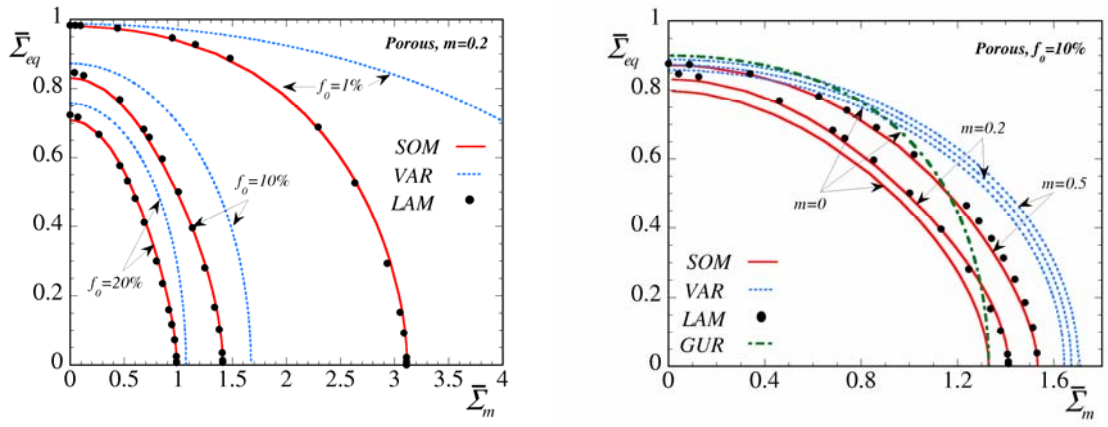

Figure 1: Stress flow potentials as a function of the porosity, f and the nonlinearity m for porous composites with cylindrical microstructure.

Furthermore, Fig. 2 shows plots of the two modes of the macroscopic strain-rate, $\overline{E}_{eq} = \sqrt{\frac{2}{3}\overline{\mathbf{E}}_d : \overline{\mathbf{E}}_d}$, with $\overline{\mathbf{E}}_d = \overline{\mathbf{E}} - \overline{E}_m \mathbf{I}$ and $\overline{E}_m = \overline{E}_{kk}/2$, with respect to the strain-rate triaxiality $X_E = \overline{E}_m/\overline{E}_{eq}$, for a nonlinearity $m = 0.2$ and several values of the porosity f. The VAR estimate underestimates the macroscopic strain-rate for all the range of the triaxialities, while the SOM is in good agreement with the LAM estimates, especially at high triaxialities, where the dilatational rate of the void, which is mainly controlled by the $\overline{E}_m$ mode, becomes crucial concerning the failure of the material.

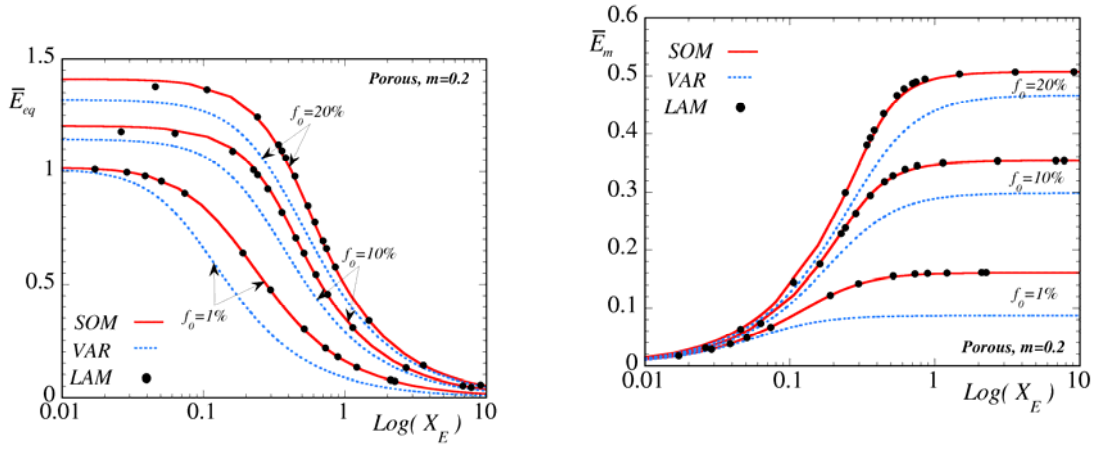

Figure 2: Macroscopic average strain-rates for $m = 0.2$ as a function of the strain triaxiality and the porosity f.

References

[1] A. L. Gurson, Continuum theory of ductile rupture by void nucleation and growth, J. Engng. Mater. Technol. 99 (1977). 2-15.

[2] P. Ponte Castaneda, The effective mechanical properties of nonlinear isotropic composites, J. Mech. Phys. Solids 39 (1991) 45--71.

[3] P. Ponte Castaneda, Second-order homogenization estimates for nonlinear composites incorporating field fluctuations. I. Theory, J. Mech. Phys. Solids 50 (2002) 737--757.

[4] G. deBotton, I. Hariton High-rank nonlinear sequentially laminated composites and their possible tendency towards isotropic behavior, *J. Mech. Phys. Solids*, **50**, (2002), pp. 2577-2595.

Viscoplastic Phase Field modelling of rafting in Ni base superalloys

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Mechanical behaviour of Ni base superalloys depends largely on the microstructure at meso scale. Initially, the alloy consists in cuboids precipitates separated by channels of matrix. When such a material is submitted to a creep loading at high temperature (around 1000°C), we observe a directional coalescence of the γ' precipitates often called rafting.
The aim of this study is to propose a Phase Field model to represent in a quantitative way the change in morphology in superalloys. The misfit stresses as well as anisotropy in elastic constants between matrix and precipitates are taken into account. Moreover several authors have pointed out the role of the plastic strain in the matrix which enables relaxation of misfit stresses between the two phases during rafting. Thus plasticity in the γ phase is introduced by the means of a viscoplastic law coupled with the Phase Field model.

ON THE GEODESIC PROPERTY OF SHEAR-BAND PATTERNS IN ELASTO-PLASTIC COMPOSITES

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Under study is the geodesic (i.e., shortest path [1,2]) character of shear bands occurring in elasto-plastic response of a planar inclusion-matrix composite. The composite's spatially random morphology is created by generating the disk centers through a *sequential inhibition process* based on a Poisson point process in plane. Two cases of composite, matrix-inclusion materials, perfect bonding everywhere, are considered:
(i) Elastic inclusions in an elastic-plastic-hardening matrix, with the matrix having the elastic response (up to the yield point) identical to that of the inclusions [3].
(ii) Both inclusions and the matrix are elastic-plastic-hardening [4], with the matrix being more compliant and weaker than the inclusions.
Figures in these two references clearly show plastic flow occurring between the inclusions at about $\pm 45^o$ to the directions of principal normal stresses.
A quantitative comparison of response patterns obtained by computational micromechanics with those found only by mathematical morphology indicates that the regions of plastic flow are very close to geodesics for a composite with all the phases being elastic-plastic-hardening, and approximately so when the inclusions are elastic [5]. Furthermore, geodesics can be computed orders of magnitude more rapidly than by, say, finite elements. Thus, the advantage of this purely geometric method is an extremely fast computation of patterns of plastic deformations as opposed to a full computational mechanics approach.

[1] Vincent, L. & Jeulin, D. (1989), Minimal path and crack propagation simulation, *Acta Stereol*. **8/II**, 487-494.
[2] Jeulin, D. (1993), Damage simulation in heterogeneous materials from geodesic propagations, *Eng. Comp*. **10**(1), 81-91.
[3] Jiang, M., Ostoja-Starzewski, M. & Jasiuk, I. (2001), Scale-dependent bounds on effective elastoplastic response of random composites, *J. Mech. Phys. Solids* **49**(3), 655-673.
[4] Li, W. & M. Ostoja-Starzewski, M. (2006), Yield of random elasto-plastic materials, *J. Mech. Mater. Struct*. **1**, 1055-1073.
[5] Jeulin, D. & Ostoja-Starzewski, M. (2000), Shear bands in elasto-plastic response of random composites by geodesics, *8th ASCE Specialty Conference on Probabilistic Mechanics and Structural Reliability*, University of Notre Dame, IN.

Kolmogorov Dispersion for Turbulence in Porous Media

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We will utilise the Self-Avoiding Walk (SAW) mapping [1] of the vortex line conformations in turbulence, to get the Kolmogorov scale dependence of energy dispersion, and the knowledge of the effect of disordered fractal geometries on SAW conformational statistics [2]. This will give us the Kolmogorov energy dispersion exponent value for turbulence in pororous media in terms of the Flory size exponent for polymers in the same.

[1] see e.g., Lectures on Statistical Physics & Protein Folding, K. Huang, World Scientific, Singapore (2005).

[2] see e.g., Statistics of linear Polymers in Disordered Media, Ed. B. K. Chakrabarti, Elsevier, Amsterdam (2005).

Long-range hydrodynamic response of complex liquids

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In viscous particulate liquids, such as suspensions and polymer solutions, the large-distance steady-state flow due to a local disturbance is commonly described in terms of hydrodynamic screening --- beyond a correlation length ξ the response drops from that of the pure solvent, characterized by its viscosity η_0, to that of the macroscopic liquid with viscosity $\eta > \eta_0$. For cases where $\eta \gg \eta_0$ we show that this screening picture, while being asymptotically correct, should be refined in an essential way. The crossover between the microscopic and macroscopic behaviors occurs gradually over a wide range of distances, $\xi < r < (\eta/\eta_0)^{1/2}\xi$. In liquid-laden solids, such as colloidal glasses, gels and liquid-filled porous media, where $\eta \to \infty$, this intermediate behavior takes over the entire large-distance response. The intermediate flow field has several unique characteristics relating to its distance dependence, concentration dependence, and temporal buildup. These general properties are demonstrated in several model systems.

Modeling of film flow of complex fluids, a review

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We discuss recent results on problems such as the flow of fluids over inclined plane or corrugated substrates, with possible Marangoni effect of thermal or chemical origin, evaporation (tears of wine), etc. obtained by systematically replacing the direct search of solutions to the Navier-Stokes equations by the study of the dynamics of the film thickness and other appropriate quantities averaged other this thickness.

The Cahn-Hilliard equation with degenerate mobility

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Often, when the Cahn-Hilliard equation is mentioned, the equation

$$u_t = M_0 \triangle(-u + u^3 - \epsilon^2 \triangle u) \quad (1)$$

comes to mind, where $u = u(x,t)$ reflects the concentration of one of two components of a binary alloy undergoing phase separation. However, in reviewing the original derivation of the Cahn-Hilliard equation, one find that it should be just as accurate if not more accurate to consider the Cahn-Hilliard with a degenerate mobility and logarithmic terms,

$$u_t = \nabla \cdot M_0 u(1-u)\nabla \frac{\Theta}{2}\{\ln u - \ln(1-u)\} + \alpha(1-2u)\epsilon^2 \triangle u. \quad (2)$$

We explain the derivation of (2) within the context of phase separation, and show how equations similar to (2) also arise, for example, in the context of thin films when gravitational and Marangoni effects are included and in modeling biofilms. Some of the quantitative differences in the behaviors predicted by equations (1) and (2) are explained, and certain similarities between the predicted behavior of (2) and that of the classical thin film equation are noted.

Features of Immiscible Steady-State Two-Phase Flow in Porous Media

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Deep inside a reservoir, the flow conditions in a representative volume element does not resemble those encountered when performing flooding experiments where the porous rock is saturated with one fluid which is then subsequently displaced by another one. Rather, what enters a representative volume element is statically the same as what leaves it.
Starting with a digitized sample of Berea sand stone measuring 3x3x3 mm^3 combined with the implementation of seamless periodic boundary conditions, we have simulated steady-state flow of a oil and water mixture at different saturations, capillary numbers and viscosity ratios.
Among the new features we find, we point out the appearance of phase transition separating a state where bubbles of one of the fluids dominate and a state where bubbles of other type of fluid dominate. The transition point depends on the capillary number, i.e. how fast the fluids flow.

Transient Evaporation of Drops on an Heterogeneous Surface

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KEY WORDS: hydrophilic and hydrophobic surfaces, high speed visualization of drying drops, lubrication model of evaporation with account of chemical and topographical heterogeneities.

Free surface phase-change problems occur in a wide variety of scientific and engineering applications. Some examples are related to evaporation of drops in ink-jet printing, agricultural spraying or biological activities such as genomics and proteomics. This work details experimental measurements and numerical simulations of evaporation of one or several drops of very different sizes placed on horizontal model substrates covering a large range of wetting behavior.

The experimental part emphasizes the similarity in the evaporation of microdrops and macrodrops. Experiments are performed on perfectly flat substrates with only minute roughness. The differences which are noted are analyzed in terms of the substrate wetting characteristics. Thus, the results allow pinpointing stick and slipping phenomenon for some substrates with intermediate wetting behavior and this is shown to depend only on the difference between advancing and receding contact angles.

Computational results are obtained using the lubrication approximation to describe the effects of capillarity, viscous spreading and mass loss. In the course of the numerical simulations, the fluid is first assumed to be pure and then to be composed of solid pigments in a Newtonian solvent with local viscosity depending on the non-volatile mixture fraction. The resulting time-dependent non-linear coupled set of governing equations is solved using finite elements. The results are compared with the experimental ones and discussed both from the point of view of macroscopic evaporation times and finer details of the drop transient profiles.

A noted complexity of this work is the inclusion of chemical and topographical heterogeneities on the solid surface which are known to have a significant effect on flow dynamics even in the absence of thermal phenomena. The surface energy of substrates is taken into account through a disjoining pressure model proposed elsewhere whilst the effect of topography is introduced in the free surface curvature. Since the effect of heterogeneity often competes with the basic instability mechanism occurring on homogeneous surfaces as shown above, the result is an elaborate interplay of various mechanisms. Finally the results obtained are examined in the framework of applications where instabilities appearing during evaporation are undesirable since they may lead to unwanted deposition of solid film in certain areas and/or visible coating defects.

Study of thermodynamic and dynamic behavior of liquids close to solidification

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Using a classical density functional approach a model for the metastable liquid sate in terms of holes present in the amorphous structure is considered. For a one component Lennard-Jones system we obtain the temperature dependence of the free volume v_f in the metastable state. A temperature T_o , similar to that of the characteristic transition of the free volume theory, is identified by extrapolating $v_f(T)$ to zero. The Kauzmann temperature T_K is also obtained here by extrapolating the entropy difference between the supercooled state and that of the crystal to zero. We compare the temperatures T_o and T_K obtained in our model with other two characteristic temperatures for glassy behavior, namely (a) the dynamic transition temperature T_c of the mode coupling theory (MCT) and (b) the glass transition temperature T_g which was obtained from studying the violation of Fluctuation-dissipation theorem. All the four temperatures, obtained from independent routes, are located with respect to the melting temperature T_m in a manner which is in agreement with experiments. Applying the same model for the crystalline solid, the importance of the presence of a small fraction of vacancies in a crystal structure is demonstrated from the consideration of thermodynamic stability. We include in the classical density functional description of the crystal the effects due to the distortion of the lattice structure surrounding the vacancy and show that the free energy of the solid is less when vacancies are present. The test density function is modified from its usual form to take into account the presence of vacancies in the lattice structure. For the Lennard-Jones interaction potential, the repulsive part is treated in terms of an equivalent hard sphere (EHS) system while the contribution from the long attractive part is treated perturbatively. The properties of the EHS in the inhomogeneous state is obtained with the weighted density functional approach. The thermodynamic behavior is studied by locating the state of minimum free energy. The dependence of the vacancy concentration on temperature at the coexistence of crystal and liquid is obtained.

The dynamics of a metastable liquid is studied in the supercooled region below the freezing temperature. This is formulated in terms of the equations of motion for the slow variables which result from the underlying microscopic conservation laws or broken symmetries in the liquid or the frozen solid. The conservation laws are expressed in terms of stochastic equations with noise. The correlated motion of the particles in the dense liquid is expressed through the nonlinear coupling of the slow modes in the equations of motion. The nature of decay of dynamical correlations developing over the long time scales is analyzed from numerical solution of the stochastic equations.

General Lecture

Discrete Network Approximation in Particle Suspensions and Biosuspensions

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We present a novel approach for calculation of effective properties of high contrast disordred composites and illustrate it by considering highly packed suspensions of rigid particles (joint works with Y. Gorb &A. Novikov and with A. Panchenko) and bacterial suspensions (joint work with V. Gyrya, based on recent experimental work by I. Aronson et al).
The main idea of this variational approach is the approximation of the original continuum problem, which is described by PDEs with rough coefficients, to a discrete network. This approximation makes the dependence of physical parameters transparent and it is obtained with a controlled error estimate.

Polygonization of Multi-walled Carbon Nanotubes

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It has long been known that the graphite modification of carbon consists of a three-dimensional stack of planar sheets of carbon atoms called graphene layers. Each grapheme layer has hexagonal structure in which a carbon atom has strong covalent bonds with three of its neighbors. This type of bonding results in a high extensional strength but low bending stiffness of individual layers. On the other hand, the interactions between the layers are of weak van-der-Waals-type so that the layers are loosely bound and can slide along each other with little resistance.

Carbon nanotubes-a recently discovered morphology of carbon-can be visualized as either one or more graphene layers rolled into a tube-a single graphene layer forms a single-walled nanotube while two or more layers form a multi-walled nanotube.

Experiments have shown that, typically, carbon nanotubes have circular cross-sections. However, under certain conditions (e.g. following heat treatment), multi-walled nanotubes can assume polygonal cross-sections. In particular, for multi-walled nanotubes of a large diameter, it has been observed that cross-sections of inner tubes are circular, while cross-sections of outer tubes are polygonal.

In this talk we present a continuum model of multi-walled carbon nanotubes. The model incorporates the elastic energy of individual layers and the energy of nonlocal van der Waals interactions between the layers. Using constrained minimization, we demonstrate that the model predicts polygonization of multi-walled nanotubes of large diameter.

ON THE LATTICE DYNAMICS OF A FRACTAL GASKET

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So far self-similarity of material systems was widely ignored in dynamical modeling. However, pioneering work was done by Kigami by introducing the harmonic calculus on a self-similar (Sierpinski) gasket [1]. The self-similar spectrum of a fractal lattice was studied numerically by Bodarenko and Levin by deducing recursion relations for the lattice Green's function of a Sierpinski gasket [2]. In this paper an attempt is made to account for the influence of self-similar symmetry on the dynamic characteristics on a fractal exact self-similar gasket. To this end the equation of motion on a fractal gasket is defined. Dynamic characteristics such as fractal lattice Green's function, and oscillator density are deduced and the effect of self-similarity is discussed.

[1] J. Kigami, A harmonic calculus on the Sierpinski spaces, *Japan J. Appl. Math.* 8 (1989), 259-290.
[2] Bondarenko A.N., Levin, V.A., Science and Technology (2005) KORUS Proceedings. The 9th Russian-Korean International Symposium, 33-35, ISBN: 0-7803-8943-3.

TOWARDS CONTINUUM MECHANICS OF FRACTAL MATERIALS

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Hans Ziegler's thermomechanics [1,2,3], established half a century ago, is extended to fractal media on the basis of a recently introduced continuum mechanics due to Tarasov [4]. In particular, it has been shown that the Green-Gauss theorem can be written in an appropriately generalized form, which in turn allows derivation of local balance laws (conservation of mass, conservation of linear and angular momenta, and conservation of energy) of a fractal. Proceeding in the same vein and employing the concept of internal variables and internal stresses, as well as the quasi-conservative and dissipative stresses, a field form of the second law of thermodynamics is derived [5]. In conradistinction to the conventional Clausius-Duhem inequality, it involves generalized rates of strain and internal variables. Upon introducing a dissipation function and postulating the thermodynamic orthogonality on any lengthscale, constitutive laws of various elastic-dissipative fractal media naturally involving generalized derivatives of strain and stress can then be derived. Passing to a non-fractal medium, one always recovers conventional forms of local relations of continuum thermomechanics. Also generalized to fractal bodies is the Hill condition necessary for homogenization of their constitutive responses. With a focus on thermoelasticity, a new form of Duhamel's differential equation of heat conduction is derived [6].

[1] H. Ziegler, Thermodynamik und rheologische Probleme, *Ing. Arch.* **25**, 58-70, 1957.
[2] H. Ziegler, *An Introduction to Thermomechanics*, North-Holland, Amsterdam, 1983.
[3] H. Ziegler and Ch. Wehrli, The derivation of constitutive relations from the free energy and the dissipation functions, *Adv. Appl. Mech.* **25**, 183-238, Academic Press, 1987.
[4] V.E. Tarasov, Fractional hydrodynamic equations for fractal media, *Ann. Phys.* **318**/2 (2005), 286-307.
[5] M. Ostoja-Starzewski, Towards thermomechanics of fractal media, *ZAMP*, in press, 2007.
[6] M. Ostoja-Starzewski, Towards thermoelasticity of fractal media, *J. Thermal Stresses*, in press, 2007.

Texture in polycrystals

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Nearly all technologically useful materials are polycrystalline, consisting of small crystallites, called grains, separated by interfaces, the grain boundaries. The energetics and arrangement of this network, its texture, are important factors in material behavior, and constitute the basic problem of microstructure. Experimentally, the inverse relationships between grain boundary populations and energy have been observed for many years. We introduce the grain boundary character distribution (GBCD), a new statistic, and offer compelling evidence for its strong dependence on grain boundary energy. In addition we demonstrate that there are natural laws for texture and the GBCD using large network simulations. We introduce a model system and analyze it with methods of continuous time random walk theory.

Effective properties of matrix composites with inclusions of arbitrary shapes

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The effective field method is applied to the calculation of the overall dielectric permittivity of composite materials consisting of a homogeneous matrix and a set of isolated inclusions. The problem is reduced to the solution of the one particle problem for a typical inclusion subjected to a constant external field. An original numerical method is proposed for the solution of the one particle problem for an inclusion of an arbitrary shape. As an example, the effective properties of composites with cylindrical inclusions of various sizes and properties are calculated.

Field statistics in nonlinear composites

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This work is concerned with the extraction of the statistics of the local fields in nonlinear composites from the effective potential of suitably perturbed composites. The idea is to introduce a parameter in the local potentials, generally a tensor, such that differentiation of the corresponding effective potential with respect to the parameter yields the volume average of the desired quantity. In particular, this provides a generalization to the nonlinear case of well-known formulas in the context of linear composites, which express phase averages and second moments of the local fields in terms of derivatives of the effective potential. Such expressions are useful since they allow the generation of estimates for the field statistics in nonlinear composites, directly from homogenization estimates for appropriately defined effective potentials. Here, use is made of these expressions in the context of the "variational", "tangent second-order" and "second-order" homogenization methods, to obtain rigorous estimates for the first and second moments of the fields in nonlinear composites. While the "variational" estimates for these quantities are found to be identical to those proposed in previous works, the tangent second-order and second-order estimates are found be different. In particular, the new estimates for the first moments given in this work are found to be entirely consistent with the corresponding estimates for the macroscopic behavior. As an example, we generate estimates for the phase averages and second moments of the fields for two-phase, power-law composites with isotropic and transversely isotropic microstructures.
The accuracy of these estimates is assessed by confronting them against corresponding exact results for sequentially laminated composites.

Influence of external stresses and pore pressure on deformation of soft crack-like inclusion in poroelastic medium

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The poroelastic médium containing a random set of inhomogeneities with different poroelastic properties is considered. The inhomogeneities in the form of flat ellipsoids are filled with a porous material having a skeleton much softer than the corresponding to the main medium (crack-like inclusions). One of the self-consistent schemes named effective field method (EFM) is used for study of the influence of external stresses and pore pressure on deformation of such inhomogeneities. The EFM allows to take into account the interaction between the crack-like inclusions in the case of non-dilute their concentration. The result of calculation of the stress and strain fields inside the inclusions is presented. Explicit formulas for the inclusion aspect ration changing are obtained and analyzed. This parameter is important for calculation of the seismic waves velocities in porous rocks and their permeability in dependence of external stresses and pore pressure. The obtained formulas are compared with ones available in literature.

Mathematical derivation of a rubber-like stored energy functional

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Rubber elasticity is usually derived using statistical physics arguments and entropy considerations on one polymeric chain. It is then induced at the continuum scale assuming some affine dependence. The stress-strain relation may then be obtained by applying linear boundary conditions on the reference cell oriented according to the principal stretch or by averaging on the orientations.
Starting from the same model for one polymeric chain, we adopt here an approach closer to that of Treloar concerning the derivation of the continuous energy. We only rely on the energy of a chain network and on minimization principles. The free energy of an elastomeric chain and the network being given, we rigorously perform a discrete to continuum limit to derive a continuous energy density. We will discuss the motivations of the variational approach and the mechanical properties of the energy density obtained, such as hyperelasticity, objectivity, isotropy and incompressibility.

A hierarchy of higher order and higher grade continua

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A hierarchy of higher order continua is presented that introduces additional degrees of freedom accounting for volume changes, rotation and straining of an underlying microstructure. An increase in the number of degrees of freedom represents a refinement of the material description. In addition to available nonlinear Cosserat and micromorphic theories, general formulations of elastoviscoplastic behaviour are proposed for microdilatation and microstretch continua. A microstrain theory is introduced that is based on 6 additional degrees of freedom describing the pure straining of the microstructural element. In each case, balance equations and boundary conditions are derived, decompositions of the finite strain measures into elastic and plastic parts are provided. The formulation of finite deformation elastoviscoplastic constitutive equations relies on the introduction of the free energy and dissipation potentials, thus complying with requirements of continuum thermodynamics. The hierarchy can also be formulated for higher grade continua based on the introduction of the second gradient of the displacement field. In particular, the question of the introduction of the gradient of temperature into the free energy function within a strain gradient theory is tackled.

Potential influence of microstructural morphology on the viscoplastic flow of two-phase polycrystals

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Linear properties of single phase polycrystals are known to be accurately predicted by the classical self-consistent scheme (SCS), the efficiency of which being due to its ability to reasonably describe the randomness of the spatial distribution of the grains in real metals. On the other hand, numerous mean field models for two-phase materials with a clear matrix inclusion morphology have been proposed, including the Willis/Hashin-Shtrikman (WHS) estimates, generalized self-consistent or pattern-based models.
Two-phase polycrystals such as austenitic-ferritic steels can be described both as polycrystals and two-phase materials so that an efficient description of their behaviour taking into account both the phase distribution and the cristallographic texture requires the combination of both above described classes of models, especially for materials with a contrast between constituents significantly higher than that observed in more conventional single phase polycrystals.
The simplest approach consisting in applying the classical equations of the SCS to the set of single crystals of both phases, assuming implicitely that the grains of both phases are randomly mixed together, provides a first estimate. It is however not able to tackle the potential effect of the phase distribution, which may vary from a hard configuration in which the harder phase would be continuous with embedded isolated grains of the softer phase to the reverse softer situation. An attempt to model such extreme situations consists in using a two-stage homogenization scheme based, first, on the classical self-consistent scheme at the smaller scale of the constitutive single phase polycrystals and second, on estimates of the WHS-type for the prediction of the properties of the blend of hard and soft phases. To do so, a separation of length scale between the grain scale and the phase scales has to be assumed but different grain shapes in both phases and "phase shapes" can be considered. These homogenisation schemes have been combined with Suquet-Ponte Castañeda's variational principle for arbitrary anisotropic nonlinear media, which is shown to be applicable to such a two stage scale transition. A noticeable influence of the phase distribution can be observed this way when the contrast between phases is sufficiently large. Comparisons with experimental data relative to austenitic-ferritic steels made of a soft BCC phase and a hard FCC phase, under plane strain compression at high temperature are however not totally satisfactory.
Possible extensions of the model are presented.

TOPIC 3

Fundamentals of fracture, defect dynamics, fatigue, and fracture dynamics on different microlevels

General Lecture

Physical and Statistical Aspects of Fracture

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The consequences of fracture can be either unacceptable in view of possible fatalities or undesirable for reasons of economy and inconvenience. It is the task of the designer to build structures which will not fail. This task is difficult to achieve because, excluding any possible sources of error, there are other sources of statistical variations, in particular those associated with the mechanical properties of the materials used to fabricate these structures.
The presentation will start with a brief introduction illustrating a number of catastrophic failures observed over the past 25 years. This will include examples taken from aeronautical industry and gas production and transportation. We will concentrate on two main modes of failure : brittle cleavage fracture in steels and fatigue failures in Ni base alloys used for the fabrication of turbine discs. Then the presentation will be divided into three parts.
The first part will be devoted to a brief overview of the physical micromechanisms responsible for these two modes of failure. It will be shown that the essence of fracture is deterministic. The randomness of fatigue and brittle fracture is related to the presence of "defects" either initially present in structural materials (microshrinkage porosities, inclusions, etc.) or which may be produced by plastic deformation (slip bands, mechanical twins, cracked particles, etc.).
In the second part of the presentation an attempt is made to show how these "defects" can be taken into account in modelling brittle fracture based on weakest link concept. Two extreme cases will be considered corresponding to defect nucleation controlled fracture and defect propagation controlled failure. It will be shown that the Weibull theory and more or less sophisticated models derived from the weakest link concept can be used to develop probabilistic linear fracture mechanics.
The third part will be devoted to statistical modelling of fatigue damage. Both high strain low cycle fatigue (LCF) and high cycle fatigue (HCF) are considered. In LCF the emphasis is laid on kinetic theories describing the evolution of multiple cracks population, while in HCF results obtained in the frame of the weakest link theory are presented. A short account of directionality aspects in multiaxial fatigue damage is given. The relative importance of volume and surface effects is also discussed.

SCALING PROPERTIES OF FRACTURE SURFACES

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Failure of heterogeneous media continues to pose significant fundamental challenges. While continuum theory has allowed the determination at least numerically of the energy flux into the crack tip process zone for any growing crack, the way this crack responds to dissipate this flux by progressing within the process zone is more problematic. Crack surface roughening is a consequence of fracture processes occurring at the micro-structure scale, i.e. at a scale out of the range of continuum theory. Such roughness generation, while resulting from material specific processes, exhibits some *universal* scaling features whose understanding has elicited much interest. In particular, we showed very recently that the statistical scaling properties of fracture surfaces can be fully characterized with the use of the *two-dimensional* (2D) height-height correlation function. This function exhibits anisotropic scaling properties, similar to Family-Viseck scaling predicted in interface growth problems, characterized by *two independent* critical exponents, the roughness exponents measured along and perpendicular to the direction of crack growth respectively. Different materials were investigated. Different sets of critical exponents were measured whether the surfaces are examined at scale below or above the size of the damaged zone. In this latter case, the exponents values can be understood by deriving a model from Linear Elastic Fracture Mechanics which describe the development of crack roughness as an "elastic" manifold creeping in a random media.

Brittle fracture and its Power-law dynamics in the RRTN model for nonlinear complex systems

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Abstract: We study the breakdown characteristics (e.g., the breakdown exponent) and the dynamics of the charge carriers in a tunneling-enhanced percolation network, named as a Random Resistor cum Tunneling-bond Network (RRTN), where we allow tunneling in the gap between two randomly thrown nearest neighbour metallic bonds only. Our earlier studies involve the dc and ac *nonlinear response*, the percolative aspects [1], the finite-temperature variable range hopping conductivity [2], dielectric breakdown [3], etc. in the RRTN. Here we study the non-equilibrium dynamics of the carriers. With two early far-from-equilibrium inverse power-law relaxations [4] extending over several decades, the dynamics has a lot of similarities with many avalanche-like, *breakdown phenomena* occurring in a wide variety of naturally occuring *driven* systems (e.g., brittle fracture, earthquake etc.) with statistically *correlated randomness*. These scale-free regimes show slow non-Debye dynamics and unconventional dynamic hysteretic curves. Beyond this regime, the dynamics is exponentially fast (acquires a time-scale).

References:

[1] For motivation and the original development of our RRTN model, see *Nonlinearity and Breakdown in Soft-Condensed Matter*, Lecture Notes in Physics **437**, A.K. Sen and A. Kar Gupta, pp. 271-287 (Springer-Verlag, Berlin, 1994). Further works on a new percolation threshold and on dc/ac responses appeared in: A. Kar Gupta and A.K. Sen, Physica A **215**, 1 (1995); A. Kar Gupta and A.K. Sen, Phys. Rev. B **57**, 3375 (1998); and in A.K. Sen and A. Kar Gupta, Phys. Rev. B **59**, 9167 (1999).

[2] A.K. Sen and S. Bhattacharya in an edited volume named *Continuum Models and Discrete Systems*, Eds. D. Bergman and E. Inan, pp.367-373 (Kluwer Acad. Publ., Dordrecht, 2004).

[3] A. Kar Gupta and A.K. Sen, Physica A **247**, 30 (1997); a schematic description of the RRTN model and its breakdown aspects do also appear in an advanced text-book named *Statistical Physics of Fracture and Breakdown in Disordered Systems*, by B.K. Chakrabarti and L.G. Benguigui, p.68 (Clarendon Press, Oxford, 1997).

[4] Two early power-law dynamics far-from-equilibrium was demonstrated by S. Bhattacharya and A.K. Sen, Europhys. Lett. **71**, 797 (2005).

General Lecture

A Physically Based Constitutive model for FCC metals with Applications to Dynamic Hardness

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Keywords: Constitutive Model, Strain Rate, Temperature, FCC metals

A constitutive model is developed in this work to describe the mechanical behavior of face centerd cubic (fcc) metals under a wide range of temperatures and strain rates. The model is based on the dependence of the activation energy on temperature, strain rate, and stress. An expression for the flow stress is proposed in terms of micromechanical terms such as mobile dislocation density and burgers vector as well as macromechanical based state variables such as stress and material constants that include threshold and transition temperature. The proposed model is used to simulate the experimental results of Oxygen Free High Conductivity (OFHC) Copper at different temperatures and strain rates in order to obtain the different model parameters. The model shows good capability in capturing the coupling between strain rate and temperature, plastic strain and strain rate, and plastic strain and temperature. The model is used to characterize the hardness at low and high strain rates for a representative strain of 8%.

Mathematical model of a crack moving along an imperfect bi-material interface

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In this work we describe a mathematical model for a Mode III crack propagating along a thin stiff/soft interphase layer separating two dissimilar elastic materials. We begin by deriving transmission conditions which model the way the load is transferred across the thin layer from one phase to the other, and then replace the layer by an imperfect bi-material interface containing "interchange points" of the boundary/ transmission conditions. We assume that the interface is straight, and the point of interchange in the boundary/transmission conditions coincides with the crack tip which moves along the interface with a constant speed. For both stiff and soft interfaces, we develop an integral equation formulation which leads to singular integral equations with fixed point singularities (normally solvable with zero indices in appropriate functional spaces). We derive asymptotic formulae for the stress and displacement fields in the vicinity of the crack tip, and construct the solution of a boundary layer problem describing the propagation of the crack within the soft interphase layer. We give the expressions for the Mode III stress intensity factor as a function of the crack speed for both stiff and soft interfaces. We also consider a delamination crack propagating along a stiff interface. We present several numerical examples which illustrate our theoretical results in connection with applications to fracture mechanics.

This work has been supported by a Marie Curie Transfer of Knowledge Fellowship of the European Community's Sixth Framework Programme under contract number MTKD-CT-2004-509809.

Euler's best column : a singular non local quasilinear equation with boundary blowing up flux condition

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In 1757, Leonhart Euler asked what would be the maximum of height of a stable column for a prescribed volume of material, and what would be the corresponding shape. Since then many authors have contributed to the subject, such as J.B. Keller, but the problem is not yet completely solved.
In a joint work with J.I. Diaz (Univ. Complutense Madrid), we show that, when the load at the top of the column is large enough, the problem as reformulated by J.B. Keller and F.I. Niordson admits a solution, then that this solution is unique and that it provides actually a unique solution to Euler's original problem.

TOPIC 4

Dislocations and plasticity

NANOINDENTATION THROUGH THE SCALES : FROM THE ATOMIC TO CONTINUUM PLASTICITY

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Keywords: Multiscale modelling, nanoindentation, discrete dislocation dynamics.

Nanoindentation is an interesting tool used to probe the local mechanical properties of a material. Although this test has been widely used and developed over the world during the past few years, it remains a lot of uncertainties regarding the interpretation of nanoindentation data. As an example the indent size effect (ISE) corresponds to the increase of hardness when the indentation depth decreases. Although the first observations of this effect were mainly due to artefacts such as a bad surface preparation or a poor shape calibration, the ISE remains measurable when great care is paid to the experiment procedure. Recent explanations invoke strain gradient theory and geometrically necessary dislocations.
In this study, we propose to simulate the nanoindentation test of FCC metals like Cu or Ni using three numerical models. At the lowest scale, molecular dynamics simulations give details of the nucleation of the first dislocation induced by the indentation. At an intermediate scale, discrete dislocation dynamics (DDD) simulations are performed to study the evolution of the dislocation microstructure during the loading. Finally, at the upper scale, finite element modelling (FEM) using crystal plasticity constitutive equations give a continuum description of the indentation induced plasticity.

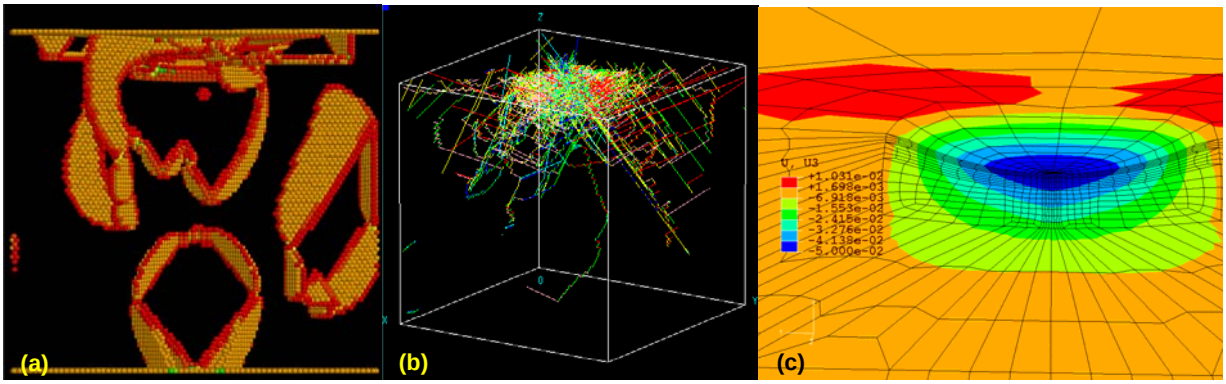

Figure 1: *The three numerical models used to study the nanoindentation test. a- Prismatic loops obtained by molecular dynamics simulations. (b)- Typical dislocation microstructure obtained during a 50 nanometer (001) indentation in Cu using dislocation dynamics. (c)- Displacement profile computed by a crystal plasticity model integrated by finite elements.*

In the presentation it will be shown how the three models are interconnected together. Basically, the MD simulations give the shape and position of the dislocation loops to introduce in the DDD model and the set of constitutive equations used in the FEM are determined by DDD simulations.
The results on the nanoindentation simulation along (111) and (110) directions will be given in term of surface relief (pile-up or sink-in) and dislocation density tensors computed within the crystal. Then, different strain gradient model of ISE are checked. Quantities like statistically and geometrically stored dislocation densities are computed from the DDD results which give insights for the length scale to use in strain gradient models.

"Plasticity" in Silica via Molecular Dynamics Simulations

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Recent Molecular Dynamics (MD) simulations and Atomic Force Microscope (AFM) experiments have revealed a process zone ahead of the crack tip in amorphous silica (a-SiO_2). MD simulations probed the atomistic aspects of dynamic fracture in SiO_2 revealing nanometer scale cavities nucleating, augmenting, and coalescing with one another up to 20 nm ahead of the crack tip [1, 2, 3]. After which these cavities were seen to merge with the advancing crack to cause mechanical failure. A similar scenario was also observed experimentally during stress corrosion ultra-slow fracture of glass using Atomic Force Microscopy (AFM) [4, 5]. Thus to gain a better understanding of the irreversible changes in structure taking place within the process zone (i.e. the zone ahead of the crack tip where pores are opening), a variety of simulations have been carried out using 1) cyclic loading and unloading in hydrostatic pressure and 2) cyclic loading and unloading in shear. Structural changes revealed by these simulations have been analyzed in various ways (static structure factor, analysis of the ring structure, evolution of the fabric tensor…).

[1] C.L. Rountree, et. al. Annual Review of Materials Research. 2002. 32:377-400.

[2] L.Van Brutzel, C. et. al. Mat. Res. Soc. Symp. Proc. 2002. 703:V3.9.1- V3.9.6.

[3] S. Prades, et. al. "A Unified Nanoscale Damage Scenario in Glasses: From Ultraslow to Ultrafast Fracture." In preparation.

[4] F. Celarie, et. al. Phys. Rev. Lett. Vol. 90 (2003), 075504/1-4.

[5] S. Prades, D et. al. Int. J. Sol. Struct. Vol. 42 (2005), 637-645.

Depinning and nucleation of crystal dislocations

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We present a discrete model of dislocations for cubic crystals that describes the core of dislocations and it approaches the correct equations of anisotropic elasticity in the far field of defects.
We analyze the depinning of dislocations near the Peierls stress and show that this transition can be understood as a global bifurcation whose character depends on the underlying dynamics. We also show how the discrete model displays homogeneous nucleation dislocations.

Homogeneous nucleation of dislocations*

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We present a mathematical theory of nucleation of dislocations is crystals. The dynamics of crystal atoms is described by a discrete elasticity model with a periodic dependence on discrete strain which changes with the type of bond. In a perfect 2D cubic lattice, edge dislocations are nucleated when a large enough shear stress is applied on the boundary. The pattern depens on the magnitude of the shear, the size of the crystal and the periodic nolinearity. Nucleation corresponds to a bifurcation in the branch of solutions describing sheared lattices as the shear grows.

*(joint work with I. Plans and L.L. Bonilla)

Modelling Dislocation Climb in Dislocation Dynamics Simulations

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Dislocation Dynamics simulations (DD) are one of the computational methods to study dynamic collective evolution of dislocations in a solid under an external loading. In this method, dislocations are considered as entities and the interaction with an external loading and between them is treated according to elasticity theory. In this work we present a method to couple the diffusion theory of point-defects with a DD simulation, in order to incorporate diffusional-climb of dislocations in the latter, as part of a larger effort to simulate creep. We make use of a 3-dimensional Discrete Dislocation Dynamics (DDD) simulation, in which each dislocation is represented by pure edge and screw dislocation segments. The DDD was utilised to study the activation of a Bardeen-Herring climb source upon the application of an external stress or under superconcentration of vacancies. Additionally, dislocation prismatic loops shrinkage and expansion, which is related to dislocation climb, was simulated in the DDD. The dynamic properties of these loops are discussed both as a function of temperature and of superconcentration of vacancies. The calculated loop shrinkage rate and its temperature dependency agree with experimental observations.

Continuum theory of evolving dislocation fields and plastic deformation

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We present the continuum theory of evolving dislocation fields and plastic deformation at the micrometer scale. The theory describes the size-dependent behaviour of materials with microstructure (e.g. composites) or of micrometer-scaled samples (e.g. thin films). To overcome the problem of averaging that appears in the continuum theory of dislocations, the concept of single-valued dislocation fields was introduced. Utilizing crystal plasticity, the description of the evolving single-valued fields of continuously distributed curved dislocations has been coupled with the small-strain continuum mechanics framework. The coupling accounts for the long-range elastic dislocation fields. The size-dependence in the original theory [Sedlaček et al., Phil. Mag. 83 (2003) 3735] was due to the non-locality related to the line tension of the curved dislocations. The line-tension represents the strongest and always present short-range dislocation interaction. Recently, the model has been enhanced by considering other short-range dislocation interactions, namely, the mutual interactions between dislocations. To this end, by generalizing the result of Groma et al. [Acta Mater. 51 (2003) 1271], we consider gradients of dislocation density perpendicular to the local dislocation line direction. The resulting back stress modifies the size dependence of the modeled material behaviour.

The resulting system of partial differential equations is a convection-diffusion problem, the numerical features of which are dependent on the dislocation interactions considered. In some cases, the problem is convection dominated and solved numerically by means of the so-called dislocation-Lagrangian method developed by Sedlaček et al. [Phil. Mag. accepted]. This is a numerical technique that enables a stable solution of the considered problem by tracking individual segments of representative dislocations in time.

We present results of several applications of the enhanced model which has been implemented for applications to two-dimensional plane-strain problems, where the continuum-mechanics part is solved by the Finite Element Method. Physical as well as mathematical consequences of the introduction of the back stress representing the short-range dislocation interactions in the model will be discussed.

Pair correlations in 3D dislocation systems

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Statistical mechanics studies of 2D systems of straight, parallel dislocations have lead Groma and co-workers to a physically established prototype continuum model for bridging the micro and mesoscales of plastic deformation of crystalline materials. Groma's model takes the form of a hierarchy of interconnected evolution equations for different order dislocation densities (similar to the BBGKY hierarchy in plasma physics), which needs to be cut at a certain level to arrive at a closed theory. To arrive at a model with a demonstratedly strong predictive power, it suffices to cut the hierarchy at first order and utilize the pair correlation functions of homogeneous dislocation systems. In this step the numerical finding is of crucial importance that dislocation pair correlations have a short range character which enables a local approximation of the correlation terms emerging in the first order evolution equations.

The authors of the present paper are involved in extending the above 2D model to the entire 3D dislocation problem by studying the statistical mechanics of curved dislocation lines. In the extended model, pair correlations are expected to play a similar role as in the original 2D one. In this talk we analyze the results of a large number of 3D discrete dislocation dynamics simulations in view of the expected form of the 3D correlation terms, with an emphasis on the spatial range and history dependence of dislocation pair correlation functions. Possible applications of these numerical findings will also be discussed.

From discrete dislocation dynamics to a phase field theory of dislocations

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A dislocation ensemble is a system of objects with long range interaction.
So the traditional methods developed for atomic systems to derive a continuum theory from the equation of motion of the individual objects cannot be directly applied. In the paper presented a set of parallel edge dislocation is considered representing the simplest possible, but already rather complex system. It is shown, that based on discrete dislocation simulation results, a link between the microscopic and mesoscopic length-scale description of the collective behavior of dislocations can be established on a rigorous manner. Furthermore, it is found that by applying the standard formalism of phase field theories the continuum theory obtained can be derived from an effective free energy functional too.
The predictions of the continuum theory are compared in details with discrete dislocation dynamics simulation results for several different problems such as Debye-like screening of stress field of dislocations, or size effects at sheet shearing.

Peierls-Nabarro Galerkin approach to instationary dislocation motion and interaction

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In the last ten years, boosted by an upsurge in multiscale approaches, the dislocation approach to plastic deformation in metals has won numerous quantitative successes. One of the present theoretical locks however concerns the fully dynamic regime, of relevance to shock loading situations and more generally to situations of high strain rate deformation where inertial effects prove important. So far, molecular dynamics (or lattice models) were the only means of addressing such cases. However, theoretical exploitations of molecular dynamic results are intrinsically difficult, partly because of the presence of noises of various origins (e.g., thermal noise), and of the difficulty to achieve special boundary conditions of relevance to dynamical studies. On the other hand, the analytical Peierls-Nabarro continuum approach to dislocations, and some of its extensions, have proved a powerful tool to help understanding complex features of dislocations, either in equilibrium or under stationary motion.
Recently, a unique three-dimensional and fully dynamic numerical generalization of the Peierls-Nabarro model has been proposed by one of us [1,2]. Aimed at studying the motion in interaction of a small number of dislocations in instationary regimes [3], it is based on a phase-field representation of the planar domains spanned by dislocation lines. Among other useful features, it allows for realistic input energetic parameters such as the so-called "Gamma-surface potential", possibly computed ab-initio. This new tool thereby combines some of the advantages of the molecular dynamics approach and of the Peierls-Nabarro approach, without suffering from their respective major drawbacks.
The present contribution provides an overview of the approach, and of some of its applications such as: the determination of pressure-dependent Peierls stresses for BCC metals; the study of the subsonic/transsonic transition for a screw dislocation, in a framework directly comparable to analytical stationary models; its use as a reference tool to help establishing an accurate equation for the accelarated or decelerated motion of screw and edge dislocations, etc.

[1] C.Denoual, Phys.Rev.B 70, 024106 (2004).
[2] C.Denoual, Comput.Meth.Appl.Mech.Engrg. 196 (2007), in press.
[3] L.Pillon, C.Denoual, R.Madec, Y.P.Pellegrini, J. Phys. IV
France 134,49-54 (2006).

TOPIC 5

New developments in continuum theory; non classical models, and discrete vs. continuum models

General Lecture

Modelling of Bloch-Floquet flexural waves in periodic plate structures and networks of beams

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The lecture addresses the results of the recent work on analysis of dispersion properties of flexural waves propagating through a doubly periodic array of inclusions/voids within an elastic plate. A version of the multi-pole method (originally due to Rayleigh) has been developed to represent the eigensolutions in the form of rapidly convergent series. The dispersion equation involves the lattice sums characterizing the geometry of the array. A particular attention is given to analysis of standing waves and also to the stop bands observed in the dispersion diagram for flexural waves.
This analysis is complemented by a model of Bloch-Floquet waves within a multi-structure represented by a network of thin walled flexural beams connecting bodies of a large mass.

Interpenetrating Phase Composites: Micromechanical analysis of deformation and damage behavior

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Composites with interpenetrating phases (IPCs) attract a growing interest of scientists and industry, especially, after the publication of the review by Clarke [1]. They are considered as a very promising group of materials for a number of applications. A number of micromechanical models have been developed for the analysis of IPCs: 3D cubic model by Daehn et al., multiphase IPC model by Feng et al., the triangular prism unit cell model by Wegner and Gibson [2], etc.

The purpose of this investigation is to analyse the effect of the microstructure and properties of IPCs on their deformation and damage behavior.

Numerical investigations of the mechanical behavior of interpenetrating phase metal/ceramics composites are presented in this work. In the numerical experiments, a series of micromechanical models of IPCs is developed, using the voxel array based code for 3D FE model generation [3]. The deformation and damage evolution in composites with interpenetrating isotropic (3D random chessboard) and graded microstructures are numerically simulated. The effects of the availability of percolation clusters from microstructural elements of each phase, their size distribution and other microstructural parameters on the constitutive behavior and damage evolution of the IPCs are analysed in the framework of computational experiments. The tensile stress–strain curves, fraction of failed elements, and stress, strain and damage distributions at different stages of loading are determined for different random microstructures of the composites. Both isotropic and gradient interpenetrating phase composites [4] are considered. It was shown that the stiffness, peak and yield stresses of a graded composite decrease with increasing the sharpness of the transition zone between the region of high volume content of the hard phase and the reinforcement free region.

References:

1. Clarke, D. R. (1992) Interpenetrating phase composites, J American Ceramic Society, 75, pp. 739–759
2. Daehn, G. S., et al, (1996) Acta Materialia, 44 (1), pp. 249-261 Feng, X.-Q., Mai, Y.-W. and Qin, Q.-H. (2003) Computational Materials Science, 28, pp. 486-493. Wegner, L.D. and Gibson, L.J. (2000) Int J Mechanical Sciences, 42 (5), pp. 925-942
3. Mishnaevsky Jr L., Automatic voxel based generation of 3D microstructural FE models and its application to the damage analysis of composites, *Matls Sci & Engnrng A*, 407, No. 1-2, 2005, pp.11-23
4. Mishnaevsky Jr L., Functionally gradient metal matrix composites: numerical analysis of the microstructure-strength relationships, Composites Sci. & Technology, 2006, Vol 66/11-12 pp 1873-1887

General Lecture

Localised modes in doubly periodic structures with defects

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The talk presents analytical and numerical models describing localised vibration modes in doubly periodic structures with defects. We consider structures containing two different materials distributed in such a way that "thin bridges" of one phase are formed in between two regions occupied by the other phase. We develop an asymptotic model that describes long wavelength vibrations of such structures and derive asymptotic estimates (two-sided bounds) for frequencies of localised vibration modes in structures involving a finite size core connected to thin ligaments of variable width. We analyse filtering properties and construct dispersion diagrams displaying stop bands for certain intervals of frequencies. We pay particular attention to disper-sion curves of low group velocity, which represent standing waves or localised vibration modes. Such localised modes occur for both Dirichlet and Neumann boundary conditions at the boundary of localisation domain. The approximations for eigen-functions for these localised modes are discussed in the paper. The asymptotic low-dimensional models are derived for both (in-plane and out-of-plane shear) elastic waves and electromagnetic waves in transverse and oblique incidence. Theoretical results are compared with the accurate finite element computations for particular types of lattice structures.

DISCRETE MODELING OF ENTANGLED MATERIALS

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Some materials appear as a disordered assembly of long flexible fibers. These entangled fibers can appear as it (metallic wools, glass wools, …) or as networks embedded in a matrix (carbon nanotubes in polymeric matrices, cytoskeleton in biological cells, …). Mechanical as well conduction properties of such entangled materials remain largely unclear, especially for volume fraction of fibers close to specific values (entanglement packing density, percolation threshold …).

We address these problems via discrete computational models. Fibers are modeled using techniques developed for the simulation of polymer chains. They are discretized by nodes or segments whose positions are the degrees of freedom of the model. Elongation stiffness, bending stiffness as well non-overlapping between fibers are schematized by means of potential energies. The system evolution is then modeled using energy minimization schemes developed for classical molecular dynamics simulations. During compressions, we follow the evolution of the number of contacts per fiber, the macroscopic stress and the total energy. Transitions in connectivity and stiffness are identified. Corresponding packing density and number of contacts are function of fiber aspect ratio. Beyond the transition, scaling laws relating stress and relative density are identified and are compared to simple analytical laws.
Concerning the electrical conductivity, entanglement of fibers is modeled as a resistance network. Distinction is made between fiber resistance and contact resistance. Important parameters were highlighted such as fiber tortuosity and fiber-fiber contact conductivity and found to influence strongly the percolation threshold and critical exponent. Assumptions are proposed to explain "non-universal" percolation behavior often observed in the literature.
In both cases (mechanical and electrical behavior), numerical predictions are compared to experimental results obtained with very different systems (carbon nanotubes embedded in polymer, steel wools, …) .

Micromechanics of micropolar and microstretch composites

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Homogenization technique for a heterogeneous material depends on the different length scales involved in the problem, typically four length scales are present in a homogenization scheme: the macro structure size L; the RVE size l; the inclusion size A and the matrix characteristic length l_m. According to different order relations of these four length scales, local or homogenized material must be idealized as different material models. For example, for the length scale relation $L >> l >> A >> l_m$, both local and homogenized materials can be idealized as classical Cauchy material model. The classical homogenization technique corresponds to this case. In this paper, we are interested in the length scale relation $L >> l >> A \approx l_m$, high order continuum model is utilized for the local material, however the homogenized material model can be still considered as Cauchy one. Two high order continuum models: micropolar and microstretch, are used to describe local material response. The Eshelby problem for a general ellipsoidal inclusion is solved for these two material models, a special micro-macro transition relation was also proposed based on local and global energy balance. With help of average effective inclusion method, the classical effective moduli of a micropolar (microstretch) composite with ellipsoidal fibers are derived in an analytical way. It is found that the effective shear modulus increases when the size of fiber decreases, especially in the range of matrix characteristic length. However the effective bulk modulus for a micropolar composite is the same as that for the corresponding Cauchy composite. For a microstretch composite, effective bulk modulus increases as the size of fiber decreases. We also extent the elastic micromechanical method to nonlinear composites, the extension is based on second order moment of stress and couple stress and secant moduli method.

It is found that the particle size has a significant influence on the nonlinear stress and strain relation of the composite, which has been confirmed by experiment.

Multifield continuum modelling for materials with lattice microstructure

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The mechanical behaviour of complex heterogeneous materials with significant fine scale sizes and textures strongly depends on their microstructural features. Lacking in material internal scale parameters, the classical continuous model is not always appropriate to describe the relevant macroscopic behaviour by accounting for the size, orientation and disposition of micro-heterogeneities. Moreover, the basic hypothesis of local uniformity of classical stress/strain fields is inappropriate in critical regions with high gradients, associated, e.g., to geometrical or loading singularities [1, 2]. These difficulties claim for developing continuous models different from the simple Cauchy one.

Focusing on composite media made of short, stiff and strong fibres embedded in a deformable matrix that also presents distributed microcracks, due to manufacturing defects or lack of cohesion, a non-standard continuum model has been formulated [3-5] within the framework of the theory of multifield continua [6]. This multifield continuum (macromodel) has additional field descriptors accounting for the presence of the microstructure and has been built up, starting from the kinematics of a complex lattice model (micromodel), by linking different material scales (multiscale modelling) via an energy equivalence criterion, in analogy with the approach of the classical molecular theory of elasticity [7, 8]. Additional balance equations suitably select the actual dynamical path in the framework of the virtual power principle.

In this work we point out how such a strategy makes it easy to describe the actual microscopic mechanical response, both in the linear and in the non-linear case. The relevant constitutive information are effectively transferred from the micro to the macro-scale by a procedure independent of the specific microscopic constitutive ingredient.

The model has been implemented in a specifically designed Finite Element computer code specifically improved to account for non-linear material behaviour. Numerical simulations have been performed with respect to a plane brick masonry wall. Different size and arrangement of bricks, as well as various non-linear constitutive assumptions for the mortar joints have been considered. Analysis of numerical results acknowledges the multifield model as more effective than the Cauchy model in describing the gross material behaviour depending on microscopic features.

References

1. Trovalusci, P. and Masiani R., Non-linear micropolar and classical continua for anisotropic discontinuous materials. *Int. J. Sol.& Struct.*, 2003, 40, 1281-1297.
2. Sluys, L. J., de Borst R. and Mühlhaus H.-B., Wave propagation, localization and dispersion in a gradient-dependent medium. *Int. J. Sol. & Struct.*, 1993, 30, 1153-1171.
3. Sansalone V., Trovalusci P. and Cleri F., Multiscale modelling of materials by a multifield approach: Microscopic stress and strain distribution in fibber-matrix composites, *Acta Materialia*, 2006, 54(13):3485–3492.
4. Sansalone, V., Trovalusci, P. and Cleri F., Multiscale modelling of composite materials by a multifield finite element method. *Int. J. Multiscale Comput. Engn.*, 2005, 3, 463-480.
5. Sansalone V., Trovalusci P., A numerical investigation of structure–property relations in fibre composite materials, to appear in P. Trovalusci (Ed.), 'Multiscale Mechanical Modelling of Complex materials and Engineering Applications', Special Issue of *Int. J. Multiscale Comp. Engng.*, 2007, 5(2).
6. Capriz, G., *Continua with Microstructure*, Springer-Verlag, Berlin, 1989.
7. Voigt, W., Lerbuch der Kristallphysik, *Mathematischen Wissenschaften*, 1910, XXXIV, 596-616.
8. Trovalusci, P. and Masiani, R., A multifield model for blocky materials based on multiscale description. *Int. J. Sol. & Struct.*, 2005, 42, 5778-5794.

TOPIC 6

Granular materials: statics and dynamics

General Lecture

Coarse graining in granular gases and solids

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As is by now rather well known, one of the properties of granular matter is the lack of scale separation between the microscales and macroscales. This fact gives rise to serious questions concerning macroscopic/continuum descriptions of the statics and dynamics of granular matter; in particular one may be concerned about the existence of convenient local (in space) and Markovian constitutive relations. These problems are in part not unique to granular matter since other rheological systems exhibit lack of scale separation (as a matter of fact, this property may be taken to define rheological systems). Also, small ("mesoscopic") systems lack scale separation by their mere sizes (this is common to granular and mesoscopic systems since typical granular systems, which are composed of macroscopic grains, contain a number of grains which is far smaller than say the Avogadro number). Indeed quite a few researchers are busy testing these continuum descriptions even in the fluidized ("granular gas") phase, where the Boltzmann equation provides a very good kinetic description. The situation is more challenging in the dense and quasistatic phases of granular matter, since there is no fundamental equation (such as the Boltzmann equation for gases) that serves as a starting point.

The talk will present a brief review of the above facts and will show that in spite of the lack of scale separation granular matter possesses regimes which are well described by near-standard constitutive relations (similar to the hydrodynamic ones in the fluidized regime, and elasticity in part of the quasi-static regime). Some corrections to standard elasticity, which occur when fine resolution is required or small systems are considered, will be presented. Certain characterizations of plastic events may enable one to go beyond elasticity and describe yield and eventually plastic flow. The latter topic is under current intensive study by numerous researchers and preliminary results will be presented, time allowing. Though the talk will focus on granular systems, it will attempt to identify results which pertain to broader classes of rheological systems, such as amorphous solids, small solid systems and the like.

Particle displacements in the deformation of amorphous materials: local fluctuations vs. the non-affine field

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PMMH-ESPCI

We describe a new characterization of displacement fluctuations in amorphous materials, obtained by subtracting the local coarse-grained displacement field from the particle displacements. We compare these fluctuations to the commonly used non-affine field (obtained by subtracting a homogeneous strain) in an elastically deformed Lennard-Jones glass. The main features of this field are captured well by the coarse-grained displacement, justifying an inhomogeneous continuum description. The local fluctuations are considerably more localized, with a correlation length smaller than the mean particle diameter (vs. about 30 diameters for the non-affine field). This suggests the definition of a new local "noise" field to be used in extended continuum models, e.g., for the description of localized events observed in the plastic regime.

TOPIC 7

Continuum theory of living structures

General Lecture

Applications of a theory of sequence-dependent DNA elasticity that accounts for intramolecular electrostatic forces

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For many problems in DNA elasticity a DNA molecule in the familiar Watson-Crick double helical form can be treated as though it is a rod-like structure obtained by stacking dominoes one on top of another with each rotated by approximately one-tenth of a full turn with respect to its immediate predecessor in the stack. These "dominoes", called *base pairs*, are formed by joining together with hydrogen bonds two nearly planar complementary nucleotide bases. Both the intrinsic geometry (e.g., curvature in the stress-free state) and the elastic properties (e.g., moduli governing bending, twisting, shearing, and coupling between such modes of deformation) depend on the nucleotide sequence in the DNA molecule. Each base pair is covalently attached to the sugar-phosphate backbone chain of one of the two DNA strands that have come together to form the Watson-Crick double-helical structure, and as each phosphate group in the backbone chain bears one electronic charge, two such charges are associated with each base pair. It follows that the electrical force exerted at a base pair is dependent on the position in space of the other base pairs in the same DNA molecule.

Yoav Biton, David Swigon, and the speaker have been developing a mathematical theory of DNA elasticity that accounts for the dependence of the mechanical properties of a DNA molecule on its nucleotide sequence and the electrostatic forces between the members of that sequence.

This talk will be about work in progress on applicatons of the theory to two areas of research in molecular biology: (i) the search for a fine scale understanding of the role played by DNA binding proteins in the regulation of gene expresson, and (ii) calculation of the dependence of the equilibrium configurations and the free energy of supercoiled DNA on nucleotide sequence and the concentration of salt in the medium.

Biofluidmechanics of reproduction

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Complex fluid-structure interactions are central to mammalian fertilization. Motile spermatozoa, muscular contractions of the uterus and oviduct, as well as ciliary beating generate forces that drive fluid motion. At the same time, the dynamic shapes of these biostructures are determined by the fluid mechanics.

We will present recent mathematical and computational models, based upon an immersed boundary framework, that promise to provide insight into these complex, coupled dynamical systems.

The human respiratory airway system: a robust transport system

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The airway system in the human lung is a complex branched structure, exhibiting up to 23 levels of branching. During the respiratory cycle, this structure acts as a pump, a transport device and an exchanger.
The transport of oxygen and carbon dioxide through this structure involves several transport mechanisms: convection in the ventilated air in the bronchia, diffusion in the distal parts of the lung (the acini) and diffusion across the alveolar membrane. It will be shown how these mecanisms interplay with the geometry of the lung, and how this interaction gives rise to a specific robustness towards external perturbations or diseases, that is crucial in living systems.

TOPIC 8

Composite media and meta-materials

General Lecture

DYNAMIC MASS DENSITY AND ACOUSTIC METAMATERIALS*

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Mass density of a composite is generally taken as the volume-averaged value of components' densities. Moreover, the same volume-averaged mass density is usually used to calculate the wave speed in the long wavelength limit, i.e., where the wavelength is much larger than the size of the inhomogeneities. In this talk I show via rigorous derivation that the dynamic mass density used in the calculation of (long wavelength) wave speed can differ significantly from the static volume averaged value. This recognition is shown to yield an excellent account of some recent experimental data, as well as to make possible the realization of acoustic metamaterials. Physical reason for the difference between two mass densities is attributed to the relative motion between the components. That is, the implicit assumption—that all components in a composite must move uniformly in the long wavelength limit—can be violated in the limit of large acoustic impedance contrast between the components. The dynamic mass density can even be negative for the locally resonant sonic materials as demonstrated both experimentally and theoretically. The implications of this finding, in the context of acoustic metamaterials, are discussed.

*Work done in collaboration with Jun Mei, Zhengyou Liu and Weijia Wen

Piezoelectric effect in composites with different polarization constituents

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In this work a problem is addressed that looks into the role of different poling characteristics in a combination of materials that have crystal symmetry 622, like Barium Titanate and PZT7-A. This composite has been studied numerically recently (Kar-Gupta and Venkatesh, 2005) in relation to potential uses as sensors and actuators by considering a simple geometry, a fiber-reinforced composite of long circular cylindrical fibres periodically distributed in a square array, whose constituents have electroelastic properties, in particular, with parallel or antiparallel polarizations. Closed-form expressions for the effective properties of this kind of composite derived recently using the asymptotic homogenization method are used to gain insight into the overall properties. Parallel and antiparallel polarizations of composites of two like materials display important differences. Opposite polarizations in constituents result in a composite with a direction of polarization as a function of fiber volume fraction, which may be either in the same, or opposite direction. The case of a non-polarized composite also arises. It is interesting to note that the longitudinal shear modulus becomes stiffened for all the fibre volume fractions. Moreover it lies between the elementary upper and lower bounds predicted in general for two such phases as expected. A similar situation is found for the out-of-plane dielectric constant. Other results are discussed.

Entropy of Microstructure

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In materials with random structure energy is not determined uniquely by any finite set of microstructure characteristics. On the other hand, in experiments and in any mathematical modeling of microstructure one can operate only with a finite set of parameters. The question arises how could one properly formulate the constitutive equations if energy is not defined uniquely. The key point of this talk is that there is a "missing" parameter in thermodynamic description of microstructure, entropy of microstructure. It can be experimentally measured via Einstein's type relation. To the author's knowledge, the necessity to introduce entropy of microstructure was recognized for the first time in connection to modeling of plasticity in samples of micron sizes (V.Berdichevsky, J. Mech. Physics of Solids, 53, 2457-2469, 2005). It is clear now that this parameter is essential in any modeling of random structures. In the talk the basic features of entropy of microstructure will be discussed, its explicit computation will be given for several random structures and the closed thermodynamic relations for entropy of microstructure will be derived.

A continuum model with microstructure for liquids with vapour bubbles

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We propose a model for liquids with bubbles calling upon the theory of continua with microstructure. In addition to the contraction and expansion of bubbles due to pressure already included in models available in the litterature on such continua, we take into account possible phase changes at the bubble's surface. To begin with, we consider here the simplest constitutive assumptions for both phases: a perfect incompressible fluid and a perfect gas.

Configurational forces that are dual to microvelocities appear in the model, leading to a generalization of the Rayleigh-Plesset bubble dynamics.
The need of calling upon results of the kinetic theory of gases, such as the Hertz-Langmuir-Knudsen's, to evaluate the velocity of phase change at the bubble wall is thus discussed in terms of working of such micro-configurational actions.

Exact results for the general case of a macroscopic conductivity tensor of a 3D composite with a 2D microstructure

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Exact linear relations are found among different elements of the macroscopic conductivity tensor of a three-dimensional, two-constituent composite medium with a columnar microstructure, without any further assumptions about the forms of the constituent conductivities: Those can be arbitrary non-scalar, non-symmetric, and non-real (i.e., complex valued) tensors. These relations enable all the elements of the macroscopic conductivity tensor of such a system to be obtained, from a knowledge of the macroscopic conductivity tensor components only in the plane perpendicular to the columnar axis. The latter elements can be found by solving the two-dimensional (2D) problem of electrical conduction in that plane, without any reference to the third dimension, which is the direction of the columnar axis. Exact linear relations are also found among different elements of the macroscopic resistivity tensor of such systems. Again, these relations enable all the elements of the macroscopic resistivity tensor of such a system to be obtained, from a knowledge of the macroscopic resistivity tensor components only in the plane perpendicular to the columnar axis.

FROM 3D IMAGING OF STRUCTURES TO DIFFUSIVE PROPERTIES OF ANISOTROPIC CELLULAR MATERIALS

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Keywords: Metallic foams, X-Ray images, morphology, transport properties

Metallic foams are porous materials which present a complex structure of three-dimensional open cells. Light weight materials such as metallic foams are more and more used in several applications [Banhart2002]. The effective transport properties are essential for these new materials. The accurate evaluation of effective transport properties becomes critical for specific uses of these new materials. Models widely used for low porosity media are more difficult to apply to high porosity materials for which effective thermal properties are highly dependent on the local morphology [Bonnet2007, vicenteMat2006]. The control of the texture of porous materials used for the optimization of compact and multipurpose heat exchangers (boiler, heat sink...) represents a significant technological stake. Indeed, the choice of foam optimized for a given application requires the correlation of the microscopic structure to transport properties (permeability, capillary pressure, thermal/heat conductivity...).

We have developed a3D morphological tools to extract geometrical characteristics of the media from X-ray images. The anisotropy of the geometry of each phase is observed and the relationship between microstructure and effective properties is analyzed. We compute directional effective conductivities using a network approach on the actual skeleton obtained from X-ray tomography images. We present a specific technique used to obtain the skeleton and the vertex-edge graph of the foam. We emphasize on geometrical tortuosity determination and impact on conductive transport tensor.

In a previous paper [vicente2006], we determined the thermal conductivity of metallic foams by using the solid phase skeleton obtained from X-ray tomography images. In order to take into account the fluid phase of the porous medium, the metallic foam is now described as two complementary networks: solid struts and interconnected pores. Morphological parameters such as throat diameter and strut length and diameter are locally assigned to the network. The conductive heat transfers are computed on this network to determine directional effective conductivities by solving the energy equation on this network. The fluid properties dependencies and the exchange law between the two phases are analyzed and compared to the literature. We realize a systematic study carried on a wide range of different Nickel foam samples.

Finally, we propose a simple model of effective diffusion properties dependence on tortuosity and porosity.

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References

[1] Banhart, J. Manufacture, Characterization and application of cellular metals and metal foams. *Progress in materials Science*, 2001. 46: p. 559-632.
[2] Bonnet J.P.; Topin F., Tadrist L. Flow laws in metal foams: compressibility and pore size effects., *Material transaction* 2007, Under review.
[3] Vicente, J., F. Topin, and J.-V. Daurelle, Open celled material structural properties measurement: from morphology to transport properties. *Material transaction* 2006. 47(9): p. 2195-2202.
[4] J. Vicente, F. Topin, J-V. Daurelle, F. Rigollet. Thermal conductivity of metallic foam: simulation on real x-ray tomographied porous medium and photothermal experiments Proc. of IHTC 13, 13th International Heat Transfer Conference., Sidney, 2006.

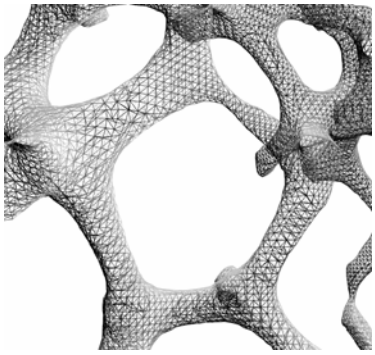

Figure 1 : Mesh

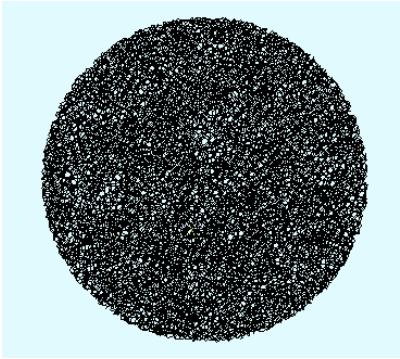

Figure 2 : Solid Network

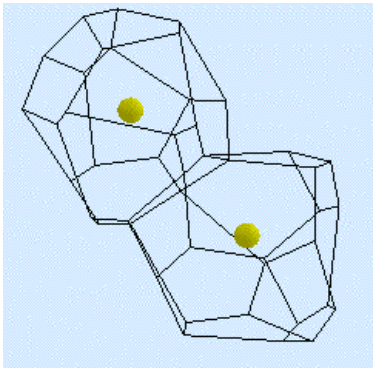

Figure 3: Two cells

Statistical Representative Volume Element for Predicting the Dielectric Permittivity of Random Media

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An efficient way to predict the dielectric permittivity of heterogeneous media makes use of numerical solutions of the corresponding partial differential solutions, before estimating the effective properties by spatial averaging of the solution. The input image can be a 3D image of the studied medium obtained by various techniques, or simulations of realizations of an appropriate model of random structure. Beside the finite element method, efficient iterative techniques operating by Fast Fourier Transform on periodic media were recently developed for micromechanics problems [8], and for the dielectric permittivity [1, 2]. This numerical approach is based on the convolution form of the Lippman-Schwinger equation appearing in a perturbative expansion of the electrical field. We use this numerical approach in this presentation.

When using numerical simulations, a natural question arises: what is the representativeness of the effective property estimated on a bounded domain of a microstructure? In other words, what is the size of a so-called "Representative Volume Element" RVE [5]? A similar question appears for engineering purpose, when working on parts with dimension of the same order as the microstructure: this occurs for instance for some devices like microbeams in micro-electronics, where a few grains only are seen across the beam. In that case the effective properties of different parts can fluctuate, so that a specific procedure may be required for the quality control in production, with a more or less important amount of rejected parts.

To answer to these questions, higher order statistical information than average values is required, but unfortunately is not available. The second order moment of the field over an infinite domain can be worked out when the effective property is known, but it does not provide any information on the fluctuations of the average made over a finite domain.

Recent developments use a geostatistical approach based on the experimental determination of the integral range [7] from numerical simulations [5]. In geostatistics, it is well known that for an ergodic stationary random function $Z(x)$, one can compute the variance $D_Z^2(V)$ of its average value $\overline{Z}(V)$ over the volume V as a function of the central covariance function $Q(h)$ of $Z(x)$. For a large specimen (with $V \gg A_3$), it is expressed to the first order in $1/V$ as a function of the integral range in the space R^3, A_3, by

$$D_Z^2(V) = D_Z^2 \frac{A_3}{V}$$

$$\text{with } A_3 = \frac{1}{D_Z^2} \int_{R^3} Q(h)\, dh$$

where D_Z^2 is the point variance of $Z(x)$. The asymptotic scaling law is valid for an additive variable Z over the region of interest V.

The effective dielectric permittivity ϵ^*, is estimated by the ratio of the space averages of the electrostatic displacement $<D>$ and of the electric field $<E>$. For an appropriate choice of the constant electric field E_0 (namely of the constant displacement field D_0) applied on ∂B and in the isotropic case, ϵ^* is obtained from the estimations of a single component of $<D>$

or <*E*>. The variance of the effective property ϵ^* is given as a function of the integral range A_3 and the point variance D_Z^2 of the relevant field. These are obtained from realizations of *Z(x)* on domains *B* with an increasing volume *V*, out of which can be estimated the parameter A_3 by fitting the obtained variance. The size of a RVE can be defined for a physical property *Z*, a contrast and, above all, a given precision in the estimation of the effective properties depending on the number of realizations that one is ready to generate. By means of a standard statistical approach, the absolute error ϵ_{abs} and the relative error ϵ_{rela} on the mean value obtained with *n* independent realizations of volume *V* are deduced from the interval of confidence.

The size of the RVE can now be defined as the volume for which for instance $n = 1$ realization is necessary to estimate the mean property *Z* with a relative error $\epsilon_{rela} = 1\%$, provided we know the function $D_Z(V)$. Alternatively, we can decide to operate on smaller volumes (provided no bias is introduced), and consider *n* realizations to obtain the same relative error. This methodology was applied to the case of the dielectric permittivity of various random media [1], and to the elastic properties and thermal conductivity of a Voronoï mosaic [5], and of real microstructures [6].

In this presentation, our approach is first validated by integral ranges obtained for the estimation of the dielectric permittivity of 2D autodual random sets (a two phase symmetrical dead leaves model [3], for which the exact effective permittivity is known), and then applied to a 3D Boolean model of spheres [4]. The effective permittivity ϵ^* and the corresponding RVE are estimated on images of $\epsilon(x)$ with increasing sizes and for an increasing contrast of permittivity. The low integral range for a low contrast of permittivity is explained from the behaviour of the covariance of the dielectric displacement field.

[1] Jeulin D., Delarue A. (2002) Numerical Homogenization of Dielectric Properties of Random Media. Application to Nanocomposites, In: *Journée doctorale 2002 Saint-Etienne (20 Novembre 2002), Signaux et milieux complexes, ISBN 2-86272-281-2*, Th. Fournel et G. Brun (eds), Presses de l'Université Jean Monnet, pp. 77-87.

[2] Eyre, D.J., G.W. Milton (1999): 'A fast numerical scheme for computing the response of composites using grid refinement', *Eur. Phys. J. Appl. Phys.* **6**, pp. 41-47.

[3] Jeulin, D. (ed) (1997): Proceedings of the Symposium on the *Advances in the Theory and Applications of Random Sets* (Fontainebleau, 9-11 October 1996) (World Scientific, Singapore).

[4] Jeulin, D., Moreaud M. (2006) Representative Volume Element for the Dielectric Permittivity of Random Media, In: *Proc. PIERS 2006 Conference*, Tokyo (Japan), 2-6 August 2006.

[5] Kanit T., Forest S., Galliet I., Mounoury V., Jeulin D. (2003) Determination of the size of the representative volume element for random composites: statistical and numerical approach, *International Journal of solids and structures*, Vol. 40, pp. 3647-3679.

[6] Kanit T., N'Guyen F., Forest S., Jeulin D. (2006) Apparent and effective physical properties of heterogeneous materials: Representativity of samples of two materials from food industry, *Comput. Methods Appl. Mech. Engrg.* 195: 3960--3982.

[7] Matheron, G. (1971): *The theory of regionalized variables and its applications.* (Paris School of Mines publication).

[8] Moulinec H., P. Suquet (1994): 'A fast numerical method for computing the linear and nonlinear mechanical properties of composites', *C.R. Acad. Sci. Paris,* **318**, Série II, pp. 1417-1423.

Representative volume element size for random elastic composites: the correlation function method

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Several existing numerical studies [1], [2], [3] show that the effective linear properties of random composites can be accurately estimated using small volumes subjected to periodic boundary conditions, more suitable than homogeneous strain or stress boundary conditions, providing that a sufficient number of realizations are considered. On the other hand, using Hashin-Shtrikman-Willis (H-S-W) approximation method for the derivation of a nonlocal constitutive equation relating the ensemble averages stress and strain for an infinite random medium, estimates of the minimum representative volume element (RVE) size are provided in [4]. Introducing the concept of periodization of random media, this paper bridges the gap between these studies. The appropriate probabilistic framework for homogenization of random media is first recalled, then the periodization concept which leads to a new definition of RVE will be presented: the smallest RVE is defined in as the "support domain" of the correlation functions of $\mathbf{c}(\omega,\mathbf{x})$, the random field of local stiffness tensor, with $\mathbf{e}(\omega,\mathbf{x})$, the random field of local strain tensor. Similarly to [4], the new definition requires ensemble averaging on many samples of the random medium. Using H-S-W approximation method, this definition allows for simple determination of minimum RVE size in agreement with [4]. Finally, the theoretical analysis is illustrated with finite element simulations of a two-phase composite [5].

Numerical simulations show that the convergence of $\mathbf{C}^{\mathrm{hom},L}$ to $\mathbf{C}^{\mathrm{hom}}$ occurs when $\mathbf{c}(\omega,0)$ and $\mathbf{e}(\omega,\mathbf{x})$ become uncorrelated for $|\mathbf{x}| \geq \frac{L}{2}$. Here, $\mathbf{C}^{\mathrm{hom},L}$ is the average overall stiffness tensor of the periodized material with a cubic unit cell of size $L > 0$. For high contrast phase, the convergence occurs for unit cell size of the periodized material larger than the minimum RVE size.

References

[1] A. A. Gusev, Representative volume element size for elastic composites: a numerical study, J. Mech. Phys. Solids 45 (1997) 1449-1459.
[2] K. Terada, T. Ito, N. Kikuchi, Characterization of the mechanical behaviors of solid-fluid mixture by the homogenization method, Comput. Methods Appl. Engng, 153 (1998) 223-257.
[3] T. Kanit, S. Forest, I. Galliet, V. Mounoury, D. Jeulin, Determination of the size of the representative volume element for random composites: statistical and numerical approach, Int. J. Solids Struct. 40 (2003) 3647-3679.
[4] W. J. Drugan, J. R. Willis, A micromechanics-based nonlocal constitutuve equation and estimates of representative volume element size for elastic composites, J. Mech. Phys. Solids 44 (4) (1996) 497-524.
[5] K. Sab, B. Nedjar, Periodization of random media and representative volume element size for linear composites, C. R. Mécanique 333 (2005) 187-195.

ON GRAIN SIZE DISPERSION EFFECTS IN METALLIC POLYCRYSTALS AND INTERNAL LENGTHS ASSOCIATED WITH (DISCRETE) INTRA-CRYSTALLINE PLASTIC HETEROGENEITIES

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Scale transition theories were developed to model the inelastic behaviour of metals in order to account for plastic heterogeneities associated with anisotropy due to crystallographic texture. This "textural" heterogeneity hides the one linked to grain size which forms a population of stochastic nature (log-normal or bi-modal distributions). In a first study [1], it was shown that grain size dispersion (in an "isotropic" aggregate with log-normal grain size distribution) has a significant influence on the macroscopic yield stress and on the evolution of internal stress distribution within the material. Here, we present last achievements considering coupled effects of crystallographic orientation/size of the grains on the macroscopic responses for IF steels (stress/strain curves, Lankford ratios etc.). Concurrently, in order to improve the local behaviour description, we propose several micromechanical approaches to describe the role of intra-crystalline plastic heterogeneities on the borders of discrete/continuum descriptions. The first one is based on calculations of elastic fields and strain energy of infinite simple or dipolar dislocation walls for which results are compared with the mean field description of the plane boundary bi-crystal. The second one (based on the Fourier transform technique) considers a spherical grain with plastic strain characterized by two characteristic lengths: grain size and spacing between plastic heterogeneities (i.e. slip bands or discrete dislocation loops). Numerical results are discussed and compared with the classic Eshelby problem associated with a uniform plastic strain in the grain.

[1] S. Berbenni, V. Favier, M. Berveiller, "Impact of the grain size distribution on the yield stress of heterogeneous materials". *Int. J. Plasticity* **23**, pp. 114-142, 2007.

Numerical FFT computations in 2D perfectly plastic pixelwise disordered porous media

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This work, of relevance to non-linear homogenization studies applied to a perfectly plastic and porous media, addresses the issue of numerically computing, by a Fast Fourier Transform method, the stress and strain fields in a 2D pixelwise disordered system. This system consists of a perfectly plastic matrix containing void pixels. As a model for a ductile damaged medium, we investigate it for the onset of plastic localization under equibiaxial or shear loading, from the point of view of mophology evolution. In particular, attention is paid to the evolution with the applied loading of clusters undergoing a plastic regime, within a nucleation / growth / coalescence scenario. Plastic cluster identification is eased by the use of a special lattice Green function in the iterative solution of the problem.
The observed different morphological regimes can be put into correspondance with some features of the macroscopic stress/strain curves.