The Nabarro–Hart–Rivlin Connection

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ABSTRACT

It would be nearly impossible for me to deliver a reasonably documented lecture on the Nabarro-Hart-Rivlin connection. I concluded this after deciding on my talk's title; wishful but not realistic. Fortunately, Ali Argon's lecture which follows will make up, in part, for this inadequacy. I will refer, thus, only to some personal experiences I had from meetings and discussions with them. I first met Hart in 1976 when I was invited for an interview at Cornell, after obtaining my PhD from Minnesota in December 1975. His first question was whether "stress" or "strain" is the fundamental variable in solid mechanics. I was educated to treat the strain and/or its rate as independent variables in constitutive equations. Hart's view was, as in Newtonian mechanics, that forces are what bring geometrical changes about. Nevertheless, a few weeks later, I received phone calls from Ali Argon and Jim Li who invited me for interviews at their schools after Hart had contacted them.

My next encounter with Hart, as well as with Nabarro and Rivlin was in 1983 in Houghton/Michigan where all three participated in the Symposium I co-organized with John Hirth on the "Mechanics of Dislocations" celebrating the 50th anniversary from the first dislocation observation with a dedication to Eshelby. At that meeting I ventured to present some preliminary ideas on the necessity of introducing diffusive-like terms in the evolution equations for dislocation densities when the material is densely populated by these defects, as well as higher order strain gradients into the constitutive equations of solids when the material enters into the strain softening regime. Nabarro commented that dislocations do not "diffuse", Rivlin commented that one cannot do mechanics at the softening regime and Hart pointed out some similarities of the approach with Cahn-Hilliards' model for spinodal decomposition. Nevertheless, the first idea led to the W-A model of "dislocation patterning" and motivated, in part, subsequent work on discrete dislocation dynamics (DDD) simulations. The second idea led to the first model for obtaining shear band widths/spacings and dispensing with mesh-size dependence in corresponding finite element calculations and motivated, in part, what is now referred to as strain gradient plasticity.

Beyond the aforementioned personal experiences and initial motivation for much of my work through these and many subsequent interactions with the N-H-R trio, I can also attest their influence on my students and co-workers. As an example, I refer to Bammann who was deeply influenced by all three and the same is true for Zbib. They both went far beyond of what I could teach them. In fact, they digested some of the fundamental issues treated by NHR and taught me how to improve on my initial formulation. This was also the case with some of my later collaborators Chang, Romanov, Zaiser, Groma, Triantafyllidis, Dafalias, Muhlhaus, and Steinmann. The things they taught me on inelasticity, dislocations/disclinations, structural media, nonlinear elasticity, finite deformation plasticity and configurational forces can be traced back to early NHR contributions.

In concluding, I should point out how the NHR work has affected my current research. The recent elimination of strain singularities with gradient elasticity theory is calibrated with the classical Peirls-Nabarro model, while Frank's most recent work on size effects in microindentation and persistent slip bands is used for a reinterpretation of these phenomena through gradient theory. The non-convexity of stress-strain graphs in polymeric materials is explored through Ed's model, while his internal variable and tensile instability theories are revisited within a gradient framework. Finally, Ronald's nonlinear elasticity and rheological models are endowed with gradient and stochastic terms to capture deformation instability and patterning phenomena.

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Nabarro, Hart and Rivlin - their Legacy on the Constitutive Relations for Inelastic Deformation of Solids: A Case Study on the Plasticity of Amorphous Silicon

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ABSTRACT

The full understanding of the physics of the constitutive connections between stress, temperature and the ensuing inelastic deformation rate of solids is to some extent still incomplete. In their distinguished careers Frank Nabarro, Ed Hart and Ronald Rivlin have all made major contributions toward this goal - ranging from all aspects of crystal plasticity to the response of elastomers. We will briefly take note of these and proceed with a discussion of a new simulation of plasticity of amorphous silicon that makes contact with the work of all three of these extraordinary men.

Recent computer simulations of plasticity of amorphous silicon have not only shed new light on the nature of the fundamental mechanisms of flow by repeated nucleation of thermally assisted shear transformations in this space network solid, but have also provided mechanistic understanding of corresponding processes in metallic glasses and glassy polymers. This permits now a penetrating overview of the mechanisms of plastic flow in all amorphous solids and clarifies the role of specific plasticity carriers in such solids referred to as liquid-like-material that plays the same role of dislocations in crystalline solids.

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Frank Nabarro; A Life In Science

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ABSTRACT

Frank Nabarro's impact was huge, and he leaves behind a legacy that will endure for long. He has influenced the lives and careers of many of us. We looked up to him as a father figure whose wisdom and integrity were almost boundless. We admired him for his brilliance as a physicist and his long list of achievements, in a career spanning almost seventy years.

His formidable international reputation is attested to by the fact that he was a Foreign Associate of the US Academy of Engineering, the only person on the African continent to be accorded that honor, and a Fellow of the Royal Society of the UK, one of only two that there were in South Africa.

In his early formative years Frank Nabarro worked with the likes of Nobel Prize winner Neville Mott, Sir Charles Frank, Alan Cottrell, Herbert Fröhlich and Jock Eshelby, some of the most eminent physicists of the day. Within a few years he had risen to a leadership position in the field of crystal lattice dislocations and plasticity. In this period he wrote a number of seminal papers which are still today highly cited. Later papers and the two books that he has published have cemented his dominance of the field. His research output continued almost unabated throughout his life. He contributed essential ideas to many topics, including the elastic theory of dislocations (which forms the basis of his monumental book "Theory of Crystal Dislocations"), work hardening, Harper-Dorn and diffusional creep, the Peierls-Nabarro stress, the effect of elastic energy on the shape of precipitate particles, crystal whiskers and the interaction of sound waves with dislocations. In recent years he turned his attention to creep resistant materials and rafting in superalloys which, with de Villiers, he surveyed in a monograph. Reference is also made to his encyclopedic series of books "Dislocations in Solids" which he edited.

Frank Nabarro played a prominent role in the Royal Society of South Africa and in the establishment of the Academy of Science of South Africa. He was a Council Member of the SA Institute of Physics (he also served as Vice President), always livening up discussions with his thought provoking views.

Frank was not only an outstanding scientist, but also a man of great culture. He possessed to a remarkable degree the ability to bridge cultures, whether scientific, political or social, and was sought out by many for his knowledge and wise counsel. The opinions he expressed were seldom bland, often questioning preconceived notions and prevailing wisdom. Through his personal attributes and extraordinary achievements he acquired legendary status in his lifetime. He was an avid reader of Marcel Proust, and had an abiding love for classical music, which he shared with his wife Margaret, who was a notable musicologist. He was Honorary President of the Johannesburg Musical Society, and in memory of his wife, he established the Margaret Dalziel Nabarro Chamber Concert Fund. Somehow, along the way, Frank and Margaret found time to raise a family of five children.

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Frank Nabarro and Dislocation Forced Crystal/Polycrystal/Composite Plasticity

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ABSTRACT

Among his many early contributions to the fundamentals of crystal dislocations and plasticity, Frank Nabarro pointed out that the experimental critical resolved shear stress corresponded to a constant force per unit length acting on a slipping dislocation[1], also known as the Peach-Koehler expression. The model consideration has interesting consequences for the orientation dependence of dislocation climb and the twin thickness dependence of deformation twinning[2]. Within slip band pile-ups at grain boundaries of polycrystals, the single dislocation forces add up to produce requisite local internal stress intensifications that are needed for general yielding and subsequent material deformations leading to material fracturing[3], thus providing an explanation of the Hall-Petch equation for an inverse square root of grain size dependence for the full polycrystalline stress-strain behavior[4], and recently extended to consideration of nanopolycrystalline strength properties[5]. For alloy strengthening, for example, of solid solutions, there are separate contributions for the hardening within the grain volumes and at the constraining grain boundary regions[6]. Such basic material strengthening approaches, that were fostered by Frank Nabarro, have been carried over, as well, to composite materials of industrial importance, including tungsten carbide/cobalt cemented carbides also involving consideration of the contiguity of the stronger tungsten carbide particles[7,8].

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Jerky-Type Motion of Dislocations: a Tribute to Frank Nabarro

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ABSTRACT

The importance of dislocations to the field of materials science and engineering lies in the fact that they are the carriers of plastic deformation in crystalline materials[1]. The mechanical properties of metals may therefore be tailored by altering the extent to which dislocations can nucleate, propagate or interact. Since metals and alloys are most common in their polycrystalline form, the interaction between dislocations and grain boundaries is of particular interest. A major drawback of experimental and theoretical research in the field of dislocations and grain-boundaries lies in the fact that most of the work has been concentrated on static structures. Nuclear spin relaxation methods in the rotating frame have been developed in the past[2] as a complementary tool for studying dislocation dynamics in metals. A strong advantage of this technique is that it detects dislocation motion in the bulk of the material, as opposed to in situ transmission electron microscopy, where the behavior of dislocations may be affected by image forces due to the proximity of free surfaces. However, information about the local response of dislocations to an applied stress cannot be obtained by nuclear spin relaxation and therefore in situ transmission electron microscopy remains a valuable tool in the study of dislocation dynamics. Direct observation of dislocation behavior during indentation has recently become possible through in situ nanoindentation in a transmission electron microscope. We have used this novel technique to study jerky-type motion of dislocations in metals with grain sizes of the order of a few hundred nanometers. It turns out that at these grain sizes, stress-induced movement of grain boundaries is an important deformation mechanism in pure Al. Furthermore, the in situ TEM indentations on both Al and Al-Mg show a considerable amount of dislocation activity prior to the first macroscopic yield point. This is a remarkable observation, as the initial contact would typically be interpreted as purely elastic from the measured loading response. The observations of incipient plasticity are illustrated by the TEM images and load-displacement data recorded during an in situ displacement-controlled indentation on Al-Mg.

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Grain Size Effects in the Elastic–Plastic Transition of Polycrystals

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ABSTRACT

Emphasis is put on the importance of analyzing properly the elastic-plastic transition in order to describe the mechanical properties of nanograined polycrystals. It is shown that the smaller the grain size of metallic polycrystals, the larger the extent of the microplastic stage. More specifically, in most fine grained polycrystals, the extent of the microdeformation stage is much larger than the conventional 0.2% proof strain. It depends both on the material and on the measurement technique.

During the microdeformation stage, the tangent modulus is very large. It is therefore inconsistent to compare measurements done for different values of the plastic strain, without carefully analyzing the elasto-plastic transition and its scale dependence. It has been shown that for very small grained specimens the elastic strain may be of the same order of magnitude as the plastic one at the macroyield. Most of the interesting length scale dependent phenomena are observed between the microscopic and the macroscopic yield stress. It is therefore inconsistent to compare measurements done for different values of the plastic strain, without carefully analyzing the elasto-plastic transition and its scale dependence.

By extracting the variation of the plastic strain rate from the measurement of the stress strain curve on thin films of various thicknesses, we have been able to evidence the large extent of microdeformation stage for tensile deformation of free standing thin films, as well as for films on substrates deformed by cyclic heating. It is shown by specific examples that the maximum plastic strain experienced by very fine grained materials, is too small to probe the whole sample. In this case, common concepts such as macroyield stress and strain hardening rate, used to represent plastic flow of standard polycrystals, are not relevant to describe the plastic deformation of nanograined polycrystals.

Specific constraints resulting from the imposed small length scale and of the shape of the specimens are discussed. An approximate criterion to determine the minimum extension of the microplastic stage will be given.

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Predicting Strain Hardening in FCC Crystals?

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ABSTRACT

Predicting strain hardening in single crystals is one of the earliest tasks assigned to dislocation theory, as a preliminary step for the investigation of polycrystal plasticity. Although the basic mechanisms governing hardening stages in single crystals are understood or identified, current models for the polycrystal are extensively based on parameter fitting. Thus, the initial objective has not yet been reached.

We present a multiscale model for single crystal plasticity, which is based on the storage-recovery framework and in which the number of free parameters is drastically reduced. It involves a constitutive formulation at the scale of slip systems, which is checked using 3D dislocation dynamics simulations. The critical part of the model involves two sets of equations. The Taylor relation is used in expanded form, taking into account the dimensionless average interaction strengths between slip systems in fcc crystals, as was done in [1]. The evolutionary law for the stored dislocation density is also expanded through the modeling of the dislocation mean free paths in each slip system. These mean free paths are found to exhibit an orientation dependence that is described in the early literature, but is systematically ignored in current models. The values of the nine dimensionless constants for fcc crystals involved in these evolutions were determined using dislocation dynamics simulations.

The orientation dependence of dynamic recovery is also modeled (after [3]), but one free parameter remains due to the present lack of atomistic input on the mechanism of mutual annihilation of screw dislocations by cross-slip. Finally, stage I is incorporated in this storage-recovery frame as discussed in [2].

The integration at the scale of the bulk material is performed using a crystal plasticity code, which computes the stress states and the lattice rotations in a model specimen. As an example, it is shown that one can recover in full detail the complex orientation dependence of the slip geometry and of the mechanical response in copper crystals at room temperature. Other potential applications and limitations of the proposed model will be discussed.

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Properties of Dislocation Microstructures during Deformation under Single Slip

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ABSTRACT

In the early stages of deformation under single slip condition, dislocations exhibit a pronounced tendency towards self-organization forming entanglements. The property of dislocations of a given slip system to spontaneously become obstacles to their own propagation was a substantial and unexpected outcome of the early Transmission Electron Microscope (TEM) explorations of the deformation of microstructures in relation with the plastic behaviour of materials. This property has been an object of constant attention ever since. It has received renewed interest with the development of computer simulation experiments and, more recently, with investigations of single crystal pillars. The scenario that accounts best for TEM observations relies on the sweeping of the prismatic loops by the mobile dislocations (Kratochvil et al), with most of the effort focused on the existence of a length scale. On the other hand, little is known about the origin and organization of the prismatic loops and the mechanism by which stable multipolar entanglements are formed. The present investigation concentrates on selected aspects related to self-organization under single slip in an effort to clarify its various constituents. The paper is organized as follows:

1. Some properties of dislocation contrast are revisited. It is shown that previously published dipole height measurements are at least doubtful in the small height limit, especially for dissociated dislocations.
2. Examples of TEM analyses of deformation microstructures are discussed in selected systems. The particular role played by dipolar configurations is emphasized. The model for the formation of loops and the further sweeping of these by mobile dislocations is confirmed experimentally by dislocation dynamics simulations. The mobility of prismatic loops along their prism cylinder is discussed based on atomistic structures determined by MD simulations.
3. Properties of dipoles are analyzed under isotropic and anisotropic elasticity in cubic systems. Several static properties are examined (e.g. the equilibrium angle and the dependence of this on dipole character and anisotropic elasticity). It is shown in addition that given a dipole height, the passing stress is maximum in the screw orientation. Implications on dislocation interactions under constrained deformation conditions, such as fatigue, are examined.

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Non-planar Dislocation Cores: A Ubiquitous Phenomenon

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ABSTRACT

Dislocation characteristics and behaviour in close-packed crystals, in particular FCC, have been habitually regarded as the paradigm of dislocation behaviour in all crystalline materials. An inherent hypothesis is that dislocation cores are planar, confined to the slip plane. This is also the basic assumption of the Peierls model and Nabarro's seminal study of the lattice friction stress, commonly called the Peierls stress. The merits and limitations of this model will be discussed first but the thrust of the contribution will be to demonstrate that it is common that for some orientations of the dislocation line the cores extend into several non-parallel crystal planes and these dislocations then control the plastic properties. The most widely recognised example is the screw dislocation in BCC metals. Hence, we present results of recent computer modelling of dislocations in transition BCC metals that reveal features such as dependence of the Peierls barrier on the applied stress tensor, leading to the significant influence of shear stresses perpendicular to the glide direction upon the plastic flow. We then show briefly that non-planar cores are encountered in hexagonal metals and many intermetallic compounds but present more details only for $L1_2$ compounds such as Ni_3Al or Pt_3Al. The general finding is that non-planar cores are the more significant the more complex and open is the crystal structure. Hence, non-planar dislocation cores are by no means limited to metallic materials but play an important role even in crystals made of organic molecules, such as, for example, the monoclinic anthracene.

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Modeling of Misfit and Threading Dislocations in Nanoscale Heterostructures

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ABSTRACT

The process of mechanical stress relaxation in lattice-mismatched epitaxial films usually proceeds via misfit dislocation (MD) formation on the film/substrate interface and is typically accompanied by the generation of a high density of threading dislocations (TDs) in the bulk of the film. In recent years there have been substantial experimental and theoretical efforts aimed at understanding the relaxation phenomena in thin films and nanomaterials, in order to reduce TD densities, in particular in III-V semiconductor compounds (for a short review see [1]). In this work, new approaches to modeling MD formation and TD reduction in nanoscale heterostructures are presented and discussed in detail.

First, it is proposed that the cross-hatch surface morphology of a growing film is directly connected with strain relaxation via dislocation nucleation and glide which results in both surface step and misfit dislocation formation [2]. This mechanism applies for materials with inclined slip planes, i.e. fcc films grown in a (001) orientation. Another specific stress relaxation mechanism is related to the inclination of TDs, which were initially normal to the film surface. This mechanism is present, for example, in GaN films with wurtzite crystal structure grown in a (0001) orientation [3].

It is argued that two fundamental issues in TD reduction include (i) the relative dislocation motion and (ii) the interactions between dislocations [4]. One type of TD motion is specific to non-relaxed (i.e. strained films) when a mobile TD produces a misfit dislocation diminishing the global stress in the film. The other type of effective TD motion takes place in growing relaxed films (buffer layers), when the point at which an inclined TD meets the film surface is laterally displaced as the film growth proceeds. The interactions among TDs are important; these being annihilation, fusion and scattering.

To characterize quantitatively the evolution of a TD ensemble, the 'interaction kinetics' equations for TD and MD densities were derived and analyzed both analytically and numerically for a set of typical film/substrate systems, i.e. epitaxial (001) growth of III-V compounds and (0001) GaN growth on sapphire, and for various conditions of the film growth [4-6].

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Dislocation Modelling of Martensitic Transformations

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ABSTRACT

For many years the cornerstone of our understanding of martensitic transformations has been based on the classical theory developed by Wechsler, Lieberman and Read [1], and Bowles and MacKenzie [2]. This model is a phenomenological treatment based on the hypothesis that the habit plane is an invariant plane of the shape transformation; it does not give physical insight into the transformation process. Recently, a dislocation model of martensitic transformations has been presented to address this shortcoming. In this model the habit plane is a semi-coherent structure containing an array of crystal slip (or twinning) dislocations and mobile disconnections (transformation dislocations), which accommodate coherency strains [3]. This model demonstrates that the interface is free of long-range strain, and accounts for the characteristic orientation relationship between the two phases. Moreover, the model demonstrates explicitly that the proposed transformation mechanism is diffusionless; lateral motion of the disconnections across the interface effects the transformation, and thereby produces the transformation displacement.

The predictions of the dislocation model are in excellent agreement with experimental observations using high-resolution transmission electron microscopy, and examples from ZrO_2, Ti alloys, PuGa and ferrous alloys will be illustrated. For the first two transformations, the classical model also gives good agreement, but is unsatisfactory for the latter two. The origin of these discrepancies will be elucidated in terms of the interface structures envisaged in the two approaches.

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New Experiments and Insights on Creep at Low Stress Levels

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ABSTRACT

Professor Frank Nabarro is well-recognized for his fundamental contributions to creep behavior at very low stress levels including his first proposal of the principles of Nabarro-Herring diffusional creep and his interpretation of Harper-Dorn creep through a mechanism incorporating the Peierls stress. Both of these creep processes occur at low stresses and both are usually characterized by a stress exponent equal to one. An important characteristic of the interpretation of Harper-Dorn creep is that it relies upon the presence of a dislocation density that is independent of the level of the applied stress. This paper describes recent experiments suggesting this assumption may be incorrect. Specifically, creep experiments were conducted using single crystals of high-purity aluminum at temperatures and stresses within the range where it is reasonable to anticipate the occurrence of Harper-Dorn creep. The results from these experiments suggest that, contrary to several earlier reports, the dislocation substructure is not independent of the applied stress and instead the network dislocation density varies with stress as a direct extension of the behavior anticipated within the conventional five-power creep regime. This paper describes these new results and addresses their significance in interpreting the flow behavior within the Harper-Dorn regime.

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Dislocations and Nanocracks in Nanocrystalline Metals and Ceramics

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ABSTRACT

A brief overview of research on dislocations and nanocracks (nanoscale cracks) in nanocrystalline metals and nanocomposite ceramic materials is presented. The key experimentally detected facts on the dislocation behavior and fracture processes at the nanoscale level are discussed. Special attention is paid to theoretical models describing the role of dislocations in plastic and superplastic deformation mechanisms, as well as nucleation and growth of nanocracks/nanovoids in nanocrystalline metals and nanocomposite ceramics. In particular, theoretical models are considered which describe conventional and specific mechanisms for nucleation of dislocations in nanomaterials. It is shown that perfect and partial lattice dislocations are effectively generatated at grain and interphase boundaries at very high stresses operating in nanocrystalline metals and nanocomposite ceramic materials. Besides, very high stresses are capable of causing the generation of dislocation loops by a nanoscale ideal shear in nanoscale grain interiors. Also, theoretical models are considered which describe conventional and specific mechanisms for nucleation of nanocracks in nanocrystalline metals and nanocomposite ceramic materials. The important role of interfacial sliding in initiation of nanocracks and their growth are discussed in detail. The sensitivity of brittle or ductile fracture modes to structural and material parameters of nanocrystalline metals and ceramics is considered. It is shown that nucleation and convergence of nanocracks cause the brittle fracture behavior of nanomaterials. At the same time, ductile fracture is carried by nanoscale voids whose growth is controlled by diffusion and plastic flow processes. Finally, we discuss the structural features capable to suppress/hamper fracture processes in nanocrystalline metals and nanocomposite ceramic materials and enhance their fracture toughness.

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Magnetoplastic Effect in Non-magnetic Crystals

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ABSTRACT

Magnetoplasticity in nonmagnetic crystals is a very peculiar phenomenon discovered in 1987 [1] and subsequently studied by many independent researchers [2-4]. The effect manifests itself in a remarkable change of the pinning force on dislocations from point defects under external magnetic field. This change is caused by an elimination of quantum exclusion of some electron transition in the system impurity-dislocation due to an evolution of a spin state in this system under a magnetic field. After the above transition, the configuration of the pinning center becomes completely different, and thus the pinning force changes as well. As a rule this leads to a softening of crystals. However, for some specific choice of doping, there are also known examples of strengthening. For instance, the hardening of NaCl(Pb) crystals in the magnetic field has been observed. Thus, the magnetoplastic effect provides a fairly rare example of a quantum phenomenon manifesting itself in crystal properties at room temperature.

Manifestations of the magnetoplastic effect were experimentally observed both in the mobility of individual dislocations and in such macro-plastic processes as active deformation ($\dot{\varepsilon}$ = const), active loading ($\dot{\sigma}$ = const), creep (σ =const), internal friction, microhardness, etc. The effect was observed in alkali halide crystals (NaCl, LiF, CsI, KCl), non-magnetic metals (Zn, Al), semiconductors (InSb, ZnS, Si) and some molecular crystals. In particular, it was found that dislocations in alkali halides and metals under a field $B \sim 1$ T in the absence of loads or any other external actions moved at macroscopic distances $l \sim 100$ mm. And the yield stress of NaCl(Ca) and LiF(Mg) crystals decreased 2-3 times under a magnetic field $B = 0.5$ T.

This work presents a short survey of main results obtained in this field. Dependencies of the mean free path l of dislocations on various physical parameters were studied, i.e on the induction B and time of magnetic treatment for different orientations of the magnetic field, on the temperature, on the type and concentration of impurities, etc. The threshold magnetic field B_c below which the effect is absent, the saturation field B_0 above which the mean free paths of dislocations remain unaltered by an increase in the magnetic induction B, and the critical frequency ν_c of rotation of a sample in a magnetic field, above which the effect disappears, were examined. The quantities B_c, B_0, and ν_c were investigated as functions of the basic physical parameters. It was found that magnetoplasticity is highly sensitive to low doses of X-ray radiation and to simultaneous action of an electric field or mechanical loading. Theoretical interpretations are proposed for all findings and dependencies observed. The interest of Frank Nabarro to the effect along with his clever questions have played an important role in our progress.

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Dislocation Avalanches and Fluctuation Characteristics of Plasticity on the Micron Scale

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ABSTRACT

The stress-strain curves of plastically deformed microcrystals display widely distributed jumps, in stark contrast with macroscopic samples where plasticity appears as a smooth process. This behavior is attributed to the collective avalanche dynamics of dislocations and may impose fundamental limits on the formability of crystalline solids on micro and nano scales.

We use three-dimensional simulations of the dynamics of interacting dislocation lines to clarify how sample size, slip geometry, cross-slip, and loading mode influence the characteristics of dislocation avalanches. The simulations demonstrate that dislocation avalanches are characterized by robust universal features (scaling exponents and functions) that do not depend on specific parameters of the dislocation dynamics or the experimental setup. Beyond demonstrating universality and reproducing quantitatively the statistical properties of deformation bursts as measured in experiment, we assess the implications of strain bursts for plastic forming processes. For sample dimensions on the micron and sub-micron scale, burst-like deformation is shown to impose fundamental limits on formability.

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Correlations in 3D Dynamical Dislocation Systems

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ABSTRACT

Metal deformation is carried at the lattice level by the motion of large numbers of lattice dislocations. The metallurgical models of deformation account only for the average dislocation behavior in crystals, while the continuum theory of plasticity completely discards dislocations in favor of continuum constitutive laws. These modeling approaches cannot capture the strong heterogeneity characterizing the collective behavior of dislocation systems. We address the question of collective dislocation dynamics in metals by the principles of statistical mechanics. A set of hierarchical kinetic equations governing the evolution of 3D dislocation systems have been developed, in which dislocations are represented in terms of phase densities for single dislocation segments, segment pairs, etc, in the space-velocity-line orientation phase space. This talk highlights this kinetic framework and focuses on the statistical basis for this type of modeling. Specifically, we present numerical simulation results of the spatial, orientation, velocity, and temporal statistics of dislocations, which are obtained by applying the concept of stochastic fiber process to the numerical data obtained using the Parallel Dislocation Simulation (ParaDiS) model. We demonstrate the anisotropic nature of dislocation line orientation distribution, the complex nature of dislocation correlations, and the anisotropy of dislocation flux in BCC crystals. We also demonstrate that dislocations are mainly correlated at short range, can be correlated or anti-correlated at intermediate range and anti-correlated at long range. In all cases, the dislocation correlation is highly oscillatory in the crystal and line orientation space, reflecting different types of dislocation structures which start to appear even at low strain levels. The theoretical method presented here and the results will be discussed in the context of development of mesoscale deformation theory based on first principles dislocation dynamics.

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The Role of Elastic Anharmonicity in Dislocation Patterning

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It is a long standing challenge of dislocation theory to understand the formation of different dislocation patterns. Over the past 50 years several different phenomenological theories were proposed to account for this self-organization phenomenon. Besides this, a vast amount of discrete dislocation dynamics simulations were performed both in 2D and 3D to identify the key dislocation phenomena responsible for pattern formation. In spite of these efforts there is no generally accepted model of dislocation structuring. It is likely that under different conditions (mode of deformation, crystal orientation, temperature, etc.) the patterning process is controlled by quite different elementary dislocation phenomena.

The simplest possible dislocation network develops in fcc single crystals oriented for single slip. According to TEM investigations up to a certain deformation level, the dislocation ensemble mainly consists of elongated edge dipoles in the easy glide plane. This dipolar character is especially dominant in fatigue. So, one would expect that under periodic external load a simple 2D edge dislocation system in single slip should arrange itself into the nearly periodic matrix structure or under certain circumstances into the ladder structure of PSB. However, there is no evidence obtained by discrete dislocation dynamic simulations performed in 2D that periodic dislocation structure forms. Moreover, 3D simulations were not clearly able to reproduce PSB formation. In our opinion this indicates that some basic physical phenomenon is missing from these computer simulations.

Recently, Nabarro and Brown[1] have suggested that the energy difference between dipoles with interstitial and vacancy types can play an important role in PSB formation. As it was realized by them in order to account for this energy difference one should go beyond linear elasticity. Allowing certain quadratic terms in the stress-strain relation they were numerically able to estimate the energy difference between the two types of dipoles. This energy difference can explain the extrusion characteristics of PSB.

In this paper we follow the approach proposed by Nabarro and Brown. Our goal is to show that even in 2D single slip, nonlinear effects may lead to the instability of the originally homogeneous dislocation state with growing perturbations in the dislocation density. It is found that a characteristic length scale proportional to the dislocation spacing is selected. At the first part of the paper a field theory of dislocations suitable to handle dislocations in a nonlinear medium is outlined. After this the extra dislocation-dislocation interaction term caused by elastic anharmonicity is calculated in first order perturbation. This results in an interaction energy difference between interstitial and vacancy types of dipoles. In contrast to the work of Nabarro and Brown, the extra energy term is calculated not only numerically but analytically. As a next step, by the generalization of the coarse graining method developed earlier[2], a continuum theory is derived from the equation of motion of individual dislocations. With this, the linear stability analysis of the homogeneous solution is carried out indicating the appearance of growing perturbations, i.e. tendency for dislocation patterning. Finally, results of discrete dislocation dynamics simulations are presented showing that the relaxed dislocation configurations are strongly influenced by anharmonicity.

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Hart's Constitutive Model for Cyclic Loading and Relaxation

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ABSTRACT

A review of Hart's model is provided that includes some recent modifications by him and others to incorporate transient and steady state phenomena (1-3). There has been an extensive amount of research in the development of a unified phenomenological model for the inelastic deformation response of metals under various temperatures and loading conditions. For a successful phenomenological model, three main conditions should be satisfied. First, it should cover important ranges of loading conditions and temperatures. Second, it should be micromechanically based –there should be a physical basis for the existence of dominant parameters of the state variable model. Third, it should contain the least number of state variables. A number of models have been presented on the basis of the existence of an athermal stress as an internal state variable [1]. Other models have been proposed based on other state variables like internal stress and hardness parameter (Hart's model). These models are investigated and modified through the years and the relation between the state variables and real physical parameters is discussed.

Hart's modified model includes large deformation processes and cyclic loading [2]. The model includes a new state variable as a "micro-hardness parameter" which represents the strength or the average lifetime of the mobile dislocations relative to the frictional glide viscous drag process. This state variable can also be used to incorporate transient phenomena and load relaxation. The results show that the model can predict the transient behavior for both cyclic loading and reloading phenomena during inelastic deformation and load relaxation. The latest attempts to incorporate the most important features of the model to some physical phenomena are also discussed within the framework of Hart's model, as it compares to recent model developments by Fred Kocks and others [3].

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An Internal Variable Approach for Structural Superplasticity

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ABSTRACT

An internal variable theory for inelastic deformation is proposed, that accounts for the essential microstructural changes during deformation. The framework of the theory is built on the basis of the well known dislocation dynamics approach. First, an internal strain tensor is introduced as the most fundamental deformation state variable, a concept first proposed by Hart. The plastic and inelastic strain rate tensors are then naturally defined together with a kinematics relation among them, by considering the time rate of change of this internal strain tensor, which in fact accounts for the microstructural evolution during inelastic deformation. The constitutive relations among the various stress variables and their conjugate deformation rate variables can then be derived based on the familiar dislocation kinetics. The theory is further extended to describe the superplastic deformation behavior, adopting the slip zone model with dislocation pile-ups as the major accommodation mechanism for grain/phase boundary sliding. The experimental results obtained from load relaxation tests of various crystalline materials are then presented and analyzed in relation to the internal variable theory for inelastic deformation. The various unresolved issues of structural superplasticity are clarified through this approach.

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An Internal State Variable Model of Micropolar Elasto-Vicoplasticity

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ABSTRACT

An internal state variable theory of micorpolar elasto-viscoplasticity is developed based upon the physics associated with dislocations and disclinations. Elastic-plastic kinematics are modified to include an additional rotational degree of freedom from which non-symmetric elastic and plastic strains and curvatures are defined. Dislocations and disclinations can then be easily identified in terms of the incompatibilities associated with the elastic deformation and elastic curvature. The state variables introduced are the nonsymmetric internal elastic strain and elastic curvature resulting from the presence of the dislocations and disclinations, as well as scalar measure of the elastic strain field associated with the statistically stored dislocations. The conjugate thermodynamic internal micro-stress and micro-moment are required to satisfy micro linear and angular momentum balances, while the macro stress (the derivative of the free energy with the respect to the macro elastic strain) satisfies standard linear and angular (symmetry of stress tensor) momentum balance laws. Expressions for the plastic velocity gradient and plastic curvature are proposed as well as an equation describing the evolution of the statistically stored dislocation density. The resulting expression describing the dissipation associated with the micro and macro stress fields follows naturally as a result of the second law, and the ramifications these restrictions on localized deformation is discussed.

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Measuring and Modeling Crystal Scale Stress States in Polycrystalline Metals

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ABSTRACT

Professor Ed Hart had an undeniable impact on the field of inelasticity and state variable modeling. His emphasis on coupling of physically-motivated models with careful experiments reinforces the idea that the "truth" lies somewhere in between. Consistent with Professor Hart's philosophy, this work describes an approach designed to understand the micromechanical state in deforming polycrystals using a crystal-based finite element modeling framework coupled with synchrotron x-ray diffraction experiments. Using a method motivated by quantitative texture analysis, lattice strain pole figure data from the in-situ loading / synchrotron x-ray experiments are used to calculate the lattice (elastic) strain tensor and the stress at every crystal orientation within the aggregate. The Cauchy stress is also evaluated with respect to lattice orientation using a finite element simulation based on an elasto-viscoplastic, restricted slip, constitutive model with multiple elements per crystal. Experimental results from copper specimens are compared directly to the simulation. In particular, the evolving crystal stress states (which can vary significantly from the macroscopically applied stress) are examined from the perspective of the single crystal yield surface. Together, the experiments and simulations are enabling us to understand the microscale stress-strain response of deforming polycrystals in a very fundamental way.

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Microstructural Modeling of Grain Subdivision and Large Strain Failure Modes in FCC Crystalline Materials

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ABSTRACT

The major objective of this work is to develop a unified physically-based representation of the microstructure in fcc crystalline materials to investigate finite inelastic deformation and failure modes and scenarios at different physical scales that occur due to a myriad of factors, such as texture, grain size and shape, grain subdivision, heterogeneous microstructures, and grain boundary misorientations and distributions. The microstructurally-based formulation for inelastic deformation is based on coupling a multiple-slip crystal plasticity formulation to three distinct dislocation densities, which pertain to statistically stored dislocations (SSDs), geometrically necessary dislocations (GNDs), and grain boundary dislocations (GBDs). This dislocation-density-based multiple-slip crystal plasticity formulation is then coupled to specialized finite-element methods to predict the scale-dependent microstructural behavior, the evolving heterogeneous microstructure, and the localized phenomena that may contribute to failure initiation for large inelastic strains. The evolution of these dislocation densities is used to predict and understand how crystallographic and noncrystallographic microstructures relate to intragranular and intergranular deformation patterns and behavior. Furthermore, a clear understanding of how GB strength changes due to microstructural evolution is obtained as a function of microstructural heterogeneities that occur at different physical scales.

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Experiments and Modelling of Mechanical Properties of SPD Nanocrystalline Materials

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ABSTRACT

Compared to classical routes to achieve nanocrystalline metals (NM), that of Severe Plastic Deformation (SPD) provides nanostructures which exhibit additional advanced properties, i.e. considerable ductility at still enhanced strength, and phase existencies under conditions where they usually do not occur [1, 2]. All these phenomena can be explained with the extended hydrostatic pressure being present during SPD, as well as the high concentrations of lattice defects far exceeding those of classical routes of achieving NM [3, 4]. For the description of hardening characteristics, an upper bound-type composite model is presented which operates in separate terms of edge and screw dislocations, and which takes into account different effects of hydrostatic pressure, especially that of suppression of diffusion providing an increased density of edge dislocations and a higher one of vacancy type defects, as it has been found by experiment [3, 4]. The model also well describes the measured decrease of grain size and grain wall thickness as a function of strain as well as of hydrostatic pressure [5]. While also other concepts recently succeeded in predicting the evolution of strength and microstructure of SPD nanomaterials [6], the reason for enhanced ductility is still under dispute [7]. One possibility is to analyze the problem in terms of Hart's instability criterion [8], essentially considering the instantaneous strain rate sensitivity which can reach very high values in case of NM and particularly in those processed by SPD.

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Ronald Rivlin and Invariant Theory

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ABSTRACT

In a series of papers published between 1948 and 1952 entitled 'Large elastic deformations of isotropic elastic materials', Rivlin [1] established the basis of the modern theory of finite elasticity and thus initiated several decades of remarkable advances in nonlinear continuum mechanics. In paper IV of this series he explicitly stated that the strain-energy function of an isotropic elastic solid can be expressed as a function of the three strain invariants of a deformation tensor, and consequently was able to solve several non-trivial problems for isotropic incompressible elastic materials. Also in the 1940s, Reiner and Rivlin independently observed that the Cayley-Hamilton Theorem could be used to formulate explicit constitutive equations for a class of non-Newtonian fluids in which the stress depends on the rate-of-deformation.

Classical matrix theory suffices when the stress depends on a single kinematic variable, but many materials have more complex behavior. Rivlin and Ericksen derived properly invariant higher-order kinematic tensors and formulated the invariance requirements for when the stress depends on several kinematic tensors. To obtain explicit results in this case required additional mathematical apparatus, which was provided by Rivlin and others, using methods based on Rivlin's generalization of the Cayley-Hamilton theorem and other matrix identities. They also showed how dependence on vectors as well as tensors can be included. These methods have subsequently been sharpened and refined by many authors, and the theory of tensor representations is now an extensive and well-developed theory that lies at the centre of non-linear continuum mechanics.

Rivlin and colleagues also systematically considered the invariance issues in the formulation of constitutive equations for various classes of anisotropic materials, and derived canonical forms for the elastic strain-energy function for all the principal types of anisotropy. In particular, his methods have been extensively applied to the mechanics of fibre-reinforced composite materials, by the introduction of a *fibre vector field* that characterizes the fibre direction.

In conclusion, we outline recent applications of invariant theory to multi-scale effects in the mechanics of fibre-reinforced materials, in which the constitutive variables include spacial derivatives of the fibre vector as well as the fibre vector itself.

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Objectivity in Solid and Fluid Mechanics

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ABSTRACT

Objectivity can be stated as a requirement of properly formulated invariance, either under a change of frame of reference or under a superposed rigid body motion, for the analytical representation of constitutive relations in both solid and fluid mechanics. The introduction of structure tensors elucidated in the best possible way the importance of representation theorems by Wang (1970), Smith(1971), Boehler(1979), Liu(1982), Zheng and Spencer(1993), to mention only a few, with the omission of Rivlin's numerous contributions on the subject within finite Elasticity. In what it appears to be his very last publication, however, Rivlin (2006) has shown again his interest in the important issue of frame indifference in regards to the kinetic theory of gases that bears consequences on the issue of turbulence modeling.

The effect of objectivity and resulting invariance requirements on plasticity theory will be succinctly presented, focusing on the concept of the Plastic Spin (Dafalias, 1985), consistency condition and the involvement of 4th order tensor-valued evolving internal variables, where some newly derived identities due to invariance will be presented. The issue of violation of objectivity and the inappropriateness of using the intrinsic spin in turbulence modeling will be the second aspect of this presentation (Dafalias and Younis, 2007) with a brief reference to the last work of Rivlin (2006).

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Pressure Measurement in Viscoelastic Fluids

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ABSTRACT

Pressure measurements in flows of highly viscous and elastic fluids are of practical importance in many manufacturing processes. Problems may arise during such pressure measurements, since high fluid viscosity and elasticity result in excessive dynamic response time of the pressure measuring systems as well as in some distortion. This is true for systems that consist of manometers as well as pressure transducers. In this work we develop an analytical model for the pressure pulse transmission in columns of viscoelastic fluids leading to pressure transducers. Basic equations are derived and analytical solutions are illustrated for a square wave pulse. Predictions of the model can be utilized to interpret correctly pressure transducer readings in fluid systems exhibiting viscoelastic behavior.

In addition, we develop a numerical model which predicts the advance of viscoelastic fluids in manometer columns used for the pressure measurement of such fluids. Basic equations are derived and solutions are obtained for the viscous case (zero order) and the linearized viscoelastic case (first order) using an expansion in terms of Weissenberg number based on the manometric time scale of the system. Both time independent and fluctuating pressures are considered.

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Second-Order Torsion due to the Rotation of an Embedded Rigid Spheroidal Inclusion

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ABSTRACT

The second-order theory of elasticity has been applied to examine the mechanics of hyperelastic materials that undergo moderately large strains. The theory was developed as a method of successive approximations for the solution of the finite elasticity problem by a number of researchers including Signorini, Stoppelli, Rivlin, Misicu, Green, Grioli, Sheng and others and extensive reviews of the topic are given by Rivlin [1], Reiner and Abir [2], Green and Adkins [3] and Truesdell and Noll [4]. The theory has been applied to a variety of problems of technological interest, involving the mechanics of rubber-like elastic materials and the seminal work of Rivlin [5] on the second-order torsion problem is considered a landmark in the development of modern non-linear elasticity. The methods available for the solution of problems in second-order elasticity are many and varied and details of these methods can be found in the references cited. The use of a *displacement function* for the solution of problems in second-order elasticity for an incompressible material was first proposed by Spencer [6], who noted that the formulation in terms of a displacement function gives rise to inhomogeneous partial differential equations for the displacement function and the isotropic pressure, governed respectively, by Stokes' operator and Laplace's operator. This paper discusses the formulation of a class of second-order torsion problems where the state of deformation is always axisymmetric. In particular, attention is focused on the application of a displacement function approach to the solution of the problem of the rotation of a *spheroidal rigid inclusion* embedded in bonded contact with an incompressible elastic solid of infinite extent. The formulation in terms of spheroidal coordinates yields *exact closed form solutions* for the second-order problem.

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Corner Instabilities in a Slender Elastic Cylinder: Analytical Solutions and Formation Mechanism

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ABSTRACT

Stabilities and instabilities are important topics in finite elasticity and structures. Here, we study one kind of instability, the corner instability. Such an instability is widespread. For example, if one compresses a block of sponge, the post-buckling state will have a profile with a corner. This instability was also found experimentally in a sufficiently short thick-walled elastic tube subject to compression, which is known as the Willis' instability phenomenon. As far as we know, there is no analytical study on this kind of instability, and the reason is probably that mathematically this is a very difficult problem: one needs to study the bifurcations of complicated nonlinear PDE's and show that the bifurcations lead to "non-smooth" solutions. Here, we shall present a novel approach to tackle the challenging problem of the corner formation in an elastic cylinder under compression and reveal the mechanism of its formation. Through a method of compound series-asymptotic expansions, we manage to derive a singular dynamical system (the vector field has a singularity at one point) together with boundary conditions to model this type of problems. We then carry out a phase-plane analysis for this system. It turns out that there is a vertical singular line, which causes a variety of bifurcation phenomena. In particular, a non-smooth solution with a discontinuity in the first-order derivative can arise, which represents the formation of a corner. From the analytical results obtained, we reveal that it is the interaction of the material nonlinearity and geometrical size which causes the formation of a corner.

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Analytical Derivation of Cosserat Moduli via Homogenization of Heterogeneous Elastic Materials

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ABSTRACT

Why do experiments detect Cosserat-elastic effects for porous, but not for stiff-particle-reinforced materials? Does homogenisation of a heterogeneous Cauchy-elastic material lead to micropolar (Cosserat) effects, and if so, is this true for every type of heterogeneity? Can homogenisation determine micropolar elastic constants? If so, is the homogeneous (effective) Cosserat material determined this way a more accurate representation of composite material response than the usual effective Cauchy material? Direct answers to these questions are provided in this paper for both two and three dimensional deformations, wherein we derive closed-form formulae for Cosserat moduli via homogenisation of a dilute suspension of elastic spherical inclusions in 3D (and circular cylindrical inclusions in 2D) embedded in an isotropic elastic matrix. It is shown that the characteristic length for a homogeneous Cosserat material that best mimics the heterogeneous Cauchy material can be derived (resulting in surprisingly simple formulae) when the inclusions are less stiff than the matrix, but when these are equal to or stiffer than the matrix, Cosserat effects are shown to be excluded. These analytical results explain published experimental findings, correct, resolve and extend prior contradictory theoretical (mainly numerical and limited to two dimensional deformations) investigations, and provide both a general methodology and specific results for the determination of simple higher-order homogeneous effective materials that more accurately represent heterogeneous material response under general loading conditions. In particular, it is shown that no standard (Cauchy) homogenized material can accurately represent the response of a heterogeneous material subjected to a uniform plus a linearly-varying applied traction, while a homogenized Cosserat material *can* do so (when inclusions are less stiff than the matrix).

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Statistical Mechanics of Non-thermal Structures and Materials

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ABSTRACT

When a random structure is loaded by far-field stresses, the elements inside will not be subject to the same forces because of structural inhomogeneities. Such a system represents an interesting analog to a thermal system at equilibrium – the structural irregularities qualify for a description by a Shannon-like entropy, and there is also the usual (e.g. elastic) strain energy. When an entropy is related to energy, one immediately steps into the familiar field of statistical mechanics, but for a strained random structure the real (Kelvin) temperature plays no role. Instead, an effective temperature which measures the relative importance of entropy versus energy exists, but this is not the Kelvin temperature because the entropy here is non-thermal. The proper statistical mechanics framework that should be used to describe such systems is therefore non-thermal.

Using low-density elastic networks as prototype systems, this work reviews recent computer simulation and experimental results that support such a non-thermal statistical mechanics framework. These results show the existence of an effective temperature in the description of these structures. As further examples, the discontinuous, jumpy flow behavior of materials observed during nanoindentation experiments, and the dynamic formation of dislocation patterns during plastic deformation or annealing of crystals are also discussed within the same statistical mechanics framework.

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Generalized Continua and Applications to the Mechanics of Heterogeneous Materials

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ABSTRACT

A unifying thermomechanical constitutive framework for generalized continua including additional degrees of freedom or/and the second gradient of displacement is presented. Based on the analysis of the dissipation, state laws, flow rules and evolution equations are proposed for Cosserat, strain gradient and micromorphic continua. The case of the gradient internal variable approach is also incorporated by regarding the nonlocal internal variable as an actual additional degree of freedom.

The consistency of the continuum thermodynamical framework is ensured by the introduction of a viscoplastic pseudo-potential of dissipation, thus extending the classical class of so-called standard material models to generalized continua.

Variants of the higher order and higher grade theories are also reported based on the explicit introduction of the plastic strain tensor as an additional degree of freedom. Within this new class of models, called here *gradient of strain* models, one recognizes the fact that, in a second grade theory for instance, the plastic part of the strain gradient can be identified with the gradient of plastic strain. Finally, formulations at finite deformation of the proposed models are provided focusing on proper decompositions of the Cosserat curvature, strain gradient and gradient of micromorphic deformation into elastic and viscoplastic parts.

A systematic procedure is then proposed to deduce the values of the additional material parameters implied by the use of higher order continua, from the microstructure of heterogeneous materials. A computational approach is developed to determine the higher order elastic moduli of Cosserat and micromorphic media according to [3,4].

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Configurational Forces at Boundaries Revisited: Impact of Surface and Line Tension in Nanoscale Materials

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The response and failure of micro- or nano-structured materials is dominated by the (internal) boundaries, e.g. by the grain boundaries within polycrystals. Configurational mechanics is concerned with changes of the material configuration of continuum bodies, i.e. with configurational changes. Thereby, configurational changes are due to the kinetics of all kinds of defects like e.g. vacancies or inclusions, cracks, interfaces or phase boundaries and the like. The defect kinetics is in turn due to so-called configurational forces. All the above cases can essentially be treated by considering the configurational changes at boundaries of continuum bodies or of their subparts. The aim of this particular contribution is to variationally derive the (quasi-static) balances of momentum and the associated stresses and forces at (external and internal) boundaries within configurational mechanics. Thereby, in particular effects of boundaries' potentials are taken into account. By doing so, the intriguing duality of deformational and configurational mechanics is revealed as a by-product. Among the motivations for this work, i.e. to consider boundary potentials, are the following observations: **(i)** Inspired by an atomistic/molecular picture of materials, which is of particular relevance in the realm of nanomechanics, it is obvious that the boundary of a continuum body (or an interface between subparts of a continuum body) displays different properties as compared to its bulk. This phenomenon is usually modelled in terms of boundary (surface) tension. The notion of a scalar valued boundary tension can be generalized to a boundary stress of tensorial nature. For a conservative case, the boundary stress derives from a boundary potential that depends on the boundary deformation gradient (quite like in the case of elastic membranes and strings). In addition, the boundary potential might depend on the surface normal or curve tangent to capture anisotropies. Typical applications of boundary free energy can be found in the field of nanomechanics. The effect of boundary stress within configurational mechanics is thus of particular interest when it comes to the assessment of defects at the nanoscale. **(ii)** In materials processing, the boundary of materials is frequently exposed to oxidation, ageing, grit blasting, plasma jet treatment etc., thus resulting in distinctively different properties in comparatively thin boundary layers. Likewise, coating materials with thin films results clearly in different properties at the boundaries. These effects could phenomenologically be modelled in terms of boundaries equipped with their own potential energy (free energy in a thermomechanical setting). **(iii)** Boundary tractions are frequently assumed to be conservative, thus in this case they can be derived from an external boundary potential that depends on the deformation. Clearly, in order to realistically describe the possibilities for mechanical loading of a continuum body, boundary tractions are of eminent importance. Nevertheless, since the consideration of boundary potentials or boundary tractions within a configurational mechanics setting poses severe difficulties due to the need to consider the geometry and kinematics of configurational changes of the boundaries, boundary potentials are often simply not considered in this context. Thus the application of configurational mechanics to realistic problems is often somewhat restricted if boundary tractions can not easily be taken into account.

As a conclusion, the case of boundary traction and boundary stress (as a tensorial generalisation of boundary tension) will be treated within the same framework. Thus, within deformational mechanics, in addition to potentials in the bulk (external and internal), boundary potentials depending in the most general case on the deformation, the boundary deformation gradient and the spatial surface normal or curve tangent with possible parametrisation in the material placement and the material surface normal or curve tangent have to be considered. For the case of configurational mechanics the role of fields and parametrisation will simply be reversed, whereby dissipational configurational forces have to be considered. This will be the basic set up for the presented developments.

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Mechanical Behavior Analysis of Polymers Based on Molecular Chain Network Model

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ABSTRACT

A computational procedure for analyzing deformation and fracture behavior of solid polymers is developed based on a molecular chain model. In the model, the polymer solid is represented by a network of non-linear elastic chains. Van der Waals forces and viscous forces acting on the chains are taken into account and are approximated to act at the node points of the network. The stiffness equation is derived by employing the principle of virtual work, in which geometrical non-linearities due to large deformations are considered. The chain slippage and the chain session are also taken into consideration. A cellular automaton modeling is introduced to generate the network of polymer chains. Several computational results are given, including tensile and compressive characteristics of polymers due to the difference of molecular weight and degradation under UV irradiation.

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Autonomous Self-Oscillating Gel in a Stationary Environment

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ABSTRACT

Gels consist of a cross-linked three-dimensional polymer network embedded in a fluid phase, which may be a pure fluid or a mixture of chemical species. These soft materials therefore present rigidity properties that are characteristic of both solid and liquid states. A well-known property of gels is their swelling-shrinking phase transition in response to a wide variety of stimuli such as temperature or pH modifications, the imposition of an electric field, the irradiation by light etc. Their capacity to significantly vary the amount of fluid phase they contain make them suitable for a wide range of applications: actuators, drug delivery devices, valves for fluidic systems, etc. [1].

We are especially interested in the volume response to chemical stimuli resulting from chemical reactions taking place in the fluid part, while sometimes involving the polymer matrix as well. Quite recently, some forms of autonomous property were endowed to develop self-oscillating gels. This was realized by allowing a chemical reaction, the concentrations of which vary periodically in time, to take place inside gels sensitive to their chemical environment [2-6]. In these experiments, that could eventually lead to novel biomimetic intelligent materials exhibiting rhythmical action, the volume changes are nevertheless slaved to the chemical oscillations.

We have, on the contrary, studied the mechano-chemical dynamics of a spherical bead of gel immersed in an autocatalytic bistable chemical reaction [7]. We show that such a sphere may exhibit autonomous volume self-oscillatory dynamics although neither the gel alone, nor the chemical reaction ever shows oscillatory behavior [see also 8]. This emergent property thus arises in a time independent environment. Our description is based on a multi-diffusive hydrodynamic theory of gels [9, 10], leading to the incorporation of viscoelastic effects in the reaction-diffusion equations [11].

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Nanomechanics of Biocompatible Microbubbles using Atomic Force Microscopy

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ABSTRACT

Microbubbles (MB) are micrometer-sized biocompatible spheres consisting of an ultra thin shell (10s of nm) encapsulating an inert gas. They are primarily used as ultrasound contrast agents to improve the visualisation of vascularity and differentiate vascular patterns of tumours non-invasively[1]. Furthermore, they have shown potential as carriers of drugs/genes for targeted drug/gene delivery. The most important obstacle in the development of the MB technology in the biomedical field remains the lack of understanding of the behaviour of individual MBs which has been compromised by the lack of experimental data. A thorough scientific knowledge of these properties would lead to their optimal use as contrast agents. To date, the mathematical modelling of MB behaviour still has limited predictive value, primarily due to a lack of reliable methods for establishing the mechanical properties of the MB shell. Models either assumed a fixed behaviour for the shell properties or used a best fit to experimental data. Atomic force microscopy[2] (AFM) provides the means to investigate the micro/nanomechanical properties of individual MBs in a direct manner.

In the present study, we used AFM tipless cantilevers and force distance nanocompression testing to measure the mechanical properties of polymeric MBs. We performed a systematic study using several cantilevers. All the force-vs-separation curves show a linear part which was associated with an effective MB stiffness, k_{eff}. We found that using relatively soft cantilevers ($k_c \leq 0.12$ N/m) the total force was not large enough to bend the stiff MB shell. Using cantilevers with $k_c \geq 0.60$ N/m we found that the k_{eff} of the MBs decreased with size showing that smaller MBs are stiffer. Applying a simple model[3,4] for the deformability of the spherical shell, the Young's modulus, E, was estimated. The values were in good agreement with the values provided by the manufacturers only for the larger microbubbles. For high applied forces, we observed mechanical instabilities which (at least in some cases) may be associated with permanent deformation and shell cracking.

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