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Material issues in nuclear applications and the role of physics-based models

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Keywords: multi-scale modelling, physics-based modelling, failure mechanisms, accelerated tests, irradiation damage, creep, fatigue, stress-corrosion cracking, degradation mechanisms, nuclear safety

Structural and functional components in future reactors will be exposed to a very harsh environment in terms of irradiation damage, high temperature and environmental impact from the coolant medium. Moreover nuclear reactor components must satisfy very high safety requirements and the design life will be at least 60 years. The design and construction of the planned demonstrators and prototypes in the next decade will be based on exiting materials such as austenitic (e.g. 316LN) and FM (ferritic/martensitic) steels [e.g. P91 (9Cr-1MoVNb)] that need to be qualified and tested for the relevant conditions. In the longer term new materials such as oxide-dispersion strengthened steels and ceramics and composites are needed to fully take account of the full potential of the future reactors. It is not possible to simulate the true operational conditions in the laboratory because of the very long time scales in for instance creep or because we simply cannot simulate the harsh conditions fully as for the very high irradiation levels. It is therefore necessary to extrapolate data from accelerated tests or from less harsh conditions. Such extrapolation requires that we understand the basic physical mechanisms and degradation modes that span several length and size scales. One example is irradiation damage where high energy neutrons introduce point defects such as vacancies and interstitials resulting in for instance hardening and loss of ductility of the material at the component scale. Models at different length scales starting from ab-initio, molecular dynamics, dislocation dynamics and crystal plasticity have been developed but we are still a long way from having true multi-scale models that link several scales. Another example is creep-fatigue where austenitic steels have cyclic hardening whereas ferritic martensitic steels are characterized by cyclic softening. This cyclic softening is believed to be caused by coarsening of the subgrains and may lead to a significant reduction in the creep-fatigue life. A third example is liquid-metal embrittlement in liquid lead alloys that seem to affect steels with a BCC structure much more than steels with a FCC structure. The presentation will give a brief overview of different materials issues for nuclear reactors that are investigated in European nuclear materials research programmes and where physics-based models and multi-scale models could be a very important tool for more accurate assessments of component behaviour and design of materials with improved properties.

Modeling of localization and microstructure evolution in metallic materials

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Keywords: Localization, strain gradient crystal plasticity, dislocation microstructure, non-convexity

Plastic deformation and its possible combination with other loadings (thermal, irradiation etc.) induce various types of dislocation microstructure evolution, which eventually result in a spatially heterogeneous deformation field. Different type of dislocation microstructures exist in metallic materials at different length scales. Typical examples at macro scale are Lüders bands, Portevin-Le Chatelier (PLC) bands, while dislocation cell structures, labyrinth, mosaic, fence or carpet structures develop at meso scale, which are mainly due to self-organization of dislocations.

The plastic localization induces macroscopic softening-hardening and stress-plateau type of responses, arising numerical issues in the solution procedure. The application of standard finite element methods yields mesh-dependent post-critical results due to loss of ellipticity of the incremental boundary value problem. In order to remedy these problems during the formation of microstructures several models have been proposed including, methods using calculus of variations in an incremental setting, non-local methods, viscous regularization techniques and Cosserat theories. A complete understanding of models which can simulate the patterning of dislocation slip or formation of dislocation substructures is not at hand. In order to contribute to this, inspired by the success of phase field models, an approach is proposed to illustrate the ability of non-convex field models to predict the emergence and evolution of dislocation slip microstructures in a rate dependent strain gradient crystal plasticity framework (see e.g. Yalcinkaya et al. [2011] and Yalcinkaya et al. [2012]).

The framework studies the plastic slip patterning in a system with energetic hardening. Both the displacement and the plastic slip are considered as primary variables. These fields are determined on a global level by solving simultaneously the linear momentum balance and slip evolution equation which is derived from thermodynamical considerations. The slip law used in this context differs from the classical ones in the sense that it includes the non-convex free energy term leading to the patterning of this field. The non- convexity is treated as an intrinsic property of the free energy of the material. The numerical examples illustrate the microstructure evolution due to different types of non-convex contributions in a multi-slip 2D plane strain analysis.

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Porosity Evolution in Ni-based Single Crystals under Creep Loading Conditions

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Single crystal Ni-based superalloys were introduced in the early 1980s and since then have been widely used in turbine airfoils in jet engines. The desire for weight reduction and the use of advanced metal cooling schemes tends to drive designs toward thinner airfoil walls. Creep tests on Ni-based superalloy specimens have shown greater creep strain rates and/or reduced creep rupture times for thinner specimens than is predicted by current theories. This is termed the thickness debit effect. To investigate the mechanism of the thickness debit effect, isothermal, constant nominal stress creep tests were performed on uncoated PWA1484 Ni-based single crystal superalloy sheet specimens with two thicknesses and under two test conditions: 760 deg. C/758MPa and 982 deg. C/248MPa. The specimens contained initial micro-voids formed during the solidification and homogenization processes. The experiments showed that porosity evolution could play a significant role in the thickness debit effect. This motivated basic mechanics studies of porosity evolution in single crystals subject to creep loading. Three-dimensional finite deformation finite element analyses of unit cells containing a single initially spherical void were carried out for various values of stress triaxiality and various values of the Lode parameter. At low values of the stress triaxiality, well separated voids can collapse into crack-like or needle-like shapes. On the other hand, if the voids are sufficiently close the voids can coalesce. Depending on void spacing, there is a transition between void collapse and void coalescence.

Nano-scale modelling of sliding contact

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While for a long time considered a traditional discipline of Mechanical Engineering, Contact Mechanics is prone to exciting developments. The study of Contact Mechanics at nanoscales, i.e. nanotribology, needs to fully account for adhesive forces, third body interactions and deformation mechanisms at contacting asperities. Understanding these factors as well as evolutions in the morphology of contact areas has the potential of explaining the origin of frictional forces and wear. This fundamental understanding is needed to guide us in the design of tailored-made lubricants and surface morphologies.

Be they at the macroscopic or nano scale, tribological problems are particularly difficult to comprehend. Different physical mechanisms (which include the environment, plastic deformation, third body interactions, phase transformations, recrystallisation) interact at disparate length scales. It is therefore not surprising that contact sciences have been primarily driven by careful experimental investigations. Nonetheless, as experiments go down in size and as computational power expands, numerical simulations become increasingly relevant to experimental work.

We begin the presentation with simulation results at the continuum scale. Finite-element calculations are conducted for normal and sliding contact of rough metallic solids. The surfaces are modelled with self-affine fractals. We discuss the dependence between applied load and the real contact area, for both elastic and elasto-plastic solids. We conclude this part by highlighting the limitations of a purely continuum approach in order to represent size effects. In the second part of the presentation, we review key atomistic (MD) simulations results from the literature. We also discuss the limitations of atomistic modeling through a scratch test of alumium. Our calculations reveal that our MD simulation window (limited in space and time) is unable to resolve the plastic clusters that develop under the indenter. This motivates the development of a multiscale framework, in which MD is directly coupled to continuum modeling. We present our latest efforts in this direction and conclude with 3D simulation results of deformable rough on rough sliding. We correlate the measured friction coefficient to surface roughness and discuss the evolution of atomic scale roughness with sliding distance.

First-principles Predictions of Solute Strengthening in Al and Mg alloys

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Alloys containing substitutional solutes exhibit strengthening due to favorable solute fluctuations within the alloy that hinder dislocation motion. Here, a quantitative, parameter free model to predict the flow stress as a function of temperature and strain rate of such alloys is presented. The model builds on analytic concepts developed by Labusch but introduces key innovations rectifying shortcomings of previous models. To accurately describe the solute/dislocation interaction energies in and around the dislocation core, density functional theory and a flexible-boundary-condition method are used. The model then predicts the zero temperature flow stress and the energy barrier for dislocation motion. Standard thermal activation theory then leads to the prediction of finite temperature flow stresses and to consistency with the ``stress equivalency'' postulate of Basinski. The model is used to predict the flow stresses of various Al alloys. Excellent results are obtained for Al-Mg and Al-Mn. Al-Fe with ppm levels of Fe is not predicted well but, using experimental results for Fe, results for the quasi-binary Al-Cr-(Fe) and Al-Cu-(Fe) alloys agree well with experiments. The model is then used to predict basal strengthening in Mg-Al. The broader core of the dissociated basal edge in Mg relative to the edge in fcc Al leads to the existence of two energy minima and thus, ultimately, a transition from flow controlled by short-range solutes to flow controlled by long-range solutes with increasing temperature. Parameter-free predictions of the finite-T flow stress are in good agreement with experiments over a wide range of temperature. Overall, this parameter-free model using first-principles input thus provides a basis for achieving the long-sought goal of computational design of alloys, within the context of solute-strengthening mechanisms.

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The role of elastic anisotropy, length scale and crystallographic slip in fatigue crack nucleation

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Fatigue crack nucleation in polycrystal ferritic steel is investigated through experimental observation of multiple large-grained, notched, four-point bend tests combined with explicit microstructural representation of the same samples using crystal plasticity finite element techniques in order to assess fatigue indicator parameters together with the roles of elastic anisotropy and length scale effects in slip development and hence in crack nucleation.

Elastic anisotropy has been demonstrated to play a pivotal role in the distribution and magnitude of polycrystal slip relative to observed crack nucleation site in the context of constrained cyclic microplasticity. Length scale effects were found not to alter substantively the distributions or magnitudes of slip relative to observed crack nucleation site, but in detailed analyses of an experimental sample, the location of highest magnitude of geometrically necessary dislocations was found to coincide precisely with the position of predicted peak plasticity and the experimentally observed crack nucleation site.

The distributions of microplasticity within polycrystyal samples were found to change quite significantly between first yield and after multiple cycles. The changes in location of peak plastic strain and accumulated crystallographic slip with cycling can be profound and need to be considered when appraising fatigue indicator parameters. In addition, effective plastic strain per cycle was, as a result, found to be a better indicator of fatigue crack nucleation than peak effective plastic strain. In nine independently tested and analysed polycrystal samples, cyclic effective plastic strain and crystallographic system peak accumulated slip were found to be good indicators of fatigue crack nucleation site, but not of subsequent (micro-structurally short) crack growth path.

Formulation of thermodynamic mean-field models for dislocation transport at finite deformation

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Keywords: dislocation line segment model, dislocation transport, phase field model

The purpose of the current work is the formulation of evolution-field relations for dislocation transport in the context of crystal plasticity and their use in the formulation of continuum thermodynamic phase-field models for the energetics and kinetics of collective dislocation motion at finite deformation.

The formulation is based on a mobile dislocation line segment model for the evolution of the state of inelastic local deformation and corresponding local dislocation distribution in the crystal as a whole. In the sense that this model can also represent the effect of dislocation climb on these states, it represents a generalization of the usual dislocation-glide / glide-system-based model. In the model, the states of inelastic local deformation and dislocation distribution are determined in

particular by the (area number) density and flux of (mobile) dislocation line segments. Besides a dependence of the evolution of the density on the corresponding flux, these relations imply that finite deformation results in an additional supply of excess dislocations transported from other glide systems onto the dislocation line in question, something which is missed in the infinitesimal case.

The general model formulation is applied in the current work in particular to the case of an idealized dislocation loop consisting of straight edge and screw segments (e.g., Kords et al., 2012). When restricted to infinitesimal deformation, a single glide system and purely edge dislocations, the resulting transport relations reduce to those formulated by Groma et al. (2007, 2010) on the basis of considerations from statistical mechanics.

In the last part of the work, the transport relations obtained in the first part are used to formulate a continuum thermodynamic phase-field model for dislocation transport (e.g., Groma et al., 2010) by analogy with the case of mass transport in multicomponent systems (e.g., Cahn and Hilliard, 1958; de Groot and Mazur, 1962). Indeed, since additional field relations are involved, the Cahn-Hilliard approach or ”model B” in condensed matter physics (e.g., Hohenberg and Halperin, 1977) is relevant. On this basis, a Cahn-Hilliard relation for the density is derived.

In addition, the dislocation flux is determined by the Peach-Köhler force as well as flow and back stresses. In particular, the latter contains a ”diffusion” due to a gradient in the ”chemical” potential derived from the density dependence of the free energy.

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Multiscale modeling applied to structural nuclear materials

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The development of models to describe the behaviour of materials subjected to neutron irradiation is an important branch of nuclear materials science, in connection with both present-day and future nuclear reactors. Many approaches can be adopted, but in recent times the one denoted as 'multiscale modeling' gained special importance. This approach is based on the recognition that the behavior of materials is ultimately the consequence of how the atoms composing them are arranged and redistribute themselves due to external events (arrival of high energy particles in case of irradiation): different distributions correspond to different responses and properties. Depending on the scale at which we observe the material, as well as on the phenomena we are interested in, it is practical to give specific names to specific atomic distributions: cavities, precipitates, dislocations, grains and their boundaries, aggregates of grains, parts of components. Likewise, it is practical to describe what happens in the material in terms of how these specific distributions of atoms evolve under the action of external events. In this way, different length scales are identified and specific physical processes turn out to be best described and understood at a defined scale. Moreover, some physical processes are extremely fast (they last less than a picosecond), while others may take years. The fundamental idea of the multiscale modeling approach is hence that each physical process determining the behavior of materials should be investigated and modeled at the most suitable length- and time-scale, using the most adequate description (specific distributions of atoms) and the most specific experimental or modeling technique for that purpose. The global response of the material will be eventually best described, on physical bases, by conveniently linking the descriptions given for the different scales.

In this presentation the multiscale nature of irradiation effects on materials will be illustrated while introducing the fundamental physical processes driving them. Tools used to model these physical processes, generally based on the extensive use of computer simulation, will be very briefly overviewed. The main challenges to be faced to achieve the goal of developing reliable models, meeting both scientific requirements and industrial expectations, within the appropriate timeframe, will be summarized.

Multi-scale dynamics of twinning processes

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Twinning is a shear dominated material transition which plays a significant role in metal plasticity, geological processes, and actuation of shape memory alloys (SMA) and ferroelectric materials. Physics based models of the twinning transformation must start from the level of a discrete twin boundary, in a similar manner to the Dislocation Dynamics approach. In particular, a quantitative knowledge of the barriers for twin boundary motion, the mechanisms for overcoming them and the kinetic relations of these mechanisms (i.e. the rate or velocity of the process as a function of the thermodynamic driving force) are required. In this work we employ combined theoretical and experimental approaches for studying the twinning processes at the microscopic scale of discrete twins.

First, we present a theoretical description of the main twinning sub-processes and show that they are all governed by several atomistic and mesoscale properties of the twin boundary. Sidewise twin wall motion is identified as the rate limiting sub-process of the overall twinning transformation, and its kinetics is analyzed in detail. Our theoretical analysis predicts that sidewise twin motion follows thermally activated (fatigue like) kinetics at low driving force values and viscous type kinetics at higher driving force values. The transition between the two kinetic behaviors is associated with overcoming the Peierls energy barrier of the periodic lattice potential.

Next, we present a unique experimental study of the twinning dynamics in the ferromagnetic shape memory alloy NiMnGa. Sidewise velocities of twin boundaries are calculated based on the distance a boundary pass during the application of a tunable magnetic pulse with almost rectangular shape. The measured velocities are plotted as a function of the driving force to obtain an experimental kinetic relation.

The formulated kinetic relations are validated experimentally, leading to quantitative extraction of all governing material parameters. In particular, nanoscale properties, such as the Peierls lattice barrier and the energy of twinning dislocations are obtained. In addition, long-scale (several tens of μm) barriers for twin boundary motion are quantitatively evaluated based on analysis of quasistatic stress-strain curves by means of a new bi-stable chain model.

Finally, it is shown how the overall obtained information can be used for modeling the frequency response of NiMnGa actuators. In addition, we discuss the importance of the obtained information for the development of improved FSMA crystals for fast magnetically induced actuation applications.

Multiscale modeling of nanocrystalline metals based on competing grain boundary and grain interior deformation mechanisms

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Polycrystals with nano-sized grains show distinct deformation mechanisms when com- pared to coarse-grained polycrystals, e.g. very high strength, tension/compression asymmetry, enhanced rate sensitivity and inverse Hall-Petch effect. Around grain sizes of 10-100 nm the dominant inelastic deformation mechanism changes from traditional dislocation mediated bulk plasticity to grain boundary processes, i.e., sliding of grains, atomic shuffling, grain boundary diffusion and generation of dislocations and void growth at grain boundaries. Hence, a predictive constitutive model of nanocrystalline metals for grain sizes in the transition range should consider both competing mechanisms to capture the physics correctly.

We present a variational based multiscale plasticity model which considers the nanocrystalline material as a two phase composite consisting of a grain interior phase and a grain boundary affected zone. An isotropic porous plasticity model is employed to describe the grain boundary affected zone, whereas a grain size dependent dislocation-mediated crystal- plasticity model is used for the plasticity of the grain core regions. The behavior of the polycrystal is then described by a conventional Taylor-type averaging scheme with a lognormal grain size distribution. We demonstrate the model capabilities through comparisons against various experiments.

Microstructural modeling of heterogeneous failure modes in martensitic steels

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Keywords: Martenstic Materials, dislocation-densities, High-Strength Steels

A three-dimensional multiple-slip dislocation-density-based crystalline formulation, specialized finite-element formulations, predictive failure models, and infinity-power integrable function based Voronoi tessellations adapted to martensitic orientations, were used to investigate large strain inelastic deformation, dislocation-density evolution in martensitic transformation, and heterogeneous failure modes in martensitic microstructures. The formulation is based on accounting for variant morphologies and orientations, secondary phases, such as retained austenite and inclusions, and initial dislocations-densities that are uniquely inherent to martensitic microstructures. The computational framework and the constitutive formulation were validated with experimental results for 10% Ni high-strength steel alloy. Furthermore, the formulation was used to investigate microstructures mapped directly from SEM/EBSD images of martensitic steel alloys.

The interrelated effects of microstructural characteristics, such as parent austenite orientation, variants distribution and arrangement, retained austenite, inclusions, initial dislocation-density, and defects, such as microcracks, and microvoids, were investigated for different failure modes such as rupture, transgranular and intergranular fracture, and shear localization over a broad spectrum of loading conditions that range from quasi-static to high strain-rate conditions.

Ab initio molecular dynamics study on the effects of mechanical strain on the chemical reactions of W+CO and Ti+H2

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Keywords: Ti, W, adsorption, desorption, disassociation, ab initio molecular dynamics, mechanical strain, binding energy

The purpose of this work is to assess the effect of mechanical strain on the binding energies of two systems, tungsten (W) and carbon monoxide (CO), and titanium (Ti) and hydrogen (H2), using an ab initio approach. Results of the research work during the past decade indicate that the effect of certain types of mechanical strain alters the adsorption process. The subject of the binding energy of hydrogen on Ti with strains is of significant amount of interest in explaining the hydrogen storage capabilities for fuel cell applications. The current work is performed to determine a strain state with high binding energy for hydrogen input and storage, and then to explore the change of strain condition that reduces the binding energy for easy release of hydrogen for combustion in fuel cells. An investigation of the adsorption of gasses such as carbon monoxide (CO) on Tungsten is of interest because of the possibility to synthesize alternate or synthetic fuel technology by Fischer-Tropsch process. The present calculations are performed using VASP and CPMD atomistic modules on 2x2 and 4x4 HCP Ti slabs in (0001) crystallographic orientation, and on 2x2 an 4x4 BCC W slabs in both (100) and (111) orientation. First the convergence within a range of cutoff energies and K-points is investigated. From the possible adsorption sites for gas molecules on the surface of the two metals, the “top” site is chosen for a representative study. The variation of the binding energy of the two systems with strain is then evaluated at a range of volumetric strains (v/v 0) from 0.98 to 1.15. From the preliminary calculations, the binding energy changes with strain. It is possible to increase the binding energy with compressive strain and reduce the binding energy with tensile strain.

Crack propagation and arrest peculiarities in steels at transient loading

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Keywords: crack propagation, Charpy specimen, stress relaxation, pulsed magnetic field, fracture surface.

Currently, one of the urgent problems of the nuclear industry is the life-time extension of nuclear power plants (NPP) reactor pressure vessel (RPV). Various numerical and experimental techniques of analyzing the behavior of cracks at transient loading are being designed and improved due to the search for additional life-time reserves. Recently, a small-scaled specimen testing has been developed. It provides more information about crack propagation and arrest peculiarities.

In the G.S.Pisarenko Institute for Problems of Strength (IPS) the experimental techniques for investigation of the crack propagation and arrest in the Charpy specimen and in the disk-shaped specimen subjected to a transient thermo loading was developed. The studies were carried out on specimens of steel 45 and RPV steel 15Kh2NMFA. Using special disruptive strain gauges and high-speed digital recording system (with a sampling rate 20 MHz), the rate of change of the crack propagation in steels with different types of loading was recorded. Numerical simulation of disk-shaped and Charpy specimen tests using finite element analyses (FEA) combined with the local damage model of Gurson-Tvergaard-Nidlman (GTN) [1,2] was performed. According to special technic, GTN parameters were determined from the results of independent tension tests of smooth specimens and impact bending tests of Charpy specimens. A good agreement between the numerical and experimental results was obtained.

Currently, the study on the effect of pulsed electromagnetic fields (PEMF) treatment to increase fracture resistance of structural elements with cracks is one of the most interesting and promising areas of research.

a b

Fig. 1: Fragments of the panoramas of fracture, a – the original image, b - the result of fractograph segmentation algorithm processing.

IPS has developed an experimental technique for PEMF treatment of object with cracks and tests. The results illustrate stress relaxation in a vicinity of the crack due to the treatment under action of PEMF. Unlike the earlier works [3-4], using FEA it was shown experimentally and numerically that an increase in fracture resistance is not associated with the thermal effects of current.

To analyze the specimen fracture surface, the quantitative analysis with segmentation algorithm of raster images of panoramas fracture technique was developed. With this technique quantitative parameters, which characterize the change in the structure during the propagation of cracks, were established (Fig. 1).

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Constitutive model for cyclic deformation response of AISI 316L based on relationships between internal stress and dislocation microstructure

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Significant changes in dislocation densities and configurations during fatigue loading make AISI 316L exhibit a complex cyclic deformation response (i.e. cyclic hardening followed by cyclic softening and finally an almost stabilised cyclic response or secondary cyclic hardening response phase before failure). Strong short-range interactions between dislocations and point defects at 300°C result in more notable primary cyclic hardening, and also secondary cyclic hardening.

In order to understand this complex cyclic response, the microstructural features responsible for internal stresses (e.g. effective stress, and inter-granular and intra-granular back stresses) have been exhaustively studied. Inter-granular back stress due to the long-range interaction of dislocations arises from imposed plastic deformation as a consequence of grain-to-grain strain incompatibility. This back stress evolves first with dislocation distribution, and then with grain fragmentation. The activity of secondary slip (including cross slip) during cyclic loading on the one hand relieves the inter-granular back stress, but on the other hand raises the intra-granular back stress due to the formation of dislocation-high/low-density regions. Back stresses are mainly responsible for the cyclic deformation response at high strain amplitudes where dislocations tend to move more quickly in a wavy manner. In contrast, effective stress, coupling with short-range dislocation interactions, plays a much less significant role on the material cyclic response for wavy slip conditions, but increasingly becomes more important for planar slip conditions. The additionally strong short-range dislocation interaction at 300°C, initially with solute atoms, and later in life with corduroy structure, however induces a significant increase in effective stress, leading to its more influential role on the material cyclic response.

The presentation will describe how the understanding obtained provides a basis for the development of a physically-based evolutionary constitutive model which aims to accurately represent the complex cyclic deformation response of the material. The developed constitutive model reflects the change in microstructural condition and its relationship with internal stress variables. The model parameters are identified by systematic evaluations of mechanical and microstructural observations from a number of interrupted fatigue tests for a single set of test condition. The capability of the model is then verified by predicting the material cyclic response for different testing conditions. The verification evaluation shows that the proposed model (1) accurately describes the history dependence of the material cyclic deformation behaviour, and (2) well predicts the long-term cyclic deformation response for test conditions different to those originally adopted from the results of relatively short term mechanical testing.

Hardening models in multilevel models of inelastic deformation based on crystal plasticity

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The correct description of the hardening is an essential problem for the description of plastic deformation, allowing us to get results in numerical experiments which well correspond with natural experiments; on the other hand, it is laid down in the hardening laws a description of the material microstructure and patterns of its evolution.

In the construction of meso level's constitutive relations is essential that these relations contain in itself (except for the constants of the material), only variable meso or macro level, so as not to complicate the procedure for identification and verification of the model and to avoid the closure problem. There are two variants of such relations: in the first case we should introduce the operators on the history of deformation without using variables that describe the evolution of meso and microstructure of the material. In the second case explicitly introduced the parameters that describe the evolution of meso and microstructure and constitutive relations are constructed in these terms. If the goal of of research is a transparent accounting physics of interaction between the carriers of plastic deformation mechanisms, including the evolution of the microstructure, the second approach is preferable, and allows simplifying the mathematical relationships.

Hardening is split into "nonoriented" and "oriented". The first type describes the hardening regardless of the direction of deformation (formation of dislocation intersections, ropes, braids, Lomer - Cottrell barriers etc), and a hardening leads to an increase in critical shear stress on many slip systems (or all at once). The second type is associated with the accumulation of elastic energy on the "pursed dislocations" (the various barriers); this energy can be (fully or partially) released at the reversal the direction of deformation. The second type can be described by the kinematic hardening (residual microstresses), or due to simultaneous changes in critical shear stress at the opposite slip systems.

By using the formalism of constitutive models with internal variables and two-level mathematical model of inelastic deformation of polycrystals based on the elastoviscoplastic crystal plasticity theory, received both general and particular form of hardening laws of mono and polycrystals, allowing to describe some well-known effects, such as the Bauschinger effect, the formation and destruction of dislocation barriers, as well as additional hardening resulting from the interaction of intragranular and grain boundary dislocations.

The analysis is completed of the interaction mechanisms of the plastic deformation carriers and lattice defects that are essential to solve the problem, hardening laws are constructed, showing good agreement with experimental data. The effects of complex cyclic loading, accompanied by the emergence and destruction of dislocation barriers of various types.

Problem of constructing images of the loading processes in the stresses and strains spaces is considered, shows the effect of hardening laws parameters on the material memory, estimates of the trace delay vector and scalar properties, depending on the ratio of the latent-deformation hardening.

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Modeling of transients as a response to changes in strain path of commercially pure aluminum

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Changes in the strain path are inherently involved in metal forming operations. Metals typically show transient behavior of the stress upon the sudden or continuous change in deformation conditions. Unexpected softening due to the strain path changes can have impact on forming due to the flow localization, leading to necking, eventually fracture. Hence, there is a need to accurately predict mechanical behavior of metals due to the changes in strain paths. Continuum phenomenological model proposed by Holmedal [1] has been implemented into hypoelastic-plastic formulation with an isotropic high-exponent yield criterion. This model has also been extended by introducing possibility to model transient work hardening which can occur during strain-path change. Eventually, such model was applied to capture transient response of as-cast CP aluminium after strain path changes introduced by sequence of rolling and subsequent uniaxial tension at various angles in order to cover large range of strain-path changes often occurred in sheet forming operations.

Degradation of carbon steels after long-term ageing

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The characteristics of nucleation and development of fatigue cracks under high-cycle loading of smooth specimens from low-carbon steel after its natural ageing for 15 years were studied [1]. The method of replicas was used to study the multiple and the localized fatigue fracture process. The replicas were taken from the lateral surface of specimens at different stages of loading, up to fracture. Cumulative distributions of the number of microcracks with respect to their length were plotted and the fracture microrelief was studied.

It was found that the fatigue strength of the aged steel decreases considerably in the high-cycle region (>10E7 cycles) in comparison with the fatigue strength of the steel in initial state. An analysis of the cumulative distributions of microcracks at different stages of multiple fatigue fracture showed that they are described well by an exponential relationship with a factor which decreases with a growing number of cycles. The development of numerous delaminations on interphase boundaries was observed on the lateral and fracture surfaces of the specimens. They served as microcrack nucleation sites and probably were the prevailing mechanism by which carbon steels fail after long-term natural ageing. It was shown that the curve of the ultrasound attenuation coefficient as a function of the number of loading cycles reflects the main regions of fatigue curve corresponding to different fatigue fracture mechanisms. An analysis of the tension data showed that the ageing of low carbon steel led to increase in both the yield and ultimate strength.

Studying fatigue characteristics and fracture mechanisms of medium carbon steel after its natural ageing for 50 years [2] confirmed the above mentioned results obtained for the low carbon steel. The comprehensive study of the multiple and the localized fatigue fracture of two naturally aged carbon steels under cyclic loading in a wide range of cycles allowed supposing that decrease in fatigue strength in gigacycle fatigue is connected to microstructural changes of material in process of its ageing during long-term exploitation.

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Climb Enabled Discrete Dislocation Plasticity of Particle Reinforced Composites

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With the exception of single crystals, all metals inherently deform non-homogeneously in the plastic regime since the constituents of the microstructure does not slip with equal ease. The gradients of plastic deformation originate because of compatibility and require the storage of geometrically necessary dislocations contributing to the overall strain hardening. This gives rise to a plastic response depending on the relevant microstructural length scale of the material.

In this study we investigate the plasticity size effects in particle reinforced metal matrix composites. We use a planar climb enabled discrete dislocation plasticity framework to study the plastic deformation and evolving dislocation structure in composites while changing particle size, reinforcement morphology and climb mobility. In the light of this systematic parametric study, we predict and explore the high temperature deformation mechanisms in composites in comparison with the glide only deformation mode common at room temperature.

We consider a doubly periodic unit cell subjected to simple shear in order to model an infinitely large composite. The matrix is an elastic/plastic single crystal with dislocation nucleation and movement takes place on the slip systems. The matrix/particle interface is impenetrable to dislocation motion and hence particles containing no dislocation source only deform elastically.

Our simulation results revealed that a distinct size effect is seen for glide only deformation with smaller being harder while size effects are less pronounced upon increasing the climb mobility. For the highest climb mobility considered, there seems to be a weak reverse size effect such that smallest particles are giving a slightly softer response. We show that this is due to i) absence of pile-ups and thus the increase in the amount of plastic slip and ii) dislocation climb motion create/annihilate vacancies which triggers a vacancy diffusion and hence a mass transport inside the material in climb enabled simulations. The reinforcement morphology has a negligible effect on the plastic hardening behaviour for glide only deformation mode whereas in climb assisted glide a softer response is attained upon reducing the overlap between the reinforcing particles while keeping their volume fraction fixed.

Physics based modelling of high temperature mechanical behaviour of tool steels

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Passenger cars are responsible for about 12% of EU CO2 emissions. Many efforts have been made to improve the fuel efficiency as well as the CO2-emmission of automotive engines. Another approach to this target is the light-weight design concept. Meanwhile traditional steel sheet structures are substituted with large size die casted light metals components in order to reduce the overall weight of the car body. High casting temperatures to completely fill the large dies cause very high thermal loads on the die. "Hot work tool steels" with a chromium content of about 5 m% are frequently used as tool materials for light metal die casting. Surface temperatures can exceed 40% of the melting temperatures of the die material where creep dominant failure may occur. Concerning the service conditions, hot work tool steels have to combine not only good creep resistance but also high hot strength, wear resistance, as well as high cyclic temperature resistance.

Existing physically based models for prediction of mechanical behaviour of metals at elevated temperatures (hot strength, creep) require knowledge of several microstructure parameters like volume fraction of carbides, mean size of carbides etc. which have to be experimentally determined. Numerous microstructure parameters that have to be determined with high experimental efforts restrict the practical applicability of these models. An alternative approach is to simulate the thermal history of the metals in order to achieve the desired parameters. Here, the physically-based microstructure simulation software MatCalc can be utilized, which proves to give quite precise results for steels with similar chemical composition.

In this study, compression tests at elevated temperatures are carried out to determine the hot-strength of the tool steel. Moreover, similar compression tests for various stress levels are conducted to determine the long term mechanical behaviour. Complementary heat treatment simulation of hot work tool steel is conducted by Matcalc in order to achieve the microstructure parameters like mean size of carbides, volume fractions and concentrations of alloying elements in matrix. The microstructure simulation is coupled with the physics-based models to predict the high temperature mechanical behaviour and results are compared with the experiments. This approach can be implemented to all kinds of hot work tool steels to predict the mechanical performance at elevated temperatures with decreasing the experimental efforts drastically.

Grain-level in-situ observations on deformation twinning

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This is two part talk. Firstly, the use of high-energy synchrotron X-rays to investigate the formation and stress evolution of tensile twins in individual Mg grains is presented. In-situ measurements are performed under compressive load where sample rotations in each step allow recording of diffraction spots from most atomistic planes of targeted grains. Analysis of these spots allows identification of individual grains through their orientation and yields their strain tensor. It is crucial to note that these grains are investigated in the bulk, in their native environment. The results show a dramatic jump in the stress state of a material region that goes under deformation twinning.

Secondly, a university lab technique, digital image correlation at the microscopic scale, will be presented as part of an ongoing study that considers the identical material system and loading schemes. These experiments are at a disadvantage in comparison to the mentioned high-end methods being surface measurements that yield no direct result on the stress tensor, yet their strength lies in statistics. Further, in principle, these methods can yield a distribution of deformation inside a grain. Preliminary results will be presented from this study that bears on the resolution limit of optical light microscopy.

Blunting and brittle cleavage of a crack in BCC and FCC metals: atomistic modeling vs. theoretical estimations

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The behaviour of crack propagation and blunting at different loading rates, temperature and crack geometry in bcc-Fe, W and fcc-Ni, Cu has been studied by molecular dynamics under load mode I. Large scale atomistic simulations coupled with a special analysis have been performed to reveal conditions at which dislocations can be emitted from a semi-infinite crack in both FCC and BCC metals.

In FCC metals the crack tip is blunted by the plastic deformation due to the nucleation and emission of dislocations. This process, however, occurs in a different manner in Ni and Cu. It can be concluded that the formation of stacking faults and twins at crack tip is particularly important for brittle cleavage. In BCC crystals the crack was found to open without plastic deformation, however, the strain work hardening has a significant dependence on temperature. The critical stress intensity factor for brittle cleavage or dislocation emission was calculated from the stress tensor measured on atoms located at the crack tip. The obtained results are discussed and compared with predictions of elasticity theory.

A criterion for the onset of void coalescence under combined tension and shear

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Keywords: ductility, fracture mechanisms, voids and inclusions, finite elements, limit-load analysis

Depending on the relative positions of voids and on the loading conditions, shear loading components can play an important role in the void coalescence process leading to ductile fracture. Yet, most void coalescence criteria including the original criterion of Thomason, and its various extensions/improvements, take only normal loads into account and neglect the contribution from shear loads to coalescence. Shear can affect both the stress/strain at the onset of coalescence and the direction of deformation localization. In this paper, first, the predictive capabilities of different coalescence criteria without shear effect are critically assessed and the expressions involved in the original Thomason criterion are fine-tuned by comparing with 3D finite element calculations performed on a unit cell containing a spheroidal void. Then, the improved Thomason criterion is theoretically extended — by using limit load analysis — to incorporate the effect of shear. The predictions of this new coalescence criterion are in good agreement with the results produced by 3D finite element calculations, for both loadings involving or not a shear component.

Identification of Plasticity parameters for models of ductile damage of nuclear facilities

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Introduction

The plastic strain represents one of the most crucial parts in the process of ductile damage. If the damage additionally affects plastic behavior of the material then we can talk about the so called tied continual damage model. In this case it is necessary to calibrate dependence of actual yield stress on accumulated intensity of the plastic strain $\sigma_Y^{True}(\varepsilon_{\ln}^{pl})$.

Method of plastic model calibration

The basic experimental ground for finding this dependence mostly uses the uniaxial tensile test on smooth samples. With this method we can determine $\sigma_Y^{True}(\varepsilon_{\ln}^{pl})$ until the sample is locally strangled. In this paper the function of $\sigma_Y^{True}(\varepsilon_{\ln}^{pl})$ has two parts. The first one, which is valid until the plastic strangling, is formed by values of true stresses and plastic strains that were computed directly from the experimental data. The second part of the dependence $\sigma_Y^{True}(\varepsilon_{\ln}^{pl})$ is replaced by convenient approximate function, which is chosen to meet the condition of tangential connection in the place of plastic strain during the strangling. The parameters of the approximation function are identified by iterative process. Therefore an optimizing script in Python was developed, which is started directly in the Abaqus software. The calibration is based on a simplex algorithm of local optimization. This algorithm makes effective optimization of several parameters in the same time.

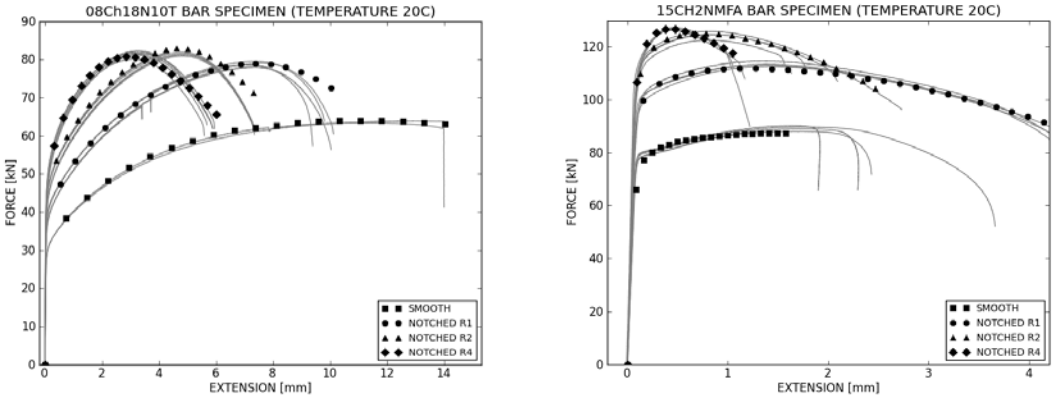

Fig.1: Comparison of the FE simulation of tensile samples with experiments

Conclusion

This paper describes the method of the calibration of the plastic part of a curve that performs an important aspect of ductile damage models. Basically two different ways of approximation of the dependence on actual yield stress and accumulated intensity of the plastic strain were defined and an effective method for their identification was designed. Identification of the independent parameters of the models is processed iteratively using an optimizing script that was developed as a part of this project. The calibration is largely corresponding with the experimental results as we can see in the Fig. 1. Our future work in the field of plasticity will be focused on the plasticity models that consider the third invariant of the deviation stress tensor and hydrostatic pressure.

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Effects of surface energy on evolution of a nanovoid in a plastic material

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Keywords: nanovoid; surface tension; finite plastic deformation; size effect; void growth; tension-compression asymmetry; pre-history yielding; intrinsic loading-unloading process

Surface effects, represented in terms of surface tension/energy, are important on the nanometer scale. Within the framework of static finite deformations, this study provides a theoretical analysis of the evolution of a nanovoid in a plastic material by considering surface effects. Based on the previous studies, this investigation accounts for the following additional factors: (1) the initial configuration is considered to be obtained by applying the surface tension onto a fictitious stress-free configuration; (2) the response under compressive hydrostatic stress is discussed as well as the tensile case. This illustrative solution provides a reasonable physical background for the following phenomena: (1) when the void size is under some critical value, finite plastic flow arises in the process from the fictitious stress-free configuration to the initial configuration, and will dramatically influence the subsequent responses; (2) the growth of nanovoids is strongly related to their sizes; (3) the tension-compression asymmetry becomes easy to understand when surface tension is included; (4) void shrinkage instability is predicted.

Homogenization-based Scale Transitions in Finite Deformation Thermomechanics

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Homogenization-based scale transitions for nonlinear purely mechanical or thermal problems exist, together with the treatment of the coupled problem in the linearized setting. However, there appears to be no consensus over how to approach the multiscale problem in the finite deformation setting with finite deviations from the equilibrium temperature. In this presentation, two different approaches will be discussed to motivate a homogenization framework that induces optimal computational efficiency, beginning with the setting of finite thermoelasticity.

First, an approach is developed on the appropriate identifications of the macroscopic density, internal energy, entropy and thermal dissipation. Thermodynamical consistency that ensures standard thermoelasticity relationships among various macroscopic quantities is invoked through the explicit enforcement of the macroscopic temperature for all evaluations of temperature dependent microscale functionals. This enforcement induces a theoretical split of the accompanying micromechanical boundary value problem into two phases where a mechanical phase imposes the macroscopic deformation and temperature on a test sample while a subsequent purely thermal phase on the resulting deformed configuration imposes the macroscopic temperature gradient. In addition to consistently recovering standard scale transition criteria within this framework, a supplementary dissipation criterion is proposed based on alternative identifications for the macroscopic temperature gradient and heat flux. In order to complete the macroscale implementation of the overall homogenization methodology, methods of determining the constitutive tangents associated with the primary macroscopic variables are discussed. Aspects of the developed framework are demonstrated by numerical investigations on model microstructures.

As the second approach, an asymptotic expansion analysis will be carried out. The treatment naturally enforces a separation of scales, thereby inducing a first-order homogenization framework that is suitable for computational implementation. Within this framework two microscopically uncoupled cell problems are again automatically recovered, where a purely mechanical one is followed by a purely thermal one. The results are in agreement with the first approach based on the explicit enforcement of the macroscopic temperature, thereby ensuring thermodynamic consistency across the scales. Numerical investigations additionally demonstrate the computational efficiency of the two-phase homogenization framework in characterizing deformation-induced thermal anisotropy as well as its theoretical advantages in avoiding spurious size effects.

Overall, the developed approach constitutes a first step towards incorporating inelastic thermomechanical effects across multiple scales and developing frameworks that can capture size effects. This microscopically decoupled analysis framework appears to be suitable for scale transitions in nonlinear multifield interface problems as well, including elastohydrodynamic lubrication and thermomechanical contact problems.

Modeling of fatigue fracture of thin finite plates with cracks based on continuum damage mechanics

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The problem of modeling of fatigue cracks growth (FCG) in thin finite isotropic plates is discussed. The finite plate with central crack is subjected to uniaxial fully reversed high-cycle loading applied perpendicular to the crack at the external boundary. The crack surfaces are considered to be entirely free from applied stresses and contact interaction of crack surfaces is not allowed for. The plates made of perfectly plastic materials are considered so the stress distribution in the vicinity of the crack tip is satisfied to crack-closure model [1] in cyclic loading which is based on modified Dugdale model.

Fatigue fracture of the plate is examined as a two-stage process of damage accumulation involving the incubation stage and the crack propagation stage. Damage accumulation is considered as "driving force" for the fatigue crack propagating. The modeling is based on the introduction of the same for both stages of the scalar parameter of damage ω as the function of the coordinate x and the number of loading cycles n. On conditions that during the incubation stage $0 \le n \le n_*$ the material of the plate is damaged but not fractured in the sense of the fracture front initiation and motion, the damage parameter equals to 0 in undamaged material and the condition that the damage parameter equals to 1 is taken as the criterion of the fatigue fracture front initiation and movement. The integral equation of the motion front of the crack is given in the following form:

$$\int_0^1 \left[1-\omega(x,n)\right]^q d\omega = D\left[\int_0^{n_*} \left[\Delta\sigma_{yy}(x,n)\right]^q dn + \int_{n_*}^{n} \left[\Delta\sigma_{yy}(x,n)\right]^q dn\right]$$

where

$$\Delta\sigma_{yy}(x,n) = \frac{\sigma_a}{\sqrt{2}}\left[\frac{\ell(n)}{x+\lambda(\ell(n))-\ell(n)}\right]^{1/2} \cdot f\left(H/W, \ell(n)/W\right)$$

$\Delta\sigma_{yy}(x,n)$ – stress state near the fatigue crack tip, $\lambda(l)$ – length of the cyclic plastic zone, $f\left(H/W, \ell(n)/W\right)$ – correction function which takes into account the effect of boundary conditions.

The values of the constants D and q specify the fatigue damage accumulation process and are determined by use of experimental data in the form of the Wohler curve which is obtained as a result of standard fatigue tests of smooth cylindrical specimens under uniaxial alternating stresses. From the equation (1) we can determine the value of damage parameter at any moment of time.

Taking into account that at the fracture front the proposed analytical solution of integral equation (1) is given in the following form:

$$\begin{cases} \dfrac{dl}{dn} = \left(1+\dfrac{1}{q}\right) D \dfrac{1}{\left[2\lambda(l)\right]^{\frac{q}{2}-1}} \times \left(\sigma_a \sqrt{l}\right)^q \times f\left(H/W, l/W\right)^q, \\ n_* = \dfrac{1}{(1+q)D}\left[\dfrac{1}{\sigma_a}\right]^q \left[\dfrac{2\lambda(l_0)}{l_0}\right]^{\frac{q}{2}} \times f\left(H/W, l_0/W\right)^{-q}. \end{cases}$$

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Abstract

This report covers the book of abstracts of the 1st International Workshop on Physics Based Modeling of Material Properties and Experimental Observations. The workshop is organized in the context of European Commission's Enlargement and Integration Action, by the Joint Research Centre in collaboration with the Middle East Technical University on 22nd – 23rd October 2012 in Ankara. The abstracts of 7 keynote lectures and 19 technical presentations are included in the book. The purpose of the meeting is to discuss the current state of the art of physics based modeling of materials and associated experimental techniques. Such approaches allow a better understanding of the degradation mechanisms and the link between the microstructure and material behavior which is necessary for the extrapolation of data beyond operational experience and for the assessment of component integrity subjected to harsh environment and long term operation.

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