09-13 June, 2014 Sevilla, Spain

SMDS2014

IUTAM Symposium on Micromechanics of defects in solids

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GENERAL INFORMATION

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41092 Seville
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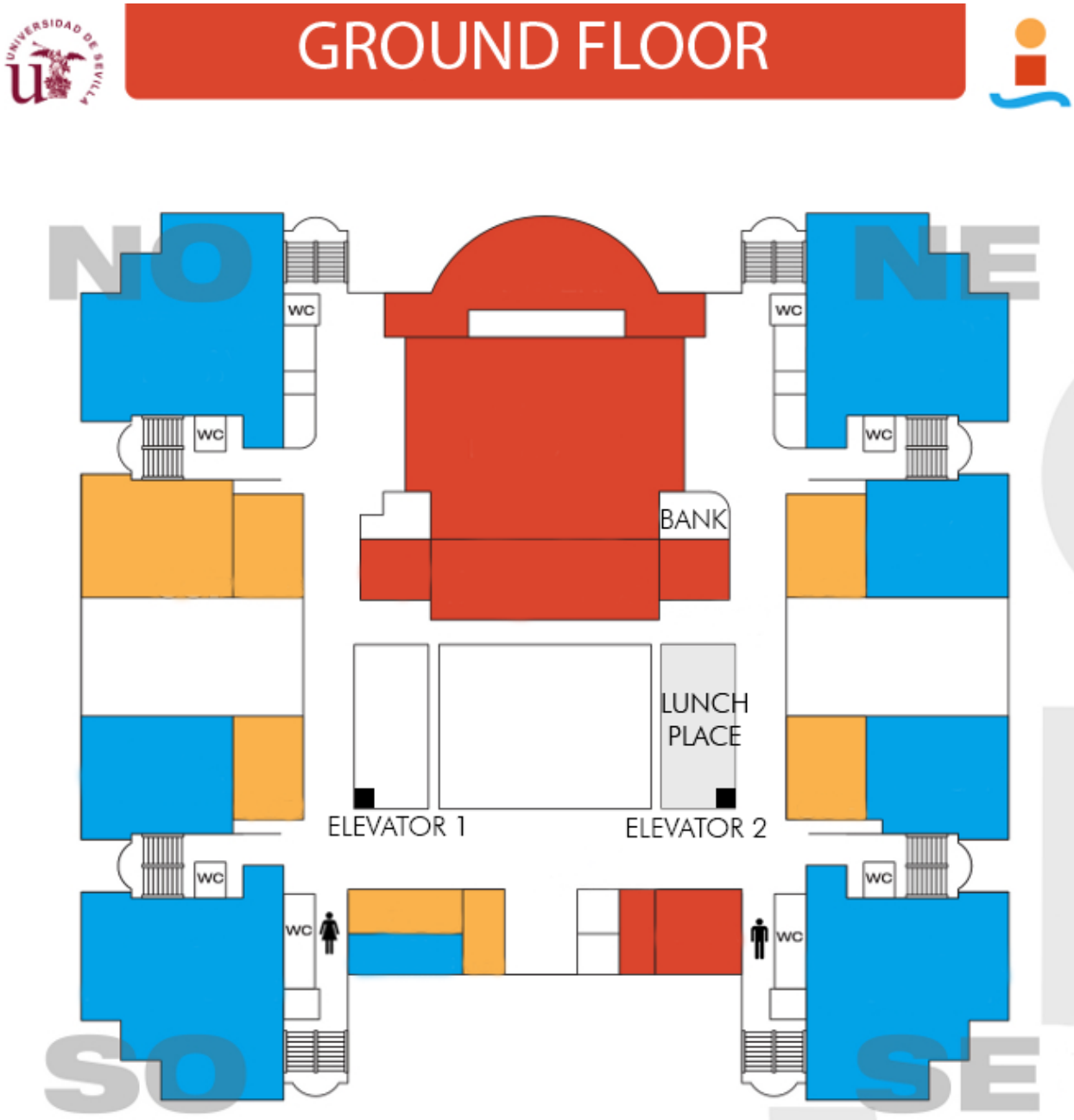
SITEMAP Ground Floor



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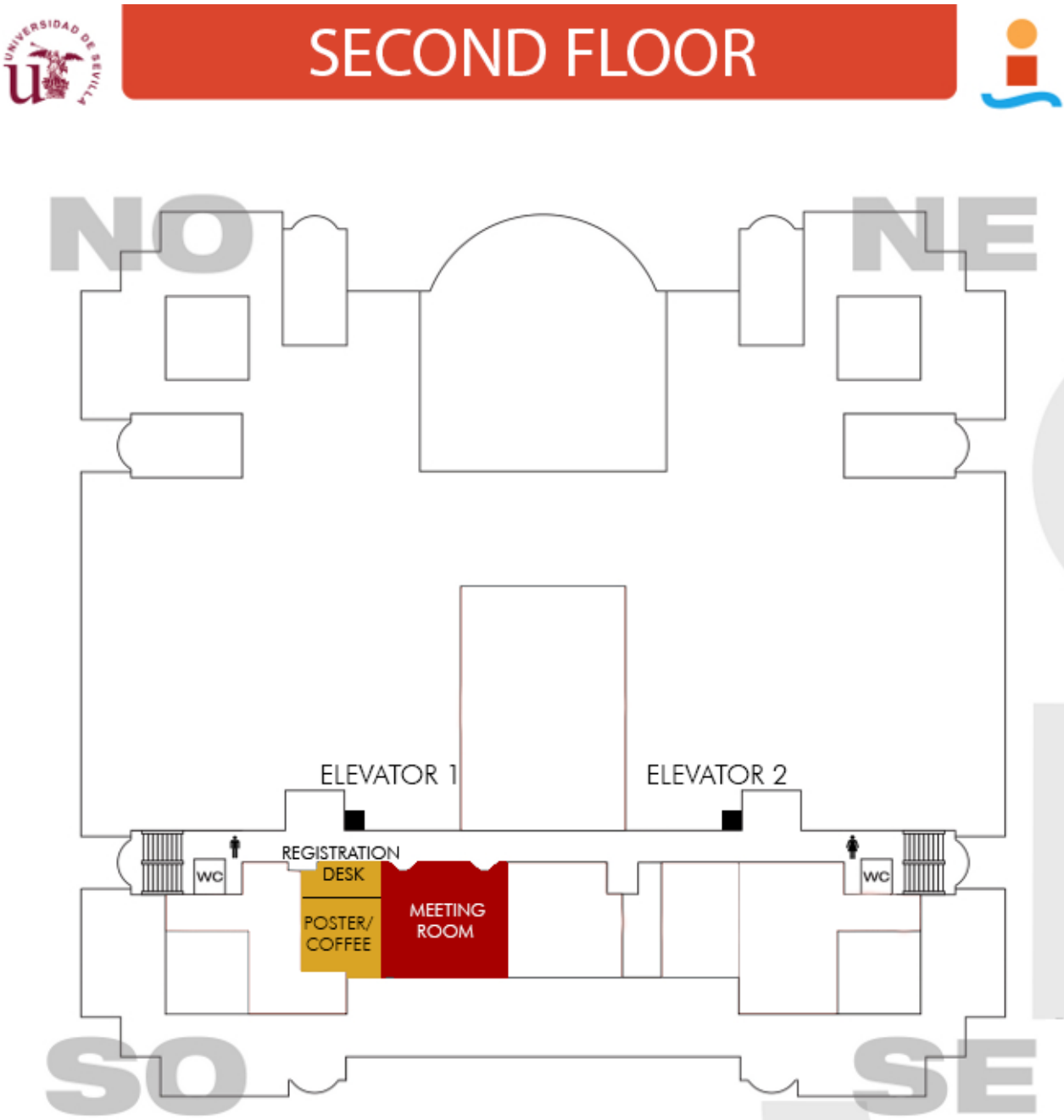

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CONFERENCE INFORMATION

Conference Venue

All talks and coffee breaks will be concentrated on the second floor of the building. The talks will take place in the *Salón de Grados*, which is equipped with advanced presentation technologies and air conditioning. The best way is to take "ELEVATOR 1" or "ELEVATOR 2" as indicated in the map.

The lunch will take place in the ground floor, next to "ELEVATOR 2" as indicated in the map.

Registration

On Monday, from 8:30 AM to 9:20AM, and Tuesday to Friday, from 8:45 AM to 9:00 AM, you will find the registration/information desk in the hall of *Sala Larrañeta*.

Upon your registration, you will receive an identification badge. Please wear your identification badge visible throughout the symposium since it will serve as admission ticket for the symposium. A delegate bag will also be given with the symposium stuff and information of Seville.

Poster Presentations

All posters will be displayed on Monday, 9 June at 9:00 AM in the *Sala Juan Larrañeta*.

The poster presentations will take place on Thursday, 12 June from 14:00 PM to 15:45 PM. The estimated time for every presentation is 10 minutes.

Coffee Breaks

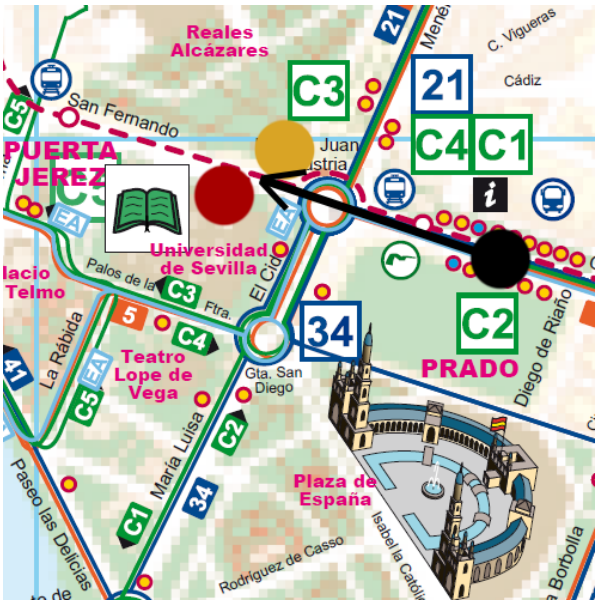
During coffee breaks beverages, cakes and fruits will be provided in the *Sala Juan Larrañeta*, where you will be able to have a look at the posters and enjoy the terrace. There will be two coffee breaks every day: 10:45-11:10 AM and 3:45-4:10 PM, except Tuesday, when other event will be carried out, and Friday.

Social Program

The visit to the main building of the University of Seville will take place on Monday, 9 June at 6:30 PM. The meeting point is indicated in the following picture. We will thank you to be there at 6:20 PM.

Later on a welcome reception will be celebrated at Oriza Restaurant, in front of the main university building.

If you go by bus, take line C1 or C2 and get off at *Prado*. In the following picture you have indicated the bus stop (black), the main university building (red) and Oriza Restaurant (yellow).



We will visit Carmona on Tuesday, a very important city during Roman and Moors periods. A bus transfer will be organized. The departure will be at 5:00 PM from Sevilla Barceló Renacimiento hotel. Afterwards the conference dinner will take place at *Los Alfares.*

We will take a tour of *Palacio de San Telmo* in two groups on Wednesday and Thursday. The meeting point is indicated in the following picture. We will thank you to be there at 6:20 PM.

Internet Access

The University of Seville is part of the international Eduroam (educational roaming) initiative. This scheme provides and facilitates inter-institutional roaming wireless network access when one is away at another institution that also uses Eduroam. Visitors from other universities that are also part of Eduroam can use their remote credentials to access ReInUS.

If it is not the case, in addition to the user name and password provided at the reception, you will also need to follow the instructions showed in: http://reinus.us.es/ On the left, click "Métodos de conexión" and "SSID eduroam". Click "in English" on the right top corner for the English version.

User: smds2014@invitados
Password: smds2014

SYMPOSIUM TIMETABLE

Hour	Monday, June 9	Tuesday, June 10	Wednesday, June 11	Thursday, June 12	Friday, June 13
8:30 – 8:45	Registration	Registration	Registration	Registration	Registration
8:45 - 9:00					
9:00 - 9:20		Viggo Tvergaard		Javier Llorca	Amit Acharya
9:20- 9:35	Welcome				
9:35 – 10:10	Alan Needleman	Erik van der Giessen	William Curtin	Amine Benzerga	Ercan Gurses
10:10 – 10:45	Michael Ortiz	P. Ponte Castañeda	Kaushik Bhattacharya	Laurent Stainier	Liping Liu
10:45 – 11:10	Coffee	Coffee	Coffee	Coffee	Coffee
11:10 – 11:45	John Bassani	Andres Jaramillo	Robert McMeeking	Vikram Gavini	
11:45 – 12:20	Xanthippi Markenscoff	Nicolas Moës	Dominique Leguillon	Celia Reina	
12:30 – 14:00	Lunch	Lunch	Lunch	Lunch	
14:00 – 14:35	Claude Stolz		Bob Svendsen	Poster Presentations (10 min. each)	
14:35 – 15:10	Lucia Nicola		Varvara Kouznetsova		
15:10 – 15:45	Dennis Kochmann		Daniel Balzani		
15:45 – 16:10	Coffee		Coffee	Coffee	
16:10 – 16:45	Jean-Baptiste Leblond	VISIT AND BANQUET (CARMONA) Departure: 17:00	Christian Niordson	Idrissi Hosni	
16:45 – 17:20	Pilar Ariza		Denis Davydov	Brian Legarth	
	Visit Rectorado and Welcome Reception (18:20)		Visit Palacio San Telmo (group 1) 18:20	Visit Palacio San Telmo (group 2) 18:20	

SESSIONS PROGRAMME

SMDS 2014 Sessions Programme

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10:10 - 10:45	2	A MICROMECHANICAL DAMAGE AND FRACTURE MODEL FOR POLYMERS BASED ON FRACTIONAL STRAIN-GRADIENT ELASTICITY S.Heyden, B. Li, K. Weinberg, S. Conti, M. Ortiz
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11:10 - 11:45	3	NON-ASSOCIATIVE PLASTIC FLOW J. L. Bassani
11:45 - 12:20	4	DYNAMIC ESHELBY MICROMECHANICS X. Markenscoff
Monday, June 9 14:00 - 15:45		
14:00 - 14:35	5	CLOSED FORM SOLUTION FOR FINITE ANTI-PLANE SHEAR FIELD FOR A CLASS OF HYPERELASTIC INCOMPRESSIBLE BRITTLE SOLID C. Stolz
14:35 - 15:10	6	PLASTIC DEFORMATION OF ROUGH SURFACES IN CONTACT R-J. Dikken, KWS Ng, L. Nicola
15:10 - 15:45	7	TAMING FORCE ARTIFACTS IN COARSE-GRAINED ATOMISTICS TO BRIDGE THE SCALES IN NANOSCALE PLASTICITY D. M. Kochmann
Monday, June 9 16:10 - 17:20		
16:10 - 16:45	8	PLANAR CRACKS WITH SLIGHTLY CURVED FRONTS: THEORICAL AND EXPERIMENTAL APPROACHES J. B. Leblond
16:45 - 17:20	9	ATOMISTIC SIMULATION OF COUPLED PROBLEMS P. Ariza

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16:45 - 17:20	9	ATOMISTIC CONTINUUM COUPLING: THE PROMISE OF STUDYING DEFECTS AT THE SUB-MICRON SCALE D. Davydov, J. P. Pelperet, A. Javili, P. Steinmann

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Thursday, June 12 16:10 - 17:20		
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VOID GROWTH AND COLLAPSE IN CREEPING SINGLE CRYSTALS

A. Srivastava[1] & A. Needleman[2]

[1] *School of Engineering, Brown University.*

[2] *Department of Materials Science and Engineering, University of North Texas. E-mail: needle@unt.edu*

Experimental observations on tensile specimens have indicated that the growth of initially present processing induced voids in nickel-based superalloy single crystals can play a significant role in limiting the creep life of these materials. In order to quantify the role of void growth in single crystals in creep loading, three dimensional finite deformation finite element analyses of unit cells containing a single initially spherical void have been carried out. The materials are characterized by a rate power law viscous crystal plasticity constitutive relation. The overall true stress components on the unit cell are adjusted so that a fixed value of stress triaxiality and a fixed value of the Lode parameter are maintained. Several crystal orientations are considered including two that are significantly anisotropic. Symmetry boundary conditions are imposed consistent with the crystal symmetry; the sides of the unit cell are not constrained to remain straight in all calculations. For significantly anisotropic crystals, the Lode parameter can have a large effect on the evolution of porosity even at relatively high values of the stress triaxiality. Whether or not a stress concentration greater than the elastic stress concentration can develop depends on the crystal orientation and the imposed stress state. Also, various void spacings are considered and, for sufficiently closely spaced voids at a low stress triaxiality value, void coalescence can occur while for widely spaced voids void collapse can occur. Whether void coalescence, void collapse or neither occurs depends on the value of the Lode parameter.

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A MICROMECHANICAL DAMAGE AND FRACTURE MODEL FOR POLYMERS BASED ON FRACTIONAL STRAIN-GRADIENT ELASTICITY

S. Heyden[1], B. Li[1], K. Weinberg[2], S. Conti[3] & M. Ortiz[1]

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[2] *Lehrstuhl für Festörpermechanik, Universität Siegen, D-57076 Siegen, Germany.*

[3] *Institut für Angewandte Mathematik, Universität Bonn, Endenicher Allee 60, Bonn, 53115, Germany.*

We formulate a simple one-parameter macroscopic model of distributed damage and fracture of polymers that is amenable to a straightforward and efficient numerical implementation. We show that the macroscopic model can be rigorously derived, in the sense of *optimal scaling*, from a micromechanical model of chain elasticity and failure regularized by means of *fractional strain-gradient elasticity*. In particular, we derive optimal scaling laws that supply a link between the single parameter of the macroscopic model, namely, the critical energy-release rate of the material, and micromechanical parameters pertaining to the elasticity and strength of the polymer chains and to the strain-gradient elasticity regularization. We show how the critical energy-release rate of specific materials can be determined from test data. Finally, we demonstrate the scope and fidelity of the model by means of an example of application, namely, Taylor-impact experiments of polyurea 1000 rods.

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NON-ASOCIATIVE PLASTIC FLOW

J. L. Bassani[1]

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Certain prominent features of plastic flow are common in a wide range of solid materials that deform by shear mechanisms, including crystalline, granular, and amorphous systems. A key element is how flow depends on the (tensorial) state of stress. Exceptional behaviors, on the other hand, are observed for FCC crystals (simple solids) which have driven much of the thinking about plasticity. Such exceptional behavior leads to so-called *associative* flow in the sense that the flow potential and yield function are taken to be the same functions of the stress tensor. Ample experimental evidence now exists that non-associated flow more appropriately characterizes plastic behavior even by mechanisms of dislocation glide, but not until atomistic simulations became sufficiently refined have we been in a position to rigorously address the issue. Clearly, frictional behavior that controls flow of granular materials is non-associative in the sense that the resistance to plastic flow depends strongly on hydrostatic pressure even in the presence of minimal volume change. Atomistic simulations have been used to rigorously construct multislip models for single crystals and polycrystals that are in good accord with experiments. At all levels, *non-associated flow* persists, and this is shown to significantly affect macroscopic deformations including strain localization. In addition, intermittent bursts of strain are predicted to arise under certain deformation histories as a consequence of non-associated flow, which is observed in many *complex* material systems.

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DYNAMIC ESHELBY MICROMECHANICS (WITH INERTIA EFFECTS)

X. Markenscoff[1]

[1] *University of California, San Diego. E-mail: xmarkens@ucsd.edu*

"Eshelby micromechanics" can be called the micromechanics based on the two celebrated Eshelby papers: The "force on an elastic singularity", or "Eshelby force" (1951), (associated with Noether's theorem and conserved integrals) and the ellipsoidal inclusion with transformation strain (1957) where the Eshelby tensor allows for the solution of inhomogeneities as well. Both of these Eshelby micromechanics building blocks are extended to dynamics with inertia. It will be presented that for *self-similarly* expanding ellipsoidal inclusions the constant stress Eshelby property in the interior holds, and the dynamic Eshelby tensor (for self-similar motion) is obtained analytically (which leads to the analytical solutions of dynamically expanding inhomogeneities). The elastodynamic evolution of moving defects (dislocations, expanding inclusion and inhomogeneity boundaries) is governed by the dynamic conservation laws (J, L, M integrals) from Noether's theorem yielding the "kinetic relations" due to inertia. For a solid containing a periodic distribution of defects, in the unit cell the defects evolve by Eshelby mechanics (J, L, M integrals) and this is carried to the macroscopic scale as macroscopic damage by asymptotic homogenization. The self-similar dynamic solutions for expanding inclusions/inhomogeneities grasp the early response of the system, along the lines of Clifton and Markenscoff (1981) for the elastic precursor decay of a plastic wave due to the transient radiation of the dislocations set in motion by the wave.

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CLOSED FORM SOLUTION FOR FINITE ANTI-PLANE SHEAR FIELD FOR A CLASS OF HYPERELASTIC INCOMPRESSIBLE BRITTLE SOLID

C. Stolz[1]

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In classical fracture mechanics, the solution of equilibrium for linearized elastostatics proposes an outer expansion of the displacement with respect to the distance of the crack tip. Some investigations must be made aimed to take into account of the nonlinear effects for determination of inner expansion in finite elastostatics or in elastoplasticity. The finite antiplane shear field near the tip of a crack in an incompressible elastic solids has been studied [4][3][6]. The local behaviour presents singularities or discontinuities of deformation gradient, depending on the shape of the stress strain curve. The stress is defined for any amount of shear γ, which is not bounded $0 \leq \gamma < \infty$.

For hyperelastic materials such polymers or elastomers rupture may occur when a maximal stretch of polymeric chains is reached. For any material direction, the stretch in an hyperelastic body is bounded by a critical value λ_c. When this value is reached, the material is broken and can not support further tension; then a damaged zone develops inside the body. The purpose of this article is to study the evolution of the damaged zone in the case of anti-plane shear. Connection with fracture mechanics is discussed.

Such a problem has been solved for linearized elastodynamics [1] and for elastoplasticity [2] in case of antiplane-shear. Connections with previous results [5] are also discussed.

Analytical solutions are also compared with numerical simulations obtained with the implementation of new types of algorithms.

References

[1] Bui H.D., Ehrlacher A.: Propagation dynamique d'une zone endommagée dans un solide élastique-fragile en mode III et en régime permanent, C. R. Acad. Sci., Série B, **290**, 273-276, (1980).
[2] Bui H.D.: Solution explicite d'un problème de frontière libre en élastoplasticité avec endommagement, C. R. Acad. Sci., Série B, **290**, 345-348, (1980).
[3] Knowles J.K.: The finite antiplane shear field near the tip of a crack for a class of incompressible elastic solids, Int. J. of Fracture, **13**(5), 611-639, (1977).
[4] Knowles J.K., Sternberg, E.: Discontinuous deformation gradients near the tip of a crack in finite anti-plane shear: an example, J. of Elasticity, **10**(1), 81-110, (1980).

[5] Neuber H: A physically non linear notch and crack model, J. Mech. Phys. Solids, 16, 289-294, (1998).
[6] Stolz C: Closed form solution for the antiplane shear field for a class of incompressible brittle solids, C. R. Mécanique, 338, 663-669, (2010).

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PLASTIC DEFORMATION OF ROUGH SURFACES IN CONTACT

R-J. Dikken[1], KWS Ng[1] & L. Nicola[1]

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The importance of plasticity in rough surface contact and friction is not yet completely understood. Even under moderate loading, plastic yield takes place not only at the summits of the contacting asperities, but also in the subsurface region. It is therefore unclear to which extent the exact surface topology is relevant in determining the plastic response of contacting bodies with rough surfaces.
This work aims to understand what is the role of plastic deformation in the surface asperities when compared to the subsurface. To this end we perform two dimensional discrete dislocation plasticity simulations of the type proposed by Van der Giessen and Needleman [1] on bodies with surface profiles approximated by sinusoidal waves. Dislocations are modeled as line singularities in an otherwise isotropic linear elasticmedium. Constitutive rules are provided for the glide of dislocations as well as their generation, annihilation and pinning at point obstacles. Results highlight that the contact pressure and shear stress at the contacts are highly localized and much higher than predicted by current contact and friction theories. Moreover, plasticity in the subsurface region is found to play an essential role in the mechanical response of metal bodies under contact loading.

References

[1] E. Van der Giessen and A. Needleman, Modelling Simul. Mater. Sci. Eng. 3 689-735 (1995).

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TAMING FORCE ARTIFACTS IN COARSE-GRAINED ATOMISTICS TO BRIDGE THE SCALES IN NANOSCALE PLASTICITY

D. M. Kochmann[1]

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The plastic deformation of crystalline solids involves large ensembles of defects whose interactions span various scales from individual atoms all the way up to the macroscale, from point defects to the intricate dislocation network to the grain structure of polycrystals. While accurate models exist for each individual scale (from molecular dynamics to discrete dislocation dynamics to phenomenological plasticity models), there is a lack of accurate albeit efficient techniques to bridge the scales, locally retaining full atomistic details while reaching to the meso- and macroscales. The quasicontinuum (QC) method was introduced to achieve such bridging solely based on interatomic potentials; yet, it still faces severe limitations (conceptually as well as based on computational expenses) which make it unattractive for many-defect systems. Here, we present recent progress in developing a new energy-based QC formulation based on novel summation rules with minimal force artifacts, improved mesh adaptation techniques, and massively-parallel capabilities in three dimensions, allowing to investigate large systems containing many defects at zero and finite temperature. We will apply the new scale-bridging technique to examples of nano- and microindentation and of nanoscale void growth and coalescence to study the underlying microstructural defect mechanisms with locally full atomistic accuracy.

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PLANAR CRACKS WITH SLIGHTLY CURVED FRONTS: THEORETICAL AND EXPERIMENTAL APPROACHES

J. -B. Leblond[1]

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This paper will present an overview of a number of recent studies of the propagation of planar cracks in mode I conditions in materials with heterogeneous fracture properties.

Theoretical works on in-plane perturbation of cracks will be reviewed first. We shall start with a seminal work of Rice of 1985 on first-order perturbation of the front of a semi-infinite crack in some infinite body, which has widely been used since to assist the interpretation of various experiments - although the geometrical conditions required for its application were frequently not met. Two distinct recent extensions of this work, due to the author and various coworkers, will then be presented: (i) one of 2011, to first-order perturbation of the front of an emerging crack lying on the mid-plane of a semi-infinite plate of arbitrary thickness; (ii) the other of 2013, to second-order perturbation of the front of a semi-infinite crack in some infinite body. An even more recent extension of both of these works, to second-order perturbation of the front of a semi-infinite crack lying on the mid-plane of an infinite plate of arbitrary thickness, will finally be expounded.

The results obtained will then be applied to the theoretical prediction, based on Griffith's criterion, of the in-plane deformation of the front of a mode I crack propagating along the mid-plane of a plate having a heterogeneous fracture toughness. It will be shown that fully explicit formulae for the shape of this front, as a function of the spatial distribution of the toughness, may be obtained up to second order in the fluctuations of this toughness. It is even possible, in the specific case of a crack encountering an isolated resistant obstacle of infinite elongation in the direction of propagation, to specify the shape of the deformed front entirely analytically (that is, without any reference to integrals to be evaluated numerically) in the two limit-cases of plates of infinite and infinitesimal thicknesses.

The formulae derived permit much more significant comparisons with observations of coplanar deformation of crack fronts encountering obstacles than Rice's original formula of 1985, since they pertain to geometrical situations corresponding much better to actual experimental conditions. This possibility will finally be illustrated by expounding the results of an experimental investigation of the detachment front of a thin film peeled from a rigid substrate with a fully controlled field of interfacial fracture toughness. The observed shape of the front is compared, in the case of an

infinitely elongated obstacle, to that predicted theoretically. The comparison does not involve any adjustable parameter since the contrast of fracture toughness is measured independently. The excellent agreement observed highlights the improvements brought by the incorporation of both influence of the finite thickness of the sample and second-order effects into theoretical predictions, and opens new perspectives in the prediction of the failure behavior of engineered heterogeneous materials.

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EFFECT OF INITIAL VOID SHAPE ON DUCTILE FAILURE IN A SHEAR FIELD

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For voids in a shear field unit cell model analyses have been used to show that ductile failure is predicted even though the stress triaxiality is low or perhaps negative, so that the void volume fraction does not grow during deformation. Here, the effect of the void shape is studied by analyzing materials where the voids have initially ellipsoidal shapes. The cell models are in plane strain, so that the voids are modelled as cylindrical holes. Periodic boundary conditions are used to represent a material with a periodic distribution of voids having different spacings in the two in-plane coordinate directions, and subjected to different average stress states. Depending on the initial orientation of the ellipsoidal voids, the principal axes of the elongated voids rotate initially in different directions relative to the shear field. After some deformation the behavior is much like that found for voids with circular cross-section, *i.e.* the voids in shear flatten out to micro-cracks, which rotate and elongate until interaction with neighboring micro-cracks gives coalescence. Even though the mechanism of ductile failure is the same, the load carrying capacity predicted, for the same initial void volume fraction, is rather different for different initial orientations of the ellipsoidal voids.

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HOW DO CONTINUUM CRYSTAL PLASTICITY TIME SCALES EMERGE FROM DISLOCATION DYNAMICS?

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The connection between lattice defects and the inelastic properties of polycrystalline metals crosses many length and time scales. While much is known about spatial upscaling from individual dislocations, via dislocation dynamics and continuum crystal plasticity to macroscopic plasticity, the transitions in time are relatively unexplored. Restricting the attention to room temperature plasticity of fcc metals, the basic question is how the picosecond timescales of lattice vibrations get coarse-grained out into the rate sensitivity as measured at macroscopic scales.

In this work, we consider just one step in this chain of scale transitions by investigating the rate sensitivity of a two-dimensional model material by means of discrete dislocation dynamics. The dislocation plasticity model has only two intrinsic timescales: one associated to the generation of new dislocations and the other implied by the dislocation mobility. By simulating the collective dynamics of discrete dislocations during multiple slip in a polycrystal material model, we study the dependence of the predicted yield strength on the applied strain rate. The rate sensitivity predicted by this simple model over more than two orders of magnitude in strain rate exhibits is similar to experimental findings for Cu and Al.

Encouraged by this succes, we zoom in to study the viscoplastic behavior of a single crystal oriented for single slip. By performing stress-controlled computations, we analyze the validity of the popular viscoplastic power-law. Preliminary results indicate that the overall plastic strain rate can be described by a power-law with exponent $\sim$30 over a range of applied stresses around the nucleation strength. From this fit, we can then extract the intrinsic viscoplastic strain, which, by virtue of the collective dislocation behavior, is significantly higher than either of the two intrinsic timescales of individual dislocations.

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THE EFFECT OF POROSITY AND ITS ANISOTROPIC EVOLUTION ON THE MACROSCOPIC RESPONSE OF PLASTICALLY DEFORMING METALS

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In this paper, we discuss a recently proposed constitutive model for the macroscopic response of viscoplastic porous materials at finite strain [1]. The model incorporates the effects of important microstructural variables in addition to the porosity, such as the average shape, orientation and spatial distribution of the pores. The model is obtained by means of a novel iterative homogenization strategy, and can be shown to provide bounds for suitable classes of microstructures. Unlike other models that have been proposed in the literature, the new model requires no fitting parameters, solely depending on the properties of the matrix phase and appropriate microstructural information. Results will be presented for the yield surfaces of ideally plastic porous materials with general ellipsoidal shape and orientation. Compared to available numerical results, the new estimates are found to be quite accurate, while they also provide more flexibility than competing models in terms of the characterization of the microstructure. In addition, evolution laws will be presented for the relevant microstructural variables [2] making use of consistent homogenization estimates for the average strain rate in the voids, which may be used to predict the evolution of the microstructure and its effect on the macroscopic response, including the possible development of shear-band instabilities.

To illustrate some of the features of the model, we will present results for the macroscopic response, microstructure evolution and possible development of shear band instabilities in rigid-plastic porous materials with power-law strain hardening under general, displacement-controlled, plane-strain loadings, i.e., combined bi-axial and simple shear straining. In this context, we focus on the subtle effects of the evolution of the internal variables—including the strain hardening of the matrix, the porosity, the (average) void-shape and the (average) void rotation—on the anisotropic response and ductile failure of the porous material. In this connection, it is noted that the evolution of the internal variables provides hardening/softening mechanisms, the competition (or synergy) among which determines the overall hardening or softening properties of the macroscopic behavior of the material. It is found that both the type and the strength of these mechanisms depends crucially on the applied loading parameters. In addition, it is often observed that an initial hardening regime in the macroscopic behavior is followed by a softening regime. This transition from hardening to softening in the macroscopic response may be identified with the onset of macroscopic strain localization. The associated critical conditions at the onset of localization will be discussed as a function of the loading parameters, including the triaxiality and Lode angle, for the entire range of loadings under investigation.

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LARGE-SCALE NON-ADIABATIC DYNAMICS SIMULATION OF MATERIALS IN EXTREME CONDITIONS

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Extreme environments may involve conditions of high dynamic or static pressure (>30MPa), high strain, and high-strain rates (> 1km/s); low or high temperature (> 1200°C); highly corrosive or erosive conditions; high-radiation fluxes (> 100dpa); and high intensity electromagnetic fields (> 15T), alone or in combination. Developing materials that can operate reliably in such environments is critical to enabling technologies required for the next-generation of energy, spatial, transportation, medical, and military systems and devices, among many others. But major breakthroughs are required in theory, computation and experiments to elucidate the chemical, atomic and molecular, processes that occur within the bulk and at the surfaces of materials subjected to extreme operating conditions. Studying these states of matter through experimental observations has proven to be extremely challenging, if not impossible, primarily because they are hard to isolate and their time scales for changes are too rapid (<1ps).

Consequently, synergistic approaches from theory and computation have taken center stage in enabling predictive calculations capable of steering experiments and material synthesis associated to extreme conditions. Yet, first-principles quantum mechanics simulation methods are inadequate for accurately describing the effects of thermal, mechanical, chemical or radiative excitations that may occur in materials operating under extreme conditions, or are impractical to use, except for very small systems (<100 atoms); including time-dependent Density Functional Theory or TDDFT. In the regime of a large number of electronic excitations, the electronic portion of the wavefunction contains contributions from many stationary states, and the Born-Oppenheimer approximation breaks down quickly. A proper model capable of capturing and tracing the inherent processes would require describing non-adiabatic coupled electronic and nuclear motions for systems with 10's-100's eV excitations over long enough periods of time (>>ps). To this end, we have been developing a mixed quantum-classical wavepacket dynamics method to simulate large electronically excited systems - called the electron Fast Forward or eFF (formerly the electron Force Field). In eFF, the electrons are defined explicitly as self- and pairwise-interacting particles via potentials derived from quantum mechanics and classical electrostatics, and their motions are propagated independently, making it possible to go beyond adiabatic dynamics.

Unlike other fermionic molecular dynamics methods, our approach achieves a balanced description of both ground- state condensed systems and highly excited

systems containing ionized electrons. eFF is uniquely suited to simulate the dynamics of materials under extreme conditions, over millions of atoms and nanosecond timescales, where many electronically excited states of matter can occur and coexist, and overcomes salient limitations of quantum mechanics methods.
We have successfully demonstrated the use of eFF in describing the thermodynamics of dense hydrogen over 0 to 100,000 K; the real-time dynamics of Auger fragmentation of diamond nanoparticles over fs ranges; electron stopping potentials in bulk materials; the dynamics of cascaded valence electron ionizations in shocked materials (e.g. polyethylene, silicon carbide and hydrocarbon molecules) during hypervelocity impact; and the electronic emissions during high strain rate brittle fracture of silicon; among others.
In this talk, I will outline the theoretical foundations of eFF, our development of effective core pseudo-potentials for high-Z elements (e.g. transition metals) in eFF, and describe some of the most salient results in modeling non-adiabatic dynamics phenomena with eFF.

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COUPLING LOCAL AND NON-LOCAL DAMAGE EVOLUTIONS WITH THE THICK LEVEL SET DAMAGE MODEL

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It is well known that damage evolution models requires a length to avoid spurious localization. We gather these type of models under the name "non-local damage models". In fact, non-locality is strictly needed only when the stress-strain curve starts to have a negative slope. Before this point, local models may be used. For instance, when damage exhibits some hardening, the stress-strain curve may be growing for quite some time before a peak point is reached.

Most if not all current non-local models are not able to distinguish between local and non-local zones, thus enforcing non-locality at every point and every instant. This leads to important computing times.

The Thick Level Set (TLS) model is a new non-local damage model [1,2,3] that allows to combine nicely zones in the domain where local model is used and zones where non-local model is used. This allows to reduce dramatically the computing time. Moreover, the TLS model is able to locate automatically zones fully damaged across displacement are allowed to be discontinuous.

The theoretical basis of the TLS model will be described. In short, it is a model in which the damage gradient is bounded (and not the Laplacian as in other modelling). The equation at stake is of Eikonal type (this explains the words level set is the name of the model). A 1D axisymmetric case will be fully developed both analytically and numerically to show the concurrent development of local and non-local damage zones.

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PREDICTING NEW AL-MG ALLOYS WITH ENHANCED DUCTILITY STARTING FROM FIRST-PRINCIPLES

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Low ductility in Al alloys is a major barrier to their replacement of steels in automotive and other applications where failure by localization limits component design. Low ductility in Al-Mg alloys has long been associated with Dynamic Strain Aging – the material is stronger at lower strain rates, which encourages localization and instabilities – but no quantitative or predictive models exist. Here, we present a hierarchical, mechanistic, multiscale model that quantitatively predicts the ductility and allows for the design of new alloys. The components of the model are:

(1) first-principles solute/dislocation interaction energies for arbitrary solutes in Al;
(2) predictive theory for solute strengthening in the absence of aging mechanisms;
(3) atomic-scale mechanism of aging via "cross-core" diffusion;
(4) effects of cross-core diffusion on two mechanisms of dislocation strengthening;
(5) full thermo-kinetic constitutive model for thermally-activated plastic flow;
(6) implementation with an FEM model to predict coupon-scale response.

The model quantitatively explains the entire scope of steady-state flow behavior as a function of strain-rate, plastic strain, temperature, and alloy composition in Al-Mg alloys, with all key inputs coming from quantum, atomistic, or dislocation-level computations. In particular, the predicted reduction in ductility of Al-Mg 5182 alloys at room temperature and strain rate of 10^{-3}/s is predicted in good agreement with experiments, tying the ductility loss directly to atomistic-scale phenomena. The model is then used to design new Al alloy compositions that have higher ductility at room temperature while maintaining the same yield and hardening behavior of the commercial alloys.

ATOMISTIC AND CONTINUUM MODELLING OF DISLOCATION DISSOCIATION, GLIDE AND TWINNING IN FCC MATERIALS

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The energetically favored state of a dislocation line or loop in fcc systems is its dissociated state, consisting of leading and trailing partial dislocations bounding a stacking fault surface. To model this and its consequences for glide and twinning, a phase-field-based model has recently been developed [2]. Building on the microscopic phase-field approach of [4], dislocations lines are modeled via their strain fields, and phase fields model the transition between thermodynamic states of "unslipped" and "slipped" on {111} planes. The free energy model is based on energy storage in the lattice, in stacking faults, and in the dislocation lines (cores). In previous related work [e.g., 1, 3], the lattice and stacking fault energy (SFE) were calculated for specific materials with the help of density-functional theory (DFT). In the current work, energy and mobility are determined using DFT-based interatomic potentials and molecular dynamics (MD). Using this approach, comparative simulation of materials with different SFEs establishes the correlation between the magnitude of the SFE and the tendency of the material to deform via twinning or glide, in agreement with MD simulations.

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GRAIN BOUNDARY PLASTICITY MODEL WITH INCORPORATION OF INTERNAL STRUCTURE AND ENERGY

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Metallic interfaces, such as grain boundaries, phase boundaries and metallization layers, play a dominant role in bulk materials, functional materials and metallic microdevices in defining their strength, reliability and life time properties. The complexity at grain boundaries results from the critical interaction between grain boundary defects and dislocations that can be accumulated, transmitted, absorbed or nucleated at the interfaces. A better insight and quantification of these mechanisms at interfaces with different characteristics can only be gained through a detailed analysis of these processes across the scales.

In this work a multi-scale approach for grain boundary interfaces is presented [1]. The grain boundary behaviour is modelled through the development of (microstructurally motivated) higher order boundary conditions within a thermodynamically consistent strain gradient crystal plasticity framework [2].

A key ingredient is the grain boundary slip law, which represents the coarse scale effect of all discrete events at the small scale. Plastic slip at the grain boundary is governed by the competition between three interface microforces. A bulk-induced microforce, derived from the bulk crystal GND densities, provides a driving force for interface normal slip which depends on the magnitude of the interface pile-up. A dissipative microforce provides a resistance to slip at the interface. An energetic microforce, acting as an interface 'back stress', is due to the (initial) intrinsic and (evolving) extrinsic defects. The evolution of the extrinsic defect is based on the conservation of the overall Burgers vector as the result of dislocations gliding in, through or from the boundary. The intrinsic defect, together with its energy, is attributed to the grain boundary structure and can be quantified based on atomistic simulations. The developed grain boundary model is implemented numerically in order to explore the influence of the interface constitutive parameters and the crystal geometry by considering a model problem consisting of a periodic bicrystal loaded in plane strain.

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APPROACH FOR THE INCORPORATION OF MICROSCOPICALLY DISTRIBUTED PROPERTIES IN DP STEELS

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Advanced high strength steels (AHSSs) enable engineering constructions with lower weight and higher energy absorption compared to conventional high strength steels, which makes them particularly attractive for automotive industry.
The enhanced material properties result from interactions of different constituents at the microscale, as e.g. ferrite and martensite in Dual-Phase (DP) steels.
The interactions are influenced by distributed properties within the individual constituents which result from e.g. eigenstresses or carbon diffusion induced during the production process.
In order to include these distributed properties in computer simulations, direct micro-macro calculations can be used.
In this context the heterogeneous fields at the microscale are numerically calculated on basis of a representative volume element (RVE) which is attached to each integration point of a macroscopic finite element problem such that the macroscopic stress is calculated by homogenizing the microscopic stresses.
An engineering approach is presented to incorporate eigenstresses and a distributed plastic yielding behavior in the ferritic matrix of DP steels.
Therein, a first step involves a volumetric expansion in the martensitic phase leading to an initial plastic deformation in the matrix phase.
In a second step these initial plastic strains are used as a local distributor for an increased yield stress in the ferritic matrix.
In order to enable relevant micro-macro calculations, e.g. sheet metal forming processes, a method is proposed for the construction of statistically similar RVEs (SSRVEs).
These SSRVEs are characterized by a significantly reduced complexity of microstructure morphology compared to RVEs as segments of real microstructures, thus leading to a decreased number of finite elements required for discretization.
The method is based on the minimization of a least-square functional formulated in terms of differences of statistical measures describing the microstructure morphology, which are calculated for a real random (target) microstructure and the SSRVE.
Numerical examples are given to show the performance of the proposed approach.

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SIZE-EFFECTS DURING VOID GROWTH MODELED BY STRAIN GRADIENT GRADIENT CRYSTAL PLASTICITY

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The intrinsic effect of size on the growth of voids and the development of void shape of initially circular voids are investigated using strain gradient crystal plasticity. A finite strain material model is employed which incorporates strain gradient hardening on the micron scale through a dissipative term. The numerical method are presented and the underlying minimum principles discussed within the context of the present finite strain implementation. The influence of the ratio of the initial void size relative to the constitutive length parameter is investigated, and results are presented in terms of slip fields as well as void growth diagrams.

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ATOMISTIC TO CONTINUUM COUPLING: THE PROMISE OF STUDYING DEFECTS AT THE SUB-MICRON SCALE

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Several staggered schemes used to couple continuum mechanics (CM) and molecular mechanics (MM) are proposed. The described approaches are based on the atomistic-to-continuum correspondence, obtained by spatial averaging in the spirit of Irving and Kirkwood, and Noll. Similarities between this and other concurrent coupling schemes are indicated, thus providing a broad overview of different approaches in the field. The schemes considered here are decomposed into the surface-type (displacement or traction boundary conditions) and the volume-type. The latter restrict the continuum displacement field (and possibly its gradient) in some sense to the atomistic (discrete) displacements using Lagrange multipliers. A large-strain CM formulation incorporating Lagrange multipliers and a strategy to solve the resulting coupled linear system using an iterative solver is presented.

Finally, the described coupling methods are numerically examined. Accuracy and convergence rates of each method are reported. It was found that the displacement (surface) coupling scheme and the Lagrangian (volume) scheme based on either discrete displacements or the H1 norm derived from continuous displacement fields provide the best performance.

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SIZE EFFECTS IN MICROPILLAR COMPRESSION: THE EFFECT OF TEMPERATURE

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Compression tests of [111] LiF micropillars with a diameter in the range 1 to 5 μm did not show any size effect on the flow stress [1]. However, more recent experimental data have shown that a strong size effect ("smaller is stronger") develops progressively as the test temperature increases. At 250°C, the micropillars of 1 μm in diameter were twice stronger than those with 5 μm in diameter [2]. Two different modelling approaches were developed to explain the development of size effects with temperature in LiF micropillars.

The first one was based on 3D discrete dislocation dynamics (3DDD) of the micropillar compression tests. Micropillars of diameters in the range 1 to 4 μm and an aspect ratio of 2 (in agreement with the experiments) were studied. The top and bottom surfaces of the circular micropillar were impenetrable to dislocations while the dislocations could leave the micropillar through the lateral surfaces and image stresses on the Peach-Koehler forces were taken into account. The three hard slip systems, [-10-1] (0-10), [0-1-1] (100) and [110] (001), that are activated during compression of LiF along the [111] direction were included in the 3DDD model, as well as the anisotropy in the mobility between edge and screw dislocations, typical of LiF. The evolution of the lattice resistance and of the dislocation mobility with temperature were obtained from theoretical considerations based on experimental results of LiF single crystals [2]. Frank-Read sources were randomly distributed in the three slip systems and the initial dislocation density was equivalent to the experimental one ($\approx 2.5 \cdot 10^{13}$ m^{-2}). The results of the 3DDD simulations were able to capture the emergence of the size effect on the flow stress of the [111] LiF micropillars with temperature. This was due to the reduction of the lattice resistance, which become comparable to the size-dependent contribution to the flow stress at 250°C. The changes in the dislocation mobility with temperature only played a secondary role in this respect.

The second approach took rigorously into account the different contributions to the flow stress of the micropillars as a function of temperature and pillar diameter: the lattice resistance, the forest hardening and the size-dependent contribution due to the operation of single arm dislocation sources. This was possible because the micropillars were obtained by chemically etching away the surrounding matrix in

directionally solidified LiF-NaCl and LiF-KCl eutectics, avoiding any use of focused ion beam methods, yielding micropillars with a controlled dislocation density, independent of the sample preparation technique. In particular, the role of the lattice resistance on the size effect of micrometer-size single-crystals was demonstrated unambiguously for the first time. This result rationalizes the different values of power-law exponent for the size effect found in the literature for FCC and BCC metals as well as for covalent and ionic solids.

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A POROUS MATERIAL PLASTICITY MODEL FOR ANISOTROPIC SOLIDS WITH NON-SPHERICAL VOIDS

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Some technologically important materials (e.g., advanced steels) fail by the linkage of microcracks without much blunting. In another class of materials the same failure process takes place in a plastically anisotropic matrix, either due to processing (e.g., Al alloys) or to the fundamental crystalline structure (e.g., HCP metals such as Mg alloys). Predictive modeling of ductile rupture in such materials requires the development of models that account for the concurrent effects of morphological anisotropy (void shape and orientation) as well as crystallographic anisotropy (texture, grain shape). As a step toward this goal, constitutive relations are derived for a type of anisotropic porous materials consisting of coaxial spheroidal voids embedded in an orthotropic matrix. A homogenization-based variational principle is formulated for the yield criterion of the effective medium and specialized to a spheroidal representative volume element containing a confocal spheroidal void and subjected to uniform boundary deformation. To obtain closed form equations for the effective yield locus, approximations are introduced in the limit-analysis based on a restricted set of admissible microscopic velocity fields. Comparisons are also carried out with numerical limit analysis calculations that employ up to 70 velocity fields. Evolution equations are also derived for the microstructure, defined in terms of void volume fraction, aspect ratio and orientation, using material incompressibility and Eshelby-like concentration tensors. The new yield criterion is an extension of the well known isotropic Gurson model. It also extends previous analyses of uncoupled effects of void shape and material anisotropy. Preliminary comparisons with finite element calculations of voided cells show that the model captures non-trivial effects of anisotropy heretofore not picked up by void growth models.

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DAMAGE IN THERMO-VISCO-ELASTIC MATERIALS: VARIATIONAL FORMULATION AND REGULARIZATION

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Thermo-mechanical coupling effects can play a significant role in the behavior of composite structures under dynamic loading, in particular those based on thermoplastics. Thermo-mechanical effects can also be exploited for predicting fatigue limits of various materials (composites, but also metals and polymers).

Modeling the progressive degradation of materials from an initial undamaged state to total failure is still a challenge in computational mechanics. Damage models can be used to describe the initial degradation of mechanical properties, while fracture mechanics is well adapted to final stages leading to fracture. The Thick LevelSet (TLS) approach, proposed by Moës et al. (2011) [1], allows for a seamless transition between damage and fracture, while providing the necessary regularization in presence of softening.

In this contribution, we will first present an application of the TLS method for the prediction of transverse cracking in layered materials (such as composite laminates). We will show how this numerical model is able to reproduce key features such as crack spacing saturation and other experimental observations. We will also discuss how this isothermal elastic damage model can be extended to thermo-visco-elastic damage within the TLS framework, and through a variational formulation.

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ELECTRONIC STRUCTURE STUDY OF AN EDGE DISLOCATION IN ALUMINUM

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This talk presents a real-space formulation of orbital-free density functional theory using finite-element basis to study the defect-core and energetics of an edge dislocation in Aluminum. Our study shows that the core-size of a perfect edge dislocation is around ten times the magnitude of the Burgers vector. This finding is contrary to the widely accepted notion that continuum descriptions of dislocation energetics are accurate beyond 1-3 Burgers vector from the dislocation line. Consistent with prior electronic-structure studies, we find that the perfect edge dislocation dissociates into two Shockley partials with a partial separation distance of 12.8 Angstroms. Interestingly, our study revealed a significant influence of macroscopic deformations on the core-energy of Shockley partials. We show that this dependence of the core-energy on macroscopic deformations results in an additional force on dislocations, beyond the Peach-Koehler force, that is proportional to strain gradients. Further, we demonstrate that this force from core-effects can be significant and can play an important role in governing the dislocation behavior in regions of inhomogeneous deformations.

This is joint work with Mrinal Iyer and Balachandran Radhakrishnan.

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F=FeFp? A MICROMECHANICAL ANALYSIS OF FINITE CRYSTAL ELASTOPLASTICITY

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The kinematic description of finite elastoplasticity based on the decomposition F=FeFp is currently standard in the continuum mechanics community. Besides its acceptance, many issues have remained unresolved, such as its micromechanical understanding, the characterization of the plastic deformation without reference to the intermediate configuration or the appropriate measure of dislocation density as a function of Fe or Fp. In this talk, we will unveil some of these issues via a careful kinematic analysis of elastoplastic deformations at the microscale.

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STUDY OF NANOSCALE DEFORMATION MECHANISMS IN NANOCRYSTALLINE MATERIALS USING ADVANCED MICRO/NANOMECHANICAL TEM TESTING

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Thin metallic films with nanocrystalline (nc) grain size are commonly used in a variety of microelectronics, coatings, microelectromechanical systems (MEMS), or stretchable electronics applications. The mechanical properties of these systems must thus be controlled or adapted to the in-service conditions, whether it is a flexible electronic device in which the metallic lines must survive large strains, MEMS microbridges which must sustain high stresses without permanent bending, or thin coatings which must not scratch under mechanical loading to preserve functionality. The mechanical properties of nc thin metallic films are directly related to the fundamental atomistic plasticity mechanisms active at the nanoscale, the associated defect distribution and topology, and the associated size effects.

The present work focuses on the investigation of the elementary defect mechanisms controlling the plastic deformation of nc metallic films. Special attention was paid to the interaction of grain boundaries and twin boundaries with the nanoscale fundamental atomistic deformation and cracking mechanisms and the resulting mechanical properties involving the strength, ductility and creep. More precisely, the investigations were performed on nc palladium and aluminium systems in the form of thin films and micro/nanowires with a high density of internal interfaces. Advanced nanocharacterization and testing methods were used to unravel the elementary processes activated at the micro and nanoscale. It mainly relies on transmission electron microscopy techniques including aberration corrected TEM and automated crystallographic orientation mapping in TEM coupled with various ex-situ and in-situ

micro and nanomechanical testing techniques. The practical outcomes consist in the development of predictive models and of improved processing routes as well as improved characterization methods towards the development of new nc materials with enhanced performances.

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EFFECT OF GEOMETRICAL ANISOTROPY ON KINKING OF A DEBONDING FIBER/MATRIX CRACK USING AFEM

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Both experiments and numerical simulations show, that failure in a composite material subjected to tension is often controlled by fiber/matrix debonding followed by matrix cracking. The fiber/matrix debonding crack arrests when its crack tip forms an angle of approximately 70° relatively to the tensile direction and subsequent damage is due to matrix cracking, as the crack kinks into the matrix [1]. Hence, in the present study is failure in an elastic composite material analyzed numerically by considering two failure mechanisms: I) fiber/matrix debonding and II) matrix cracking. Fiber/matrix debonding is modelled using a standard bilinear cohesive law, whereas matrix cracking is analyzed by the Augmented Finite Element Method (AFEM) [2]. The AFEM adopts standard shape functions in combination with an embedded cohesive law in order to represent several arbitrary crack paths and has proven to be a computationally effective tool. Plane strain, single fiber unit cell analyses with periodic boundary conditions are carried out and focus is on different loading conditions and geometrical anisotropy arising from the orientation of the non-circular reinforcement cross sections as well as the uneven fiber distributions, see [3]. Results are presented in terms of macroscopic stress-strain response curves as well as contour plots of field values. Depending on the interfacial strength cohesive and the matrix strength a rather sudden drop in stress will occur. The crack that kinks away from the interface initiates at a position found to be depending on the geometrical anisotropy and it propagates perpendicular to the tensile direction.

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PDE DYNAMICS OF LINE DEFECTS IN SOLIDS

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The talk will describe a PDE framework to deal with the dynamics of dislocations leading to plasticity in solids. Dislocations are defects of deformation compatibility/integrability in elastic response. The presented framework will be illustrated through examples involving interesting questions at the quasi-static and supersonic time scales and atomic and tectonic length scales. Time permitting, kinematics and energetics of grain and phase boundary interfacial defect structures will be discussed.

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MICROSTRUCTURAL MODELING OF SEMICRYSTALLINE POLYMERS

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Polymers, being the typical constituent of plastics in industry, have wide range of application areas in modern life. Among polymers, semicrystalline polymers (SCP) form a subset with a significant interest; owing to their remarkable deformability and toughness, good impact strength, very low gas-permeability, superior wear resistance. With notable examples of high-density polyethylene (HDPE), Nylon-6, poly(ethylene terephthalate) (PET), isotactic polypropylene (iPP); semicrystalline polymers have been used in applications such as electrical insulation systems and substrates for flexible electronic devices to plastic bags, piping systems, liquid and gas containers. Semicrystalline polymers are composed of crystalline structures and amorphous polymer chain networks and therefore they exhibit deformation mechanisms of both crystalline materials and amorphous polymers. They can be considered as two-phase materials consisting of a soft amorph phase and a hard crystalline phase, where percentage of crystalline phase can normally vary from 10% to 80%. One of the most common microstructures observed in melt crystallized semicrystalline polymers is the spherulite microstructure. In a spherulite microstructure, crystalline lamellae are embedded in a matrix of amorphous material and grow out from a common central nucleus in radial directions. The crystalline lamellae are 3 to 20 nm thick, whereas spherulite diameters are normally in the range of 2 to 100 microns. Complicated and hierarchical microstructure of semicrystalline polymers, results in deformation mechanisms that involve complex and multistage processes.

In this work, mechanical behavior of semicrystalline polymers is studied by direct finite element modeling of a spherulite microstructure under different loading conditions. Finite element meshes of idealized spherulite microstructures are constructed where different constitutive models are assigned to crystalline phase and amorphous polymer phase regions. A crystal plasticity model, which takes into account the crystalline slip constraints induced by covalently bonded strong polymer chains is used for the crystalline phase, while elastic microsphere model is employed for the amorphous phase. Effects of several parameters, such as spherulite size and degree of crystallinity, on the mechanical behavior are studied. Furthermore, it is shown that the model captures the evolution of inhomogeneous plastic deformation activity in spherulite microstructure reported in the literature.

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FLUCTUATIONS OF BIOLOGICAL MEMBRANE

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In this talk we formulate a mechanical and electrical model of biological membrane. Following the general framework of continuum mechanics, we formally derive a flexoelectric theory for membrane. Moreover, the thermal fluctuation has a significant effect on the apparent/renormalized properties of the membrane. We present statistical calculations of the renormalized properties of flexomembranes, its implication on the interaction force between membrane, and the proposed experiments for probing electro-mechanical properties of biological membranes.

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TLS APPROACH FOR DAMAGE MECHANICS UNDER ANTIPLANE SHEAR

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The initiation and growth of cracks play an important role in structural behavior of quasi-brittle materials such as concrete. Thus an accurate and efficient modeling of such phenomena is strongly needed. However, fracture mechanics is not generally adapted to the modeling of the degradation of such solids under mechanical loading. The initiation of defects requires damage modeling in order to describe the gradual loss of local stiffness. Damage is usually modeled by a scalar variable d, which value is 0 for undamaged material and 1 for totally damaged one. The classical model is local and is governed by a normality rule. The locality of this model leads to spurious localization in computational simulations: damage is concentrated in a zone of nonphysical size (similar to the elements size). Several approaches are useful to solve this problem. For instance, averaging quantities over a zone with some characteristic length, constitutive laws based on damage gradient or on deformation gradient, phase-field methods or variational approaches have been proposed for this purpose. All these methods impact the classical local models over the whole domain at all time.

To reduce computation time, a new approach was introduced in [1], [2] and [3] called Thick Level Set damage model. TLS reduces the non-locality to a small area in the domain. Damage is assumed to be zero all over the rest of the domain. The TLS model is also able to deal with local non-zero damage but this case will not be addressed in this paper. In the non-local damaged area, damage value only depends on the distance to its boundary, which is called damage front. Damage increases continuously from 0 to 1. Total damage $d=1$ is reached at a distance l_c from the front. One of the most important advantages of this model is to easily link damage models with fracture mechanics: a totally damaged zone naturally appears when damage front moves in the material. It is simply located by the level set of value l_c. X-FEM enrichment is then used to allow discontinuous displacements across the crack.

Such a model introduces a characteristic length l_c but also a function d(phi) representing damage dependence on the level-set. Thus results depend on the choice of l_c and d(phi). The influence of this function is studied in the case of an self-similar quasi-crack propagation in antiplane shear an homogeneous elastic material. A joint computational and analytical study is performed.

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SHAPE EVOLUTION OF AN EMBEDDED GRAIN UNDER COUPLED GRAIN BOUNDARY MOTION

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Microstructure plays a central role in evaluating the effective properties of crystalline solids. Studying the evolution of grain shape and size is important to understand the overall behavior of polycrystals. If the grain size is of the order of microns, the evolution usually occurs by grain boundary (GB) migration without changing the orientation of the grains (cf. Ch. 5 of [1]). In nanocrystalline materials, however, GB motion has been observed to be accompanied by the rotation of the grains (cf. Sec. 7.2 of [2]); such a motion is called coupled GB motion [3].

We study the shape evolution of an embedded grain in two systems: (i) a bicrystal where a long isolated cylindrical grain is embedded in a larger grain, (ii) a tricrystal where a long cylindrical grain is embedded at the interface of the planar GB of a larger bicrystal. The kinetic laws which provide the evolution equations are derived within the framework of irreversible thermodynamics. The kinetic relation for the bicrystal under normal GB motion is a nonlinear parabolic PDE, whereas for the tricrystal there is an additional kinetic law governing the motion of the triple junctions. Under the coupled GB motion the kinetic relations include an additional ODE governing the rotation rate of the grains. The grains are assumed to be rigid, and hence the orientations are homogeneous in each grain. In both the systems it is only the embedded grain which is assumed to be rotating, and the outer grains, being much larger, are considered to remain stationary. The overall grain rotation includes a tangential motion of the GB which is geometrically coupled with the normal motion and a viscous sliding between the grains along the GBs. The shape accommodation required for maintaining continuity across the GBs is accomplished by diffusion along the GBs.

For studying the bicrystal we have used the level set method to solve the nonlinear PDE. The results include evolution of circular and non-circular GBs. When the sliding is absent, the GB shape remains self-similar, but the shape changes in the presence of viscous sliding. The effects of anisotropy in both GB energy and kinetic coefficients have been studied. For the tricrystal, we have considered isotropic GB energy and isotropic kinetic coefficients. The presence of triple junctions retards the overall dynamics of misorientation and GB evolutions.

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CRACK-TIP FIELDS IN STRAIN GRADIENT PLASTICITY

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Experiments have shown that metallic materials display strong size effect at the micro and sub-micron scales. Attributed to geometrically necessary dislocations associated with non-uniform plastic deformation, this size effect is especially significant in fracture problems as the plastic zone adjacent to the crack tip is physically small and contains strong spatial gradients of deformation. Since conventional plasticity possesses no intrinsic material length, several continuum strain gradient plasticity (SGP) theories have been developed through the years in order to incorporate this size effect.

In this work, the influence of the plastic size effect on the fracture process of metallic materials is analyzed numerically through a SGP theory established from the Taylor dislocation model. Since generally large deformations take place in the vicinity of the crack, the chosen SGP theory, that does not involve higher order stresses and where the plastic strain gradient comes into play through the incremental plastic modulus, is developed in order to allow for large strains and rotations. The material model is implemented in a commercial finite element software by means of a user subroutine and crack tip fields are evaluated thoroughly in the framework of both infinitesimal and finite deformation theories by means of a boundary layer formulation. An extensive parametric study is conducted and differences with conventional plasticity in the stress distributions ahead of the crack-tip are quantified.

As expected from the literature, the stress level given by the SGP theory is much higher than that predicted by classical plasticity in the vicinity of the crack. When comparing large and small deformation theories, finite element results show a significant increase in the magnitude and the extension of the differences in the stress distributions originated from the plastic size effect when finite strains are taken into account. This is due to the fact that the strain gradient increases the resistance to plastic deformation, lowering crack tip blunting and, consequently, avoiding the local stress triaxiality reduction characteristic of the conventional plasticity predictions. The meaningful increase in size obtained for the distance ahead of the crack tip in which the plastic strain gradient significantly alters the stress distribution reveals that the plastic size effect could not only influence the modelling of void growth and cleavage fracture, as seen in the literature, but also void coalescence and ductile-to-brittle transition. Since the range from the crack tip where differences arise between the stress fields of SGP and conventional plasticity theories is in the order of the length between two neighbored microvoids.

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DYNAMIC SPHERICAL CAVITY EXPANSION IN TRANSFORMATION HARDENING ELASTOPLASTIC SOLIDS: THEORETICAL AND FINITE ELEMENT ANALYSIS

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Cavitation instability arises when an embedded cavity, within the solid, expands spontaneously upon application of constant load, subjected either at the cavity wall or in the remote field. That critical level of load, to induce cavitation, is the quasitatic cavitation pressure. If the applied load is higher than that critical level, dynamic cavitation will evolve implying that the cavity expands with finite velocity. Over the years, cavitation phenomena has been widely accepted as a basic mode of failure in solids which is related to fracture initiation and penetration processes. Available studies on dynamic spherical cavity expansion (e.g.: Durban and Masri, 2004; Cohen et al., 2010) focus on hardening and non-hardenig elastoplastic solids and pressure sensitive materials. In those studies the theoretical formulation of the field response bypasses the transient behavior by assuming self-similar expansion. Hence, the present study attempts at a computational model of dynamic cavitation which agrees with the theoretical models at the steady-state limit and is able to predict the transient behavior, including the time required for the theoretical steady-state response to evolve and the possible appearance of shock waves. The analysis focusses on a family of transformation hardening materials which exhibit martensitic transformation at high loading rates. A systematic comparison between theory and computations is conducted and agreement between both methodologies is found. As opposed to the observations reported for different dynamic problems (e.g.: Rodríguez-Martínez et al., 2013; Zaera et al., 2014) in which the transformation hardening has large influence on the material response, we show here that martensitic transformation barely affects cavitation instability.

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STUDY OF DEFECTS IN GRAPHENE USING A TIGHT BINDING MODEL

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We present an assessment of the stability of structural defects in graphene and how these defects might alter its electronic properties. Additionally, we also exhibit the power of the discrete dislocation theory (DD) developed by Ariza&Ortiz [1, 2]. In order to carry out this study, we first use the discrete dislocation theory to compute the harmonic atomic structure of dislocations, employing a tight binding model [3]. The benefits of using a tight binding potential relies on its ability to predict changes on electronic properties due to the existence of defects while requiring less computational time than ab initio simulations. Straight afterwards, using an extension of the DD theory, we are able to obtain the relaxed atomic structure by taking into account the non-harmonic part of the potential. Finally, we study the electronic properties due to defects and the thermal stability of these defects by inserting the discrete dislocation configurations predicted by the DD theory and its extension into molecular dynamics calculations as initial conditions.
In particular, we use Sandia National Laboratories Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS).

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FINGERING INSTABILITY DURING TENSILE PLANAR-CRACK PROPAGATION IN STRONGLY HETEROGENEOUS TOUGHNESS FIELDS

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A qualitative view at the problem of crack propagation in a heterogeneous toughness map consists in considering the competition between elasticity and toughness heterogeneities: while material elasticity tries to maintain a straight crack front, local variations of toughness deform it. As a result, the front roughens and the macroscopic effective resistance of the material can be strongly modified. A quantitative approach to this problem is to find the perturbed front geometry that leads to equality between the local stress intensity factor and the local toughness along the crack front. In general, the geometry of the crack is not known a priori and must be determined as part of the solution. For a weakly heterogeneous toughness media, first order perturbation approaches (see *e.g.* Rice, 1985) are valid so that it becomes possible to derive analytical results on the front geometry at equilibrium (see *e.g.* Lazarus, 2011). Here, we study the impact of highly heterogeneous toughness fields on tensile crack propagation. First, we study the problem with second-order developments for half-plane crack propagating in some heterogeneous toughness field. Second, we study this problem numerically with take into account arbitrary crack front deformations induced by high toughness contrasts and in particular, we focus on the propagation of a tensile penny-shape planar crack within an axisymmetric heterogeneous toughness field. To compute the variations of stress intensity factor along the crack front arising from its progressive deformation, a perturbation approach based on Bueckner-Rice weight function theory is used iteratively (see *e.g.* Bower & Ortiz, 1990, Lazarus, 2003). For
small enough toughness contrasts, as predicted using analytical first-order developments, the crack front deforms until reaching an equilibrium state for which the local stress intensity factor equals the local toughness value at each point of the front. The front keeps then a stationary shape all along the failure process. For larger contrasts, however, we observe that such an equilibrium state is never reached. Instead, some parts of the crack front remained pinned by strong impurities, while some other parts advance continuously, resulting in a constantly growing fingering crack pattern. The mechanism at the origin of this fingering instability is discussed in linked to the screening effect induced by the finger.

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STRESS-DEFORMABLE STATE OF ISOTROPIC SHELL FOR ARBITRARILY GAUSSIAN CURVATURE WITH NON-THROUGH THICKNESS CRACKS AND CIRCULAR HOLE

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The work is devoted to determining the stress-strain state of isotropic shell for arbitrary Gaussian curvature with defects system (two non-through thickness (internal) cracks directed along the one principal shell curvature and the circular hole located in the center of the structure (Fig. 1)). The shell is assigned to orthogonal coordinate system with x, y axes in the directions of structure geometric symmetry and is subjected to an external balanced load - the uniform tension along the y axis.

In this study, we used the line-spring model, allowing us to reduce the three-dimensional problem to a two-dimensional one. As a result, cracks are modeled as mathematical shell middle surface cuts.

The problem was reduced to a system of seven boundary integral equations. To ensure the uniqueness of the solution, one corresponding differential equation linking the unknown functions was added.

In the numerical solution of the problem the special quadrature formulas for singular integrals of Cauchy type were used for the reduction of integral equations system to a linear algebraic equations system. We applied the finite difference method for the reduction of differential equation to a linear algebraic equation. The defects influence on each other for different Gaussian curvature shell has been investigated.

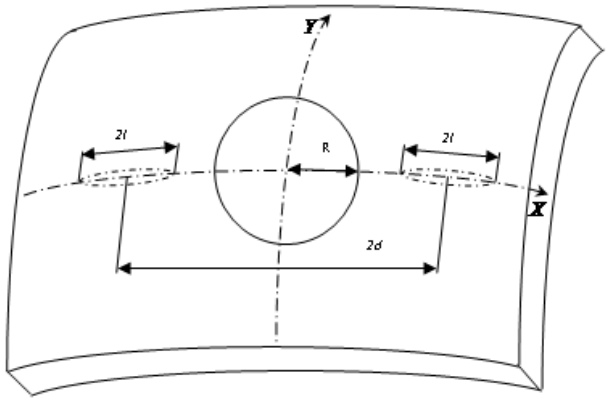

Fig.1 The shell with circular hole and non-through thickness cracks.

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MODELING FAILURE OF PCM SYSTEMS IN HEAT STORAGE APPLICATIONS

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One of the main challenges in concentrated solar power (CSP) plants is the storage of thermal energy during daylight hours and later release in the night. Within this context, phase-change materials (PCM) have proven to be a smart solution in order to store and return the energy relying on their large latent heat [1].

In general, PCM exhibits very low conductivity; therefore, different solutions are currently being studied in order to increase the effective conductivity of heat storage systems. In this work, a composite material consisting in paraffin wax as the PCM inclusion and a matrix of higher conductivity as the host material is subjected to thermal cycling and its thermomechanical behavior is characterized by means of finite element modeling.

Thermal expansion of materials with different thermal properties may induce damage in the host structure; for this reason a coupled heat transfer and mechanical model is used in order to describe the phase change process of the PCM along with the potential damage in the host material. Although this problem has been recently addressed by means of a unit cell analytical model [2], in the presence of more complex geometries a numerical approach as the one presented herein is demanded.

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MULTIPLE RELAXATION IN A PEIERLS-NABARRO MODEL FOR PARALLEL SLIP PLANES

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We study the behavior of an elastically deformed crystal with dislocations on finitely many parallel slip planes. Our model is based on that introduced by Koslowski, Cuitiño, and Ortiz, featuring a periodic Peierls potential for all slips, and linear elasticity for bulk deformations.

For small lattice parameters, the energy for nonconstant slips is known to grow logarithmically. The Gamma-limit of the rescaled energies is finite only for integer-valued slips with bounded variation, and is concentrated along the jump lines of the slips, i.e. on edge dislocations.

For two parallel slip planes with slips u and v, the limit energy varies based on the scaling of their distance h with the lattice parameter ε.

For a constant distance h, the limit energy is the sum of two single-plane energies $I(u)+I(v)$, with no interaction.

For a small distance $h=O(\varepsilon)$, the limit energy is the single-plane energy applied to the sum of the slips $I(u+v)$.

For $h=\varepsilon^{\beta}$ with $0<\beta<1$, the limit energy is still of line-tension type, but short-range interactions are relaxed before being added to long-range interactions. The total energy is then relaxed again, yielding a line-tension energy of the form $[(I_{short})^{rel}+I_{long}]^{rel}(u,v)$.

Furthermore, slips of minimal energy exhibit microstructure at length scales ε and h as well as macrostructure.

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MATERIAL MODELING OF CARDIAC VALVE TISSUE

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With around three billion heartbeats during an average life span, cardiac valves regulate the blood flow through the organ and are subjected to varying loads and stresses based on their specific location. Hereby, a key element of the cardiac cycle of the human heart is the opening and closing of the four heart valves, viz. the mitral, tricuspid, aortic as well as the pulmonary valve. However, relatively little is known about the material properties of the leaflet tissues, which fundamentally contribute to determine the mechanical response of the valves. The present study aims to provide data and insight into the material behavior of porcine heartvalve tissue from samples spanning all of the different valve and leaflet types and under uniaxial as well as biaxial loading. The tests show a fair degree of reproducibility and the data are clearly indicative of a number fundamental properties of the response of heart-valve tissue, including a progressively stiffening response with increasing elongation and a marked anisotropy in the elasticity of the tissue. Furthermore, a composite material model is devised and fitted to the experimental data set in order to characterize and represent analytically the mechanical response of heart-valve tissue.

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