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3rd International Workshop on Physics-based Models and Experimental Verification

Book of abstracts

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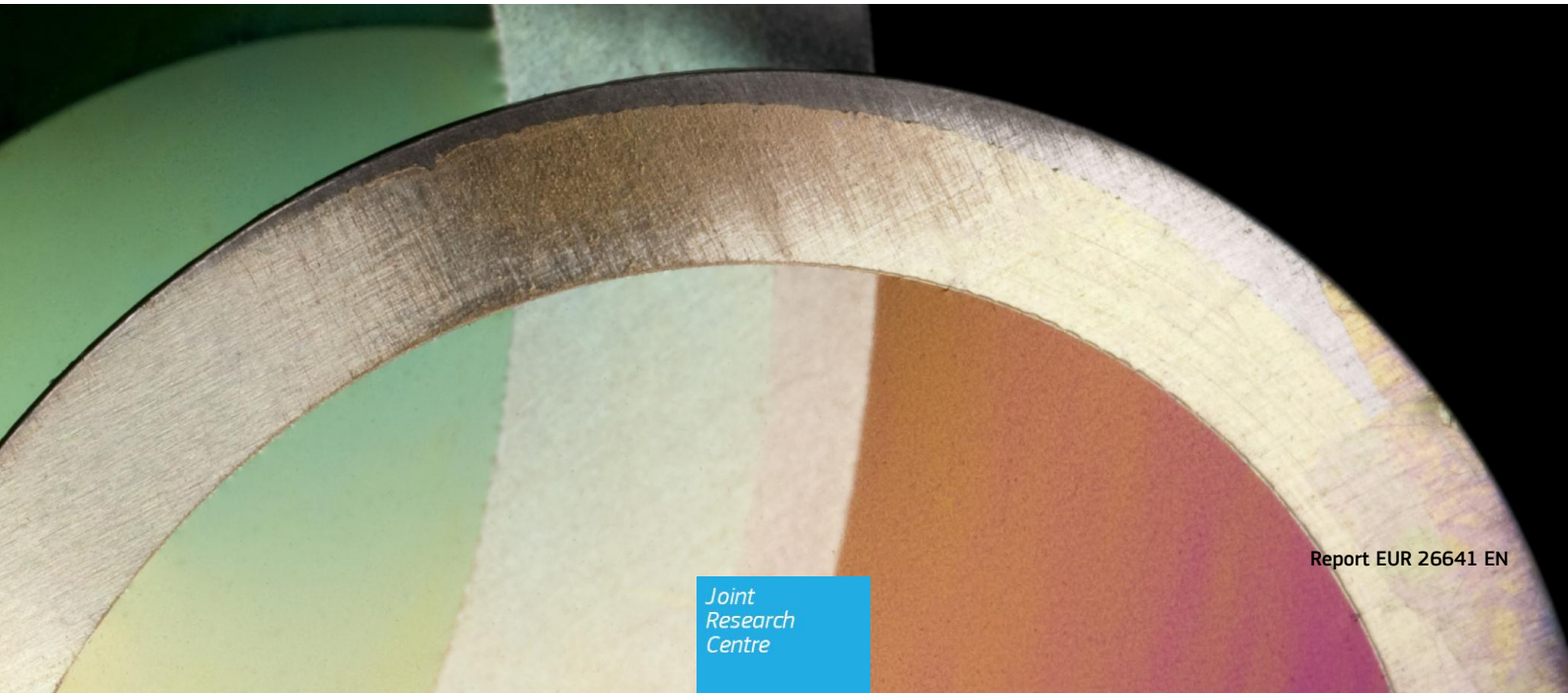

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Abstract

This report contains the abstracts of keynote lectures, oral and Poster presentations at the 3nd International Workshop on Physics Based Modelling of Material Properties and Experimental Observations, with special focus on creep and plastic in metallic materials. The workshop was organized in the context of European Commission's Enlargement and Integration Action by the Joint Research Centre in collaboration with University of Oxford, Middle East Technical University and Max Planck Institute, June 2- 4, 2014 in Çeşme Turkey. By "physics-based" we refer to models that address microstructures and associated thermodynamic non-equilibrium mechanisms and processes at different length and time scales. Such models include molecular dynamics, dislocation dynamics and crystal plasticity. The ultimate goal is to combine several models into a multi-scale approach to address complex material properties and also application to industrial components. The workshop presentations give an overview of different physics-based models and associated experiments. It provides examples of how such can be used for improved understanding and more reliable predictions but also discussed the limitations and future research needs.

3rd International Workshop on Physics-based Models and Experimental Verification

Book of Abstracts

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Introduction

This is the third Workshop on Physics-Based Models and Experimental Validation funded by the European Union's Enlargement and Integration Programme with creep and plastic deformation of metals as the focus theme this year. In addition to provide a platform for collaboration and exchange of information between researchers in EU Member States and the target countries, the Workshop also aims to bring together students and international experts, scientists addressing more basic research with code developers and industrial end-users and to provide cross-cutting by involving scientists from different sectors such as nuclear, aerospace and automotive.

Material is the key for the development of our future society such as new energy system, transport system and electronic equipment. The material properties, performance of components in different environments and associated material degradation mechanism depend on the microstructure and chemical composition of the material. By "physics-based" we refer to models that address microstructures and associated thermodynamic non-equilibrium mechanisms and processes at different length and time scales. Such models include molecular dynamics, dislocation dynamics and crystal plasticity. The basic foundation for such models were established in the 20th century but the further development and application to industrial problems is of more recent date thanks to the dramatic improvement of computational power. The ultimate goal is to combine several models, including continuum based phenomenological models, into a multi-scale approach to address complex material properties and also application to industrial components. Although one of the drivers for physics-based models is to replace the need for expensive material testing, experiments will be needed to develop, calibrate and validate physics-based and multi-scale models. Thus the integration of physics-based models and innovative experimental techniques are clearly coupled. The physics based models can be used for design of new materials with tailored properties or reducing the cost and time for development of new materials using physics-based models integrated with experiments. This research is therefore singled out as a key priority in broader research programmes.

The Workshop consists of ten keynote lectures, 19 oral presentations and a Poster session with over 50 posters. New developments and applications of the various physics-based models as well as some cases for scale bridging will be presented. There are also presentations on specific experimental techniques and on some that address the applicability for industrial applications.

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TECHNICAL PROGRAM

Cesme, Turkey, June 2-4, 2014

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Monday June 2

09:00 – 09:20 Opening of Workshop

09:00 – 09:20 *The need for physics-based multi-scale models and experimental validation,* **K-F Nilsson**, European Commission - JRC, The Netherlands

09:20 – 10:40 Key Note Lectures (Session I)

09:20 – 10:00 *Homogenizing metal plasticity: on the role of interfaces & dislocation climb,* **Marc Geers**, Eindhoven University of Technology, The Netherlands
10:00 – 10:40 *Climb-enabled discrete dislocation plasticity,* **Vikram Deshpande**, University of Cambridge, UK

10:40 – 11:10 Coffee Break

11:10 – 12:30 Oral Presentations (Session I)

11:10 – 11:30 *Climb Enabled Discrete Dislocation Plasticity of Particle Reinforced Composites,* **Can Ayas,** Delft University of Technology, The Netherlands
11:30 – 11:50 *Interaction of dislocations with grain boundaries: a hybrid atomistic-continuum approach,* **Dmitry Terentyev**, SCK-CEN, Belgium
11:50 – 12:10 *Mechanical properties of Single Crystalline Nanoparticle*, **Dan Mordehai**, Technion University, Israel
12:10 – 12:30 *The Continuum Dislocation Dynamics (CDD) theory: microplasticity, dislocation patterning and towards formation of persistent slip bands*, **Stefan Sandfeld,** Friedrich-Alexander-University Erlangen-Nürnberg, Germany

12:30- 14:00 Lunch

14:00 – 15:20 Key Note Lectures (Session II)

14:00 – 14:40 *Dislocation nucleation-limited deformation in Au nanowires: experiments and simple models*, **Cynthia Volkert**, Georg-August-Universitat Göttingen, Germany
14:40 – 15:20 *Static and dynamic mechanical studies of micron-sized Cu performed at variable temperature*, **Gerhard Dehm**, Max-Planck Institute for Iron Research, Germany

15:20 – 15:40 Coffee Break

15:40 – 17: 10 Oral Presentations (Session II)

15:40 – 16:00 *Rigorous quantification of the grain growth microstructure in 2D and 3D*, **J. K. Mason**, Bogazici University, Turkey
16:00 – 16:20 *Mechanical properties of KH2PO4 single crystals with embedded nanoparticles and organic molecules*, **A. Kosinova**, Institute for Single Crystals NAS of Ukraine
16:20 – 16:40 *Multiscale Deformation Heterogenity in Twinning Magnesium Investigated with in situ image correlation*, **Can Aydiner**, Bogazici University, Turkey
16:40 – 17:10 *Fracture of brittle crystals experiments, modeling, and atomistic calculations,* **Dov Sherman,** Technion-Israel Institute of Technology, Israel

****

Tuesday June 3

09:00 – 10:20 Key Note Lectures (Session III)

09:00 – 09:40 *Plasticity in hard materials – testing at the microscale and high temperatures*, **Sandra Korte-Kerzel** - RWTH Aachen, Germany
09:40 – 10:20 *A critical review of strain gradient theory*, **Norman Fleck**, University of Cambridge, UK

10:20 – 10:40 Coffee Break

10:40 – 12:00 Oral Presentations (Session III)

10:40 – 11:00 *Finite element studies on wedge indentation and flat punch molding using a higher order strain gradient theory*, **Sumit Basu** - IIT Kanpur, India.
11:00 – 11:20 *Mesoscale modeling of microstructure evolution using level sets*, **Håkan Hallberg** - Lund University, Sweden
11:20 – 11:40 *The Thermodynamics of strain gradient placticity*, **Albrecht Berthram** - Magdeburg University, Germany
11:40 – 12:00 *Homogenization of dislocation dynamics*, **Lucia Scardia** – University of Glasgow, UK

12:00 – 13:30 Lunch

13:30 – 14:10 Key Note Lectures (Session IV)

13:30 – 14:10 *Micromechanical modeling of the mechanical behavior of martensitic steels and comparison with experimental data*, **Maxime Sauzay**, CEA, France
14:10 – 14:50 *Creep at the micro and macro scales*, **Alan Cocks** – University of Oxford, UK

14:50 - 16:50 Coffee Break + Poster Session

16:50 – 18:10 Oral Presentations (Session IV)

16:50 – 17:10 *Dislocation density based plasticity model accounting for creep*, **Lars Erik Lindgren**, Luleå University of Technology, Sweden
17:10 – 17:30 *A Thermodynamically Consistent Cyclic Thermoplasticity Model*, **Marko Čanađija**, University of Rijeka, Croatia
17:30 – 17:50 *Thermoplasticity coupled creep damage model for predicting behavior of P91 steel*, **Babur Deliktas**, Uludag University, Turkey
17:50 – 18:10 *Prediction of creep-rupture properties for austenitic stainless steels undergone neutron irradiation*, **Andrey Buchatsky**, Central Research Institute of Structural Materials “Prometey”, Russia

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Wednesday June 4

08:40 – 10:00 Key Note Lectures (Session V)

08:40 – 09:20 *Design Codes vs. Physics-based models: complementary or incompatible?*, **Wolfgang Hoffelner**, RWH Consult GmbH, Switzerland
09:20 – 10:00 *Microstructural aspects of dynamic shear localisation in metals*, **Daniel Rittel**, Technion Israel Institute of Technology, Israel

10:00 – 10:20 Coffee Break

10:20 – 11:20 Oral Presentations (Session V)

10:20 – 10:40 *In-service corrosion-hydrogen degradation of structural steels and its experimental modeling,* **H.M. Nykyforchyn**, National Academy of Sciences of Ukraine, Ukraine
10:40 – 11:00 *Advanced Materials for Future Nuclear Energy Technologies*, **Mert Efe**, Middle East Technical University, Turkey
11:00 – 11:20 *Integrated experimental-numerical analysis of microstructural strain and stress evolution in bulk nanostructured alloys*, **Cem Taşan**, Max-Planck Institute for Iron Research, Germany

11:20 - 11:30 CLOSING OF WORKSHOP

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Opening and Keynote lectures

In the order of the programme

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The need for physics-based and multi-scale models and their experimental validation

Karl-Fredrik Nilsson

European Commission, Joint Research Centre, Institute for Energy and Transport
P.O Box 2, 1755 ZG, Petten, The Netherlands

By "physics-based" we refer to models that address microstructures and associated thermodynamic non-equilibrium mechanisms and processes at different length and time scales. Such models include molecular dynamics, dislocation dynamics and crystal plasticity. "Mechanism" or "process-based" would perhaps be a better term for such models since "Physics-based" suggests that phenomenological based continuum models are less based on physics. In fact physics-based and more traditional continuum mechanics models are complementary. For instance basic physics based models can relate how model parameters in the phenomenological models depend on microstructural features. The physics-based models have a great potential to provide a better understanding of material properties and degradation phenomena of materials to:

- Predict material properties from a given microstructure and chemical composition;
- Design new materials with tailored properties or improve properties of existing material by optimized processes;
- Predict long-term degradation such as creep or thermal ageing or behaviour in extreme environments such as neutron irradiation, by extrapolation from accelerated test data to operational conditions;
- Provide transferability between data from specimen tests to industrial components.

Physics-based models can be used to explain phenomena such as dynamic strain ageing, precipitation hardening, how grain size affects creep rates and hardening. Moreover any modelling of microstructural evolutions is based on appropriate physics-based models. In most cases properties depend on features at different length scales and it is necessary to combine models at different length and time scales by employing some type of scale-bridging; progress is being done for instance to model grain boundaries by combining dislocation dynamics and crystal plasticity. The ultimate goal, however, is to have a multi-scale approach that integrates models at the relevant scales. It should be stressed that the development of physics-based models must be integrated with dedicated experimental work for development and calibration of specific model as well as validation test to verify the up-scaling to components and materials.

The basis for the physics-based models were established in the 20th century, but the development of implementation of physics-based models as a tool for quantitative predictions would not have been possible without the dramatic increase in computational power. But at the same time it is clear that computational power will never be sufficient. The hunt for the key mechanisms and the reduction of complex problems to simpler ones without losing the key features remains the most challenging task which must be directed by expert opinion and experience.

Homogenizing metal plasticity: on the role of interfaces & dislocation climb

Marc Geers[1], Maeva Cottura[1], Benoît Appolaire[3]
Esteban Busso[2], Samuel Forest[2], Aurélien Villani[2]

[1] Eindhoven University of Technology, Dept. Mech. Engng., The Netherlands
[2] MINES ParisTech, Centre des Matériaux, Evry, France
[3] ONERA, Châtillon, France

Many metallic systems are nowadays operated in a regime where the evolving mechanical properties are not simply dependent on dislocation glide mechanisms within the underlying crystals only. This is typically the case for climb-assisted deformation and creep mechanisms, which are known to contribute significantly at higher temperatures in pure metals, solid solution alloys, particle strengthened and multi-phase metals. Moreover, in modern thin film systems for micro-electronics or micro-electro-mechanical systems (MEMS), climb mechanisms already contribute to a significant extent at only mildly elevated temperatures or even room temperature.

The role of climb in plasticity has been addressed in several papers in a purely phenomenological manner, where constitutive equations incorporate the contribution of climb. The focus of this contribution is to break through the phenomenological nature of these approaches at the crystal plasticity level, by coupling deformation to dislocation motion assisted by glide and diffusional climb. For this purpose, a state-of-the-art crystal plasticity model needs to be used, which properly incorporates short-range dislocation-dislocation interactions. The backbone of the crystal plasticity framework is based on a strain gradient crystal plasticity model enriched with dislocation transport physics.

For the coupling with vacancy diffusion at the local scale, a thermodynamically based variational framework is used that links the climb of a single edge dislocation to the diffusion of vacancies. Attention is given to the governing equations and physics of the vacancy diffusion process, the driving forces acting on a dislocation to climb and the intrinsic coupling between both. The climb law is therefore diffusion-controlled. The problem is studied at the meso-scale, where pile-ups against particles can be resolved explicitly, i.e. a scale at which it is meaningful to preserve a direct coupling between the mean vacancy flux and the dislocation climb process. A rate-dependent strain gradient crystal plasticity formulation is adopted, which accounts for the net sign of the dislocation population. The dislocation problem can be described in a fully conservative manner with transport equations. Since the analysis is carried out at the meso-scale, all dislocations are assumed to be able to participate in the climbing process. The corresponding transport equations for the dislocations are updated to incorporate climb. In order to incorporate the effect of the dislocation climb on the plastic deformation tensor, the crystallographic split of the plastic velocity gradient tensor is extended for the climb kinematics associated to each slip system.

The innovative aspects of this contribution are: (1) a fully coupled crystal plasticity model through which climb is controlled by the diffusion of vacancies; (2) an extended strain crystal plasticity model, that incorporates the climbing dislocations in the governing transport equations; (3) a global-local approach to separate the scales and assess the influence of the local diffusion problem on the global plasticity problem; (4) a kinematically enriched crystal plasticity model, which directly incorporates the climb kinematics in the crystallographic split of the plastic velocity gradient; (5) illustrative examples that emphasize the role of climb nearby interfaces that impede the glide motion.

A Coupled Framework For Climb-Assisted Glide In Discrete Dislocation Plasticity

Vikram Deshpande

Department of Engineering, Cambridge University, Trumpington Street, Cambridge CB2 1PZ, UK

It is now well established that the plastic deformation of crystalline solids is size dependent at the micron scale for a range of loading conditions. While there are many underlying reasons for these size effects, attention has been primarily focussed on situations where plastic strain gradients are generated. Models typically tend to over-predict the experimentally observed size effects as they neglect a range of dislocation relaxation mechanisms. These mechanisms include dislocation cross-slip and dislocation climb. Dislocation climb requires the diffusion of vacancies and hence significant amounts of dislocation climb only occur at temperatures above a third of the melting temperature - in these cases mass transport reduces the plastic strain gradients and thereby reducing the effect of specimen size. However, even at lower temperatures, dislocations can surmount small obstacles with the aid of small amounts of climb. This prevents the build-up of large dislocation pile-ups which consequently again relaxes stresses.

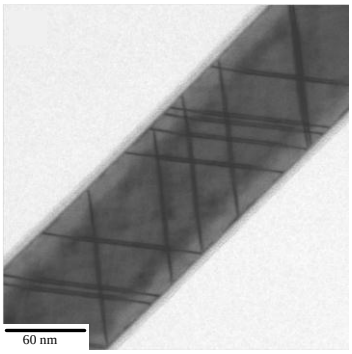
The coupling of vacancy diffusion with dislocation motion is a true "multi-scale" problem as vacancy/dislocation interaction is essentially a dislocation core effect. We present a two-dimensional discrete dislocation plasticity framework coupled with vacancy diffusion wherein dislocation motion occurs by both climb and glide. The effect of dislocation climb is explored for a range of problems including size effects in bending of crystals, metal-matrix composites and passivated films. Dislocation climb typically tends to reduce strength enhancements that occur with decreasing size but in some surprising cases can also result in strength increases.

Dislocation nucleation-limited deformation in Au nanowires: experiments and simple models

Cynthia A. Volkert

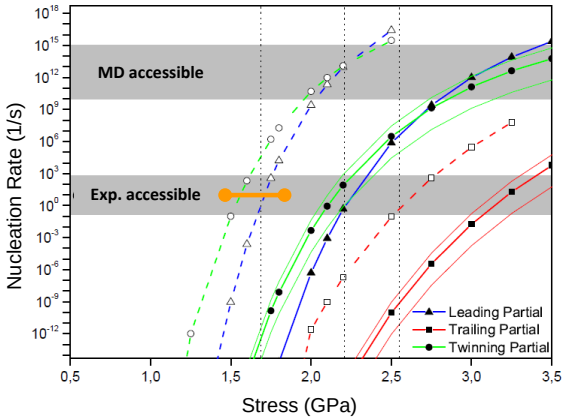
Institute of Materials Physics, Georg August University Göttingen, Göttingen, Germany

Nucleation remains one of the central puzzles of materials science and is often the rate-limiting and microstructure-determining step in transformations and processing. Since we rarely have the temporal and spatial experimental resolution necessary to directly interrogate nucleation, we must rely on comparing resultant microstructures with models to indirectly test our understanding. In this presentation I aim to describe the surface nucleation of dislocations by comparing experimental observations of the defects introduced by straining single crystal Au nanowires with predictions of classical nucleation theory.



(left) Bright field TEM image of planar defects formed in a single crystal Au nanowire during straining.

(right) Predictions for dislocation nucleation rates at flat (solid lines) and stepped (dashed line) Au surfaces. Experimental observations are indicated with the horizontal line.



Deformation of metal samples is usually controlled by dislocations interacting with each other or with microstructural features. However, the existence of nucleation-controlled deformation in materials has been appreciated for years. It is particularly relevant for nanoscale materials where there is a high probability of having an initially dislocation free microstructure and of the dislocations running out of the sample before they interact to form new dislocations. The study presented here is based on nanoscale, high crystal quality Au wires. The high crystal quality ensures well-characterized sites for nucleation on the wire surfaces and the small cross-sectional dimensions of the wires (between 20 and 300 nm) limits the generation of dislocations by dislocation reactions. By measuring stress-strain curves and comparing with resultant deformation morphologies and microstructures, a picture of the underlying nucleation process during deformation emerges.

Small Scale Mechanical Testing: More than just a fashionably tool?!

Gerhard Dehm

Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

In the last decade miniaturized mechanical compression, tension and bending experiments have been developed using focused ion beam milling or lithographic processes to fabricate small samples from thin films and/or bulk materials. Many of the experiments provided new insights on the interplay of sample dimensions, dislocation density, and mechanical strength of single crystals. However, miniaturized mechanical testing also suffers from limitations which may lead to misinterpretations. In this talk a critical overview on the challenges of micro-mechanical testing is provided. Additionally, current examples of micro-mechanical bending, compression and tension experiments combined with electron microscopy and/or μLaue investigations are presented with the aim to shed light on the deformation mechanisms at interfaces in materials.

Plasticity in hard materials – testing at the microscale and high temperatures

Sandra Korte-Kerzel

Institut für Metallkunde und Metallphysik, RWTH Aachen University

Plasticity in many hard materials is still not understood, although it is important in many applications from defect formation and migration in semiconductors over failure in cutting tools to the often very limited plasticity at ambient conditions in high temperature materials. The lack of experimental studies in these materials is mainly due to their brittleness and the resulting difficulties encountered in mechanical testing at low temperatures. In addition, many hard materials possess a rather complex crystal structure, which may lead to strong anisotropy. In this case, conventional testing methods avoiding fracture, like indentation, do not yield sufficiently detailed data, as directional properties are difficult to extract.

In nanomechanical testing a size effect on cracking can be exploited to overcome these problems and to lead to plasticity being favoured over cracking at small scales even in uniaxial compression. Being able to suppress cracking in small specimens therefore allows the study of plastic flow in hard and brittle materials by machining compression samples at the micrometerscale. At this scale, single crystals are easily obtained from single grains macroscopically polycrystalline samples and permit the study of individual slip systems in anisotropic crystals by targeting grains of particular orientations.

This approach allows the study of plasticity at room temperature, but in order to understand plasticity and its thermal activation more fully and to bridge the gap to application temperatures, the ability to test at elevated temperatures is also essential.

In this talk, a comprehensive study on silicon using microcompression at room and elevated temperatures will be presented along with the technical background and further examples from experimental studies on more complex crystal structures and high temperature materials.

A critical review of strain gradient theory

Norman Fleck, John Hutchinson and John Willis

University of Cambridge, UK

A critical examination is made of two classes of strain gradient plasticity theories currently available for studying micron scale plasticity. Both classes fit within the variational framework of Fleck and Willis. One class is characterized by certain stress quantities expressed in terms of increments of strains and their gradients, while the other class employs incremental relations between all stress quantities and the increments of strains and their gradients. Implications stemming from the differences in formulation of the two classes of theories are explored for two basic examples having non-proportional loading: (i) a layer deformed into the plastic range by tensile stretch with no constraint on plastic flow at the surfaces followed by further stretch with plastic flow constrained at the surfaces; and (ii) a layer deformed into the plastic range by tensile stretch followed by bending. The marked difference in predictions by the two theories suggests that critical experiments will be able to distinguish between them.

MICROMECHANICAL MODELING OF THE MECHANICAL BEHAVIOUR OF MARTENSITIC STEELS. COMPARISON WITH EXPERIMENTAL DATA

Maxime Sauzay

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INTRODUCTION

Metals and alloys with initial high dislocation density and small (sub)grain size are generally prone to large softening during cyclic or creep loading. This softening behaviour is characterized by stress amplitude decrease during strain-controlled tests (Fig. 1 a) and short stationary stage followed by long tertiary stage showing increasing strain rate during creep, even before necking and intergranular damage become influent macroscopically. This behaviour is observed for various metals and alloys: martensitic steels [1,2], bainitic steels [3] and ultrafine-grained polycrystals [4], whatever the crystallographic structure. Two main microstructure observations partially explain this softening behaviour: the dislocation density decreases strongly and (sub)grain size increases largely (Fig. 1 b), mainly due to low-angle boundary (LAB) vanishing. A multiscale model based on the most probable annihilation mechanisms has been developed and predictions compared to experimental data and observations for various materials and loading conditions.

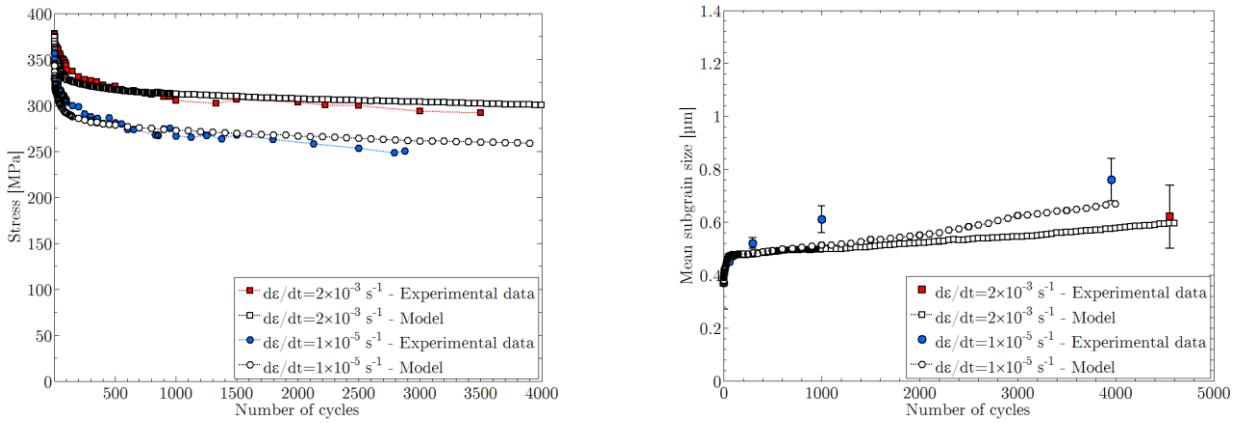

Fig. 1: a) predicted and experimental evolutions of the maximum peak stress during cyclic loading. Strain-controlled test, amplitude: ±0.35%; b) predicted and measured evolutions of subgrain size in similar conditions. Measurement by transmission electron microscopy. Tempered martensitic steel grade 92, 550°C.

CONSTITUTIVE LAWS AND HOMOGENEIZATION PROCEDURE

In the as-received condition, each crystal is assumed to be full of dislocations and LABs. Depending on the considered material, crystals represent martensite blocks, ferrite blocks or grains which boundaries are large-angle ones. These crystals are embedded in a matrix which mimics the behaviour of the whole polycrystal following the self-consistent hypothesis. For low-strain amplitude cyclic loading, the thermo-elastic localization rule proposed by Kröner [5] is used whereas the Molinari viscoplastic tangent localization rule [6] is adopted more generally, such as in the case of creep.

At the crystal scale, isotropic elasticity is used as well as thermal activation of viscoplastic glide. The hardening laws are based on the forest obstacles (isotropic shear stress) and tension line effects induced by the bowing-out of dislocations, which introduced a first (sub)grain size effect (Fig. 2 a). The hardening law linking the kinematic shear stress rate with the viscoplastic slip one has been deduced from geometry considerations and the Orowan law (Fig. 2 a). Finally, the evolution laws of free screw and edge dislocation densities take into account a production term based on the bowing-out mechanism which introduces a second (sub)grain size effect [7,8], and annihilation terms based on the spontaneous annihilation between

two close parallel dislocations of opposite signs. An additional annihilation term arises from the interactions between incident free dislocations and LAB dislocations (Fig. 2 b) [9]. Such annihilations lead to LAB dislocation lineic density decrease during viscoplastic deformation and finally LAB vanishing and (sub)grain size increase [9]. All parameters have physical meaning and their possible ranges of variation such as the ones of the initial values of dislocation density and (sub)grain size are known following either literature or our measurements. An extensive parametric study has shown that the predictions are stable with respect to the parameter values. Only two parameters should be adjusted, using two experimental macroscopic tensile curves at different strain rates, but no cyclic data. These two parameters are the activation free energy and volume which may be linked to thermally-activated interactions of gliding dislocations with various obstacles such as solid solution, nanometric precipitates… and then could not be evaluated following a more straightforward way.

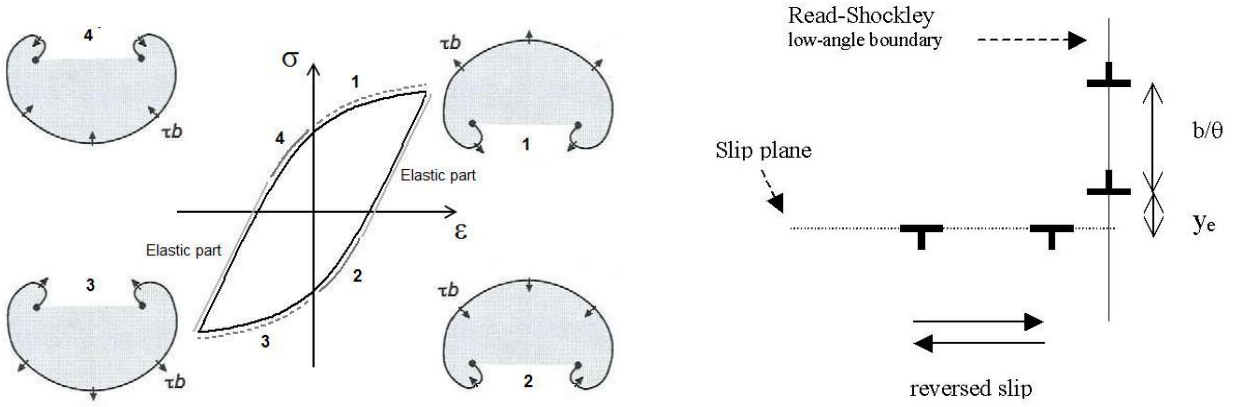

Fig. 2: a) bowing-out of a dislocation loop during tensile loading and reverse glide during compression loading; b) sketch of the annihilation process occurring between a LAB dislocation and a free dislocation of opposite sign gliding toward the symmetric tilt LAB (b: Bürgers vector length, θ: LAB misorientation, y_e: edge dislocation annihilation distance).

RESULTS

The cyclic behaviour of tempered martensitic steels at high temperature is first discussed. Twenty-four easy slip systems are considered taking into account their crystallographic structure which is very close to the body-cubic centred one. The predicted macroscopic softening behaviour is in agreement with experimental data (Fig. 1 a). At the microscopic scale, the simulated evolutions of both dislocation density and subgrain size are close to the measured evolutions (Fig. 1 b). The effect of strain rate is rather well reproduced. The respective effect of viscoplastic strain amplitude and loading multiaxiality is correctly predicted too. They both trigger softening partly because the induced numbers of activated slip systems are higher and consequently the probabilities of dislocation annihilation are higher at high amplitude or for high triaxiality (tension-compression version alternated shear for instance). Simulations of the cyclic behaviour at room temperature are encouraging as well. It should be noticed that the predictions are stable with respect to material parameter variations, which is required because the values of some of them may not be evaluated very precisely such as the screw annihilation distance.

The microstructure evolutions observed during creep of similar steels are fairly predicted as well, such as the ones of (sub)grain size and mean LAB misorientation, whatever the considered material: 12Cr [9] or 9Cr martensitic steel [10], Eurofer 97 steel [11] or even ECAPed Fe10%Cr steel [9].

CONCLUSIONS

Such multiscale modeling based on both physical recovering mechanisms and mean-field homogeneization leads to predictions in rather fair agreement with experimental data concerning cyclic and creep softening of steels. Work is in progress concerning:

- the effect of time-dependent recovering mechanisms such as climb which has been implemented in the used numerical code and precipitation which should be taken into account in long term creep or creep-fatigue tests

- the comparison between predictions and experimental data in the case of ultra-fine grained materials.

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Design Codes vs. Physics-based models: complementary or incompatible?

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Physics-based models consider frequently isolated effects in idealized materials (binary or ternary alloys).The results contribute to a basic understanding of specific materials behaviour but it is difficult to generalize them for a class of technical materials with its wide scatter of chemical compositions and microstructures. Design codes provide rules, procedures and materials data which allow safe design of components acting under usually complex service exposure. Also the microstructure cannot be fixed. A well known example is the change from martensitic (at the outside) to bainitic in the center as a result from different cooling rates in large forgings. For residual life assessments mainly fracture mechanics concepts are employed which don't need too much of physics-based modeling. Considering these differences between modeling and design it might look like a real incompatibility between the two worlds. However, this must not necessarily be the case. Modeling can provide elementary insight into materials behaviour particularly with respect to optimization of chemical composition. The current understanding of radiation damage is based on materials modeling because the time during which initial damage develops is too short for experiments which might change with the use of free electron lasers in the future. Prediction of the mechanical behaviour of components under service or component life assessments under creep-fatigue seem at least for the next future to be outside the range of physics-based modeling. However, also in such situations modeling might help to understand typical effects like cyclic softening or hardening occurring in components. The lecture will show design related examples where modeling is not expected to bring significant contributions but also others where modeling could at least punctually help to improve design procedures in the future. Design and residual life assessments based exclusively on computers using „in silico"-procedures is not expected to become a realistic tool for the next decades even when computer power steadily increases. Using a „dedicated scale" approach with experimental validation for single effects is expected to be a more powerful contribution of modeling to design than a multiscale approach chaining several space- and time scales to understand the behaviour on the macroscale. Real collaboration between modelers and design oriented individuals or groups would help to strengthen mutual understanding. However, it takes unfortunately currently not place as would be necessary.

PHYSICAL ASPECTS OF ADIABATIC SHEAR FAILURE

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Adiabatic shear failure is a dynamic failure mechanism that has been extensively investigated since the early 1940's. The prevailing assumption is that thermal softening plays a dominant role as a destabilizing factor leading to the formation of localized shear surfaces, referred to as adiabatic shear bands (ASB). Considered as an instability, the phenomenon has been quite successfully modelled using perturbation analysis which leads to the prediction of a critical failure strain.

In the recent years, we have re-examined the prevailing assumption of a dominant thermal softening from an experimental point of view, showing that for a sufficiently large number of materials studied, thermal excursions are of a quite limited extent for several alloys that indeed fail by ASB, but at relatively small strains, such as Ti6Al4Vand maraging steel among others. This observation has led to the identification of a critical value of the strain energy (density), with emphasis on its athermal component, the so-called stored energy of cold work (SECW). This parameter is particularly attractive as it ties smoothly the mechanics of ASB formation and its physics through microstructural evolutions.

In this presentation, we will review some of the more important results in this subject, related to the measurement and rate-dependence of this critical value of the SECW. Emphasis will be put on the identification and the interplay between the 2 main deformation mechanisms, namely dislocations slip and twinning. A fully coupled numerical model, in which the microstructural evolutions are included, will be described. This model can be used to differentiate microstructural from thermal softening, and the contribution of each mechanism.

The main outcome of this work is that, whereas perturbation analyses are quite adequate to represent ASB formation, we suggest that the perturbation should not solely concentrate on thermal fields and associated softening effects, but also consider softening microstructural evolutions to provide a more complete picture.

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Oral presentations

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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 as the constituents of the microstructure does not slip with equal ease. The gradients of plastic deformation 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.

Engineering materials for applications, such as jet propulsion and turbine blades that necessitates mechanical performance at elevated temperatures. Consequently, there is an increasing need to improve the fundamental understanding of plasticity at elevated temperatures and the relevant size effects.

In this study we present a small strain two-dimensional discrete dislocation plasticity framework coupled to vacancy diffusion in order to study plasticity at elevated temperatures when dislocation climb is active. The effect of particle size upon strength of the composite is investigated under pure shear. The composite consists of elastic particles in a plastic matrix oriented for single slip and the volume fraction of reinforcing particles remains fixed. Our calculations show that plasticity size effects are present when deformation is by only dislocation glide whereas size effects are reduced when dislocation climb is permitted. A key distinction between the climb enabled deformation and glide only deformation modes is the activation of a diffusional deformation mechanism in addition to the dislocation slip when significant amount of climb is permissible. Finally, we contrast predictions of the coupled framework with an ad-hoc model in which dislocation climb is modelled based on a quasi steady-state solution.

Interaction of dislocations with grain boundaries: a hybrid atomistic-continuum approach

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In polycrystalline metals and metallic alloys (such as steels and superalloys), plasticity mediated by bulk dislocations is inevitably connected to the grain boundary-dislocation interactions processes, whose complete understanding is yet to be achieved. Atomistic simulations is a natural way to proceed with the investigation of the plasticity in polycrystalline metals. Here, the interaction of dislocation pile-up with several types of tilt grain boundaries in BCC and FCC metals (Fe, W, Ni, Cu, AL) has been studied using a hybrid atomistic-continuum approach. The classical molecular dynamics (MD) tool was combined with a solver for the loaded dislocation pile-up, so the fixed boundary conditions were provided using linear elasticity theory. Large scale MD simulations were coupled with a special analysis enabling to distinguish dislocations, stacking faults, grain boundary interfaces and other discrete lattice defects. The interaction of dislocation pile-ups (containing several dislocations) was investigated at different loading rates, ambient temperatures and grain boundary configurations.

Dislocation pile-ups modify both the stress state and the residual defects at the intersection with dislocations. A multiple dislocation absorption into the boundary is also observed for the pile-ups containing several dislocations. The results of the simulations clearly reveal a competition between three principal processes, which are absorption, transmission and reflection. The obtained results are discussed and compared with predictions of elasticity theory.

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Mechanical properties of Single Crystalline Nanoparticle

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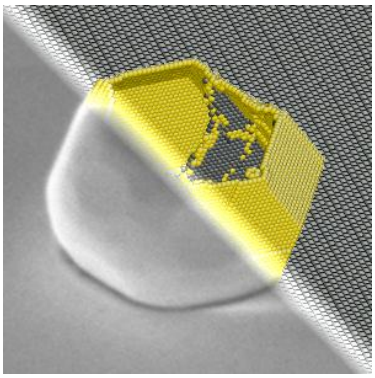
It is well established that materials can drastically change mechanical properties when their size is reduced to the nanoscale, mainly because of an increase in surface to volume ratio and of lowering the amount of defects in the lattice. Recently, we suggested employing nanoparticles as specimens to study strength at the nanoscale [1,2]. An ensemble of faceted, single-crystal, mobile-dislocation free nanoparticles is produced on a sapphire substrate via dewetting of thin-films. The nanoparticles were indented with a sharp tip or deformed under compression. In this talk, we discuss how the mechanical response of the nanoparticles to compression and indentation depends on material properties and crystal structure, which manifests itself through the underlying dislocation mechanism.

For instance, an indentation size effect is observed experimentally in Au nanoparticles, which is rationalized with large-scale molecular dynamics (MD) simulations as the competition between dislocation storage and depletion on free surfaces. In addition, the dependence of their yield stress under compression on their size can be described by a power law, with an exponent that is rationalized quantitatively from MD simulations and finite elements analysis. Based on these results, a model is proposed for dislocation nucleation at stress gradients at the nanoscale. This model clarifies similar size effects calculated in other FCC metals and to some extent in BCC metals. However, the size effect vanishes in MD simulations of Ni3Al intermetallic nanoparticles because of their geometry. An analysis of the dislocation evolution in Ni3Al nanoparticles shows that partial dislocations are nucleated at the vertices, shearing the nanoparticle with large complex stacking faults planes. These few examples demonstrate how the combination between the experimental results and atomically-informed dislocation mechanisms allow us to study mechanical properties at the nanoscale.



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The Continuum Dislocation Dynamics (CDD) theory: microplasticity, dislocation patterning and towards formation of persistent slip bands

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Metal plasticity is governed by the motion of dislocations, and predicting the interactions and resulting collective motion of dislocations is a major task in understanding and modeling plastically deforming materials. Despite all efforts and advances in the last decades this task has not yet been fully accomplished. The reason is that discrete models which describe dislocation systems with high accuracy are only computationally feasible for small systems, small strains, and high strain rates. Classical continuum models do not suffer from these restrictions but lack sufficiently detailed information about dislocation microstructure. This is particularly problematic when the underlying dislocation microstructure becomes strongly anisotropic. In the simplest case this can be observed when ensembles of dislocations approach grain boundaries where piling up of dislocations leads to anisotropy of their orientation distribution. Another class of strongly heterogeneous behavior can be observed during plastic deformation when dislocations form metastable patterns of high densities. A third type of dislocation structure arises from anisotropic annihilation, as observed e.g. in the 'matrix' and 'persistent slip band' microstructures of fatigued FCC metals where preferential annihilation of screw dislocations leads to microstructures which are dominated by edge dislocation dipoles.

Our CDD simulations represent the same dynamics as DDD simulations but in a continuum framework and is thus in general not limited by the number of dislocations or the accumulated plastic strain We present the theoretical foundations of the 'Continuum Dislocation Dynamics' (CDD) theory [1,2] and discuss the steps which are required in order to describe the evolution of intrinsically anisotropic and/or confined dislocation microstructures in a systematic manner. We then analyze dislocation pattern formation in terms of mechanisms and the "similitude principle" and derive scaling relations for CDD-/ Kröner-Nye-type continuum models of dislocations. Finally, we present the necessary conceptual steps towards physically based modeling of fatigue and the concomitant slip localization: we demonstrate that CDD enables us to simulate the bowing-out of screw dislocations including the deposition of edge dislocations. This will allow for simulation of PSBs exclusively based on dislocation mechanics of curved lines together with a minimum set of rules for e.g. dislocation annihilation.

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Rigorous quantification of the grain growth microstructure in 2D and 3D

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While a variety of approaches have been proposed to simulate the evolution of grain boundaries during grain growth, comparing the results of different simulations or the results of simulations with a physical microstructure remains difficult. We suggest that this is partly due to the absence of a rigorous definition of the conjectured steady state grain growth microstructure, and partly due to the inability to adequately measure the approach to that state. We address this situation by placing a metric on the space of grain boundary network topologies. Specifically, we use the frequencies of local grain boundary configurations to encode the statistical features of the grain boundary network topology as a discrete probability distribution. This allows us to calculate a distance between microstructures that indicates the degree of their topological similarity or difference, and to rigorously quantify the grain boundary network topology of the grain growth microstructure.

Mechanical properties of KH_2PO_4 single crystals with embedded nanoparticles and organic molecules

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The search for new nonlinear-optical media for optoelectronics and nonlinear optics, possessing high conversion efficiency of laser radiation, stimulated creation of composite materials on the basis of dielectrics containing nanoparticles and organic molecules. The enhancement of frequency conversion efficiency was obtained for KDP crystal/TiO_2 nanoparticles composite system versus KDP single crystal in picosecond range of laser pulses [1] and for KDP crystal containing Urea molecules for nanosecond laser pulses [2]. The studying of impurities effect on mechanical properties of the matrix is the important part of characterization of new composite materials.

Here are presented the results of strength properties studying of KDP crystals with embedded TiO_2 nanoparticles and Urea molecules. Crystals were grown from water solutions by temperature lowering method. The values of Vickers microhardness, fracture toughness and laser damage threshold for crystal samples cut out from the prismatic {100} and pyramidal {101} growth sectors are compared.

It is established that the mechanical strength of KDP crystals containing Urea is higher in comparison with that of pure crystals. For KDP+Urea crystals the microhardness value H_V is found to change from 2.24 GPa to 1.74 GPa while increasing the load P from 10 to 200g, respectively. For pure KDP crystals the microhardness value is within the limits 1.45÷1.70 GPa. The effect is pronounced for the (001) crystal face (see Fig. 1), which is related to special Urea molecules arrangement in the crystal bulk.

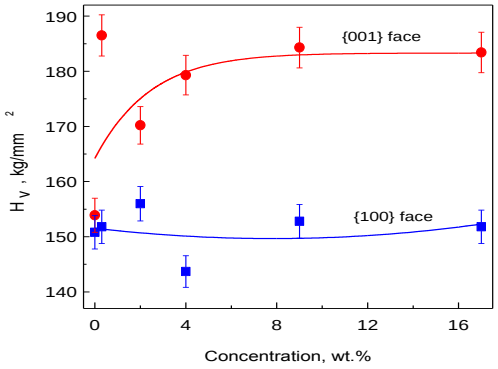

Fig. 1. – Variation of Vickers microhardness with Urea concentration in growth solution (P=100 g).

TiO_2 nanoparticles unlike organic molecules contribute to decreasing of Vickers microhardness and fracture toughness of KDP crystal at their concentration in growth solution 10^{-3} wt.% and higher. This fact is due to high internal stresses and crystal lattice discontinuities namely breaking of hydrogen bonds. In the range of TiO_2 concentration 10^{-4}-10^{-3} wt.% laser damage threshold is 3-fold reduced relative to pure KDP (at nanosecond laser action).

The obtained results are discussed in terms of structural changes in KDP crystal, changes in molecular interaction forces and the mobility of point and line defects.

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MULTISCALE DEFORMATION HETEROGENEITY IN TWINNING MAGNESIUM INVESTIGATED WITH IN SITU IMAGE CORRELATION

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The complex strain fields that emerge at the onset of extensive deformation twinning in Magnesium alloy AZ31B has been investigated in situ with multiscale digital image correlation (DIC). A two camera setup has been used to yield full-field deformation maps on two orthogonal faces of a gradually strained prismatic sample. The sample is cut off from a rolled plate such that the two examination faces are perpendicular to the normal and transverse directions of the plate (abbreviated as ND and TD, respectively) while the rolling direction is aligned with the compression axis. In this setting, not only the crystallographic texture favors the tensile twin mode but the nominal plane of shear of the operating twin mode is statistically ordained to coincide with TD-normal plane. Picking, in consequence, the TD face to be the primary examination surface, deformation fields have been determined at subgrain resolution (DIC subset and nominal grain size, 12 and 50 µm, respectively) by scanning with a microscopic lens at each load. In an in situ setting, a unique combination of microscopic DIC resolution and statistical significance (~5000 grains) is achieved that enables a full bridging of the crystallite and sample scales at each load point. Intense strain heterogeneity is revealed abruptly at all length scales in the form of banded strain patterns: At the macroscale, the strain in the sample is locally accommodated by the sudden emergence/advance of shear bands whose macroscale strain content at initiation is around 1%. The fact that these bands are volumetric and span across the sample is determined by the ND-face observation that reveals horizontal traces of strain localization. Bands from conjugate and families exhibit sequential activation. At the granular scale, another set of strain patterns are resolved inside a macroscopic band of either family with very high strain heterogeneity levels, whose extent is comparable to the twin transformation strain (principal values). Traversing the initial regions of the twin plateau in fine steps with in situ observation, the strain heterogeneity is found to explode, rather than gradually evolve, yielding uniquely shaped strain histograms at the subgrain scale which persist until the next macroscopic band arrives at the particular locality. The primary findings of this work has been published in Aydıner, C. C. ; Telemez, M. A, *International Journal of Plasticity* **2014**, *56*, 203-218. http://dx.doi.org/10.1016/j.ijplas.2013.12.001.

Fracture of brittle crystals-
Experiments, modeling, and atomistic calculations

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Keywords: Brittle Crystals; Slow Crack; Cleavage; Energy-Speed Relationship

The way brittle crystals break is still debated. Two approaches exist with no clear conclusion yet. The first approach is the continuum based elastodynamic Freund equation of motion that formulates the energy-crack speed relationship and shows that crack can initiate at Griffith barrier of 2γ, twice the free and relaxed surface energy of the material, and propagates at speeds from zero to CR, the Rayleigh free surface wave speed. The second is based on atomistic calculations, suggesting that atoms on the crack front are stuck in their potential well and need much higher energy to initiate and therefore can't start at speed below significant portion of CR.

Experiments and atomistic calculations over the last two decades have demonstrated that cracks in silicon crystal initiate at energy higher by over 50% the Griffith barrier and at speed as high as 2,000 m/sec. This is well known as lattice trapping effect, manifests that cracks in brittle crystals are actually trapped by the potential well and 'bursting' upon initiation. These findings set the fundamentals of crack dynamics in brittle materials with long range order.

Contrary, our cleavage experiments have shown recently that cracks in silicon crystal can propagate at speeds much lower than the lattice trapping speed and at energies that is comparable with the Griffith barrier. Furthermore, the energy-speed relationship well obeys Freund equation of motion at the low energy regime. This was achieved by high resolution fracture experiments enabling to manipulate the energy flow to the crack tip. To achieve slow cracks, the initiation energy should be as closed as possible to the Griffith barrier and the energy flow to the crack tip should be as much as possible low, conditions that we were able to achieve by our new experimental method.

The basic feature of crack propagation in brittle crystals is the curved crack front, motivated by the transition from plane stress condition on the free surfaces to plane strain in the interior of the specimen, which indicates on double kinking as the bond breaking mechanisms, enabling crack initiation at Griffith barrier and propagation near this value. This was supported by modeling and confirm by molecular dynamic simulations.

Investigations into the origins of plasticity in glassy amorphous polymers

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Several commercial amorphous polymers in the glassy state exhibit considerable ductility. In an attempt to understand the origins of plasticity in these materials We have performed well designed molecular dynamics (MD) simulations on carefully equilibrated macromolecular ensembles of a generic model of an amorphous glassy polymer. The intrinsic uniaxial stress–strain behaviour in these materials is characterized by an elastic part, yield followed by strain-softening and steep hardening at large strains. We are particularly interested in the phenomena of post yield strain softening and strain hardening that are typical of these materials. Existing constitutive theories of glassy polymers rely on the so called rubber elastic analogy where strain hardening is assumed to be the result of the affine orientation and subsequent stretching of an underlying entanglement network. Using MD simulations and a continuum thermo-mechanical framework, we isolate the plastic free energy associated with the back-stress that governs hardening. We show that the hardening owes its origin to the non-bonded part of the force-field and is related to the increase in the number of close binary contacts between parts of macromolecular chains that are pushed into close proximity due to compressive deformation. The strain softening is a result of a burst of free volume evolution that accompanies a sudden unstable volume expansion occurring right after yield as the polymer undergoes a deformation induced disordering. This is accompanied by a sharp increase in the room available for changes in dihedral conformations. These conformational changes are mainly responsible for accommodating the plastic deformation as many of them are unable to flip back to their original conformations even after unloading. Finally, by fitting the uniaxial responses obtained from the MD simulations with a standard constitutive model, we show that the barriers between the torsional states govern the small strain behaviour while the strength of the non-bonded interactions govern hardening.

Mesoscale modeling of microstructure evolution using level sets

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Mesoscale models of microstructure evolution, for example due to recrystallization, have historically been established using a number of different methodologies such as Monte Carlo Potts formulations, cellular automata, phase fields and front tracking algorithms [1]. Since introduced in [2], the level set method has gained attention as a promising approach to tracing of the evolution of interfaces in a wide range of physical systems. Applications also lie in mesoscale simulations of microstructure evolution due to the ability of the level set method to represent, for example, grain boundaries in polycrystal microstructures with high spatial and temporal accuracy. In addition, employed in a finite element setting, the use of level set-based RVE models provides new possibilities in multiscale modeling of crystalline materials.

Recognizing that the level set method has not yet reached its full potential when it comes to microstructure modeling, a number of developments of the method were recently proposed in [3], where also simulations of dynamic discontinuous recrystallization were performed. The suggested developments include an "interface reconstruction" method which has a number of useful implications. One example is the clear geometrical definition of grain boundary triple junction points, in contrast to standard level set implementations where triple junctions lead to artificial voids between the level sets. Another benefit is the possibility to prescribe boundary conditions along grain boundaries. A third gain is the observation of the possibilities by which gradient effects within the individual grains can be included, based on the distance information held in the level sets.

The present contribution discusses the level set formulation, proposed in [3], and its application to modeling of aspects of microstructure evolution in polycrystal solids. Possibilities related to mesoscale modeling of recrystallization and grain growth, formation of stored energy gradients due to dislocation pile-ups at grain boundaries and the evolution of grain boundary texture will be highlighted. The latter is based on the incorporation of anisotropic grain boundary properties in terms of grain boundary energy and mobility, which is an elaboration of the model in [3].

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The Thermodynamics of Gradient Elasticity and Plasticity

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The intention of this paper is to give a thermodynamical framework for the modeling of gradient effects in elastoplasticity. It is based on an approach by Ref. [1] and generalized to such gradient materials. In this case, not only higher kinematical variables are used, but also a thirdorder stress tensor is needed, see Ref. [2]. The theory is based on the assumption of identical thermoelastic behaviour in all elastic ranges which means that all measurable thermoelastic properties are not affected by plastic deformations. This concept has been introduced by Bertram Ref. [3] in the context of large deformations. In the present contribution, however, we limit ourselves to small deformations for the sake of simplicity and clearness.

After exploiting the assumption of identical thermoelastic behaviour, an example with a complete set of the thermomechanical constitutive equations is given, which generalizes the classical J2-theory to gradient plasticity. Then the restrictions from the second law of thermodynamics are worked out. The example still contains an arbitrary anisotropy. Finally, its reduction to the isotropic case by means of representation theory is shown. The example is formulated in a rather general matter, thus leaving enough space for specific models in particular applications, see Ref. [4]. An extension to finite deformations can be found in the preprint of Ref. [5]

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HOMOGENISATION OF DISLOCATION DYNAMICS

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It is well known that plastic, or permanent, deformation in metals is caused by the concerted movement of many curve-like defects in the crystal lattice, called dislocations. What is not yet known is how to use this insight to create theoretical predictions at continuum scales. It would be natural to take a sequence of systems with increasing numbers of dislocations, and derive an effective description in terms of dislocation densities. A mathematical procedure that proved to be very successful for the micro-to-macro upscaling is based on Γ-convergence, a variational convergence that is well known in the mathematical community and has been already applied to a variety of problems in materials science.

In [1] and [3] we used Gamma-convergence to derive a continuum description of the behaviour of walls of dislocations close to an obstacle, starting from a discrete model of the dislocation inter- actions. Our rigorous approach led to a family of upscaled models that we compared with other theories proposed in the literature, offering a selection criterion to identify the hidden assumptions in some of the previous derivations.

These first results provided a good starting point for the study of dislocation systems, in the static case. However, macroscopic plasticity is heavily dependent on dynamic properties of the dislocation curves. This motivated us to go further and try to extend our results to the dynamical case. In [2] we considered a discrete energy modeling the interactions among positive edge dislocations, in the single-slip case. We coupled the energy with a dissipation that allows dislocations to move only along their own slip planes. Moreover, we chose a mass preserving dissipation, and hence we did not allow sources or sinks for dislocations and only focused on the dynamics of a system of dislocations whose number is conserved in time. We analysed the asymptotic behaviour of the energy-dissipation system described above in the limit for a large number of dislocations, and we derived a limit evolution law for dislocation densities. This evolution law can be compared to the main models used in literature.

There are several steps we are going to take in the near future towards more realistic and complex systems, including the boundary-layer analysis for pile-ups of dislocations at an obstacle, the analysis of dislocation dipoles, and the multiple slip case.

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Dislocation density based plasticity model accounting for creep

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Previous work adapted a dislocation density based plasticity model [1] for AA 5083 [2]. However, temperature dependent coefficients were used for obstacle controlled glide indicating that some high temperature deformation mechanisms were missing. The current work has simplified the used model, constant coefficients, and added dislocation creep. It is at time of writing not clear if grain boundary sliding must also be accounted for. The used model has the following format, based on Bergström [3] as well as Frost and Ashby [4].

The flow stress is assumed to be an additive contribution

$$_{y}s = s_G + s_{HP} + s^* \tag{1}$$

The s_G term is an athermal stress due to long-range disturbances of the lattice due to immobile (forest) dislocations. It is called athermal, as thermal vibrations cannot assist the dislocation to overcome the disturbance of the lattice. s_{HP} is the grain size, Hall-Petch, effect. It is also a long-range contribution and accounts for the effect of stress concentrations at grain boundaries and the additional stress required to transmit the plastic deformation across grains.

The long-range stress term, s_G, in Eq. (1) is due interactions with the dislocation substructure [26]. It is an athermal stress contribution written as

$$s_G = amGb\sqrt{r_i} \tag{2}$$

where □ is a calibration factor, m is the Taylor factor, □$_i$ is the density of immobile dislocations and G is the temperature dependent shear modulus and b is the magnitude of the Burgers vector. The equation is combined with an evolution equation for the dislocation density. The short range term can be obstacle controlled glide

$$\sigma^* = \tau_0 G\left(1-\left(\frac{k_B T}{\Delta f_0 G b^3}\ln\left(\frac{\dot{\varepsilon}_{ref}}{\dot{\varepsilon}^p}\right)\right)^{1/q}\right)^{1/p} \tag{3}$$

Where t_0, Df_0, p and q are taken as calibration parameters. k_B is Boltzmann's constant. It can also be dislocation creep

$$\dot{\varepsilon}^p = A_c \frac{D_{eff}}{b^2}\frac{Gb^3}{k_B T}\left(\frac{\sigma^*}{G}\right)^n. \tag{4}$$

D_{eff} is effective self diffusivity, and A_c a calibration parameter. The mechanisms that requires lowest stress is taken as s^*.

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A Thermodynamically Consistent Cyclic Thermoplasticity Model

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The paper proposes a new model suitable for rate independent cyclic thermoplasticity. Therefore, it is especially suitable for low cycle fatigue in metals under nonisothermal regime. Starting from a carefully defined potential, the procedure is based on a variationally consistent numerical scheme that minimizes the incremental potential. Proposed model is based on the non-associated plasticity enabling nonlinear kinematic hardening and damage evolution. To keep framework as simple as possible, only isotropic scalar damage is assumed. Damage model relies on the continuum damage mechanics approach initially developed by the Lemaitre and Chaboche. Nevertheless, the proposed approach can accommodate rather complex material responses. It should be emphasized that the model does not involve the so-called Taylor-Quinney factor. The factor is widely used in popular finite element codes, mostly in the form of constant factor that multiplies dissipated plastic work. First deficiency is that this factor is not actually a constant, but rather a function of temperature, strain and strain rate. Rather straightforward extension can address this issue. However, the circumvention of Taylor & Quinney factor is of utmost importance in cyclic plasticity problems, since the model proposed by Taylor & Quinney can lead to the violation of the second-law of thermodynamics, as demonstrated within this paper. The current model does not suffer from such shortcomings. The part of the expended plastic work that is converted into heat follows consistently from energy minimization.

To obtain results as realistic as possible, heat exchange through conduction, convection and radiation is assumed. All material properties can be selected to be temperature dependent. Therefore, both type of problems – mechanically dominated, where mechanical process are source of heat and thermally dominated, where thermal effects lead to the change in material properties can be simulated. Regarding kinematics, the finite strain regime is assumed. A numerical example comparing numerical solution to experimental results is provided demonstrating efficiency of the proposed model.

Thermoplasticity coupled creep damage model for predicting behavior of P91 steel during Small Punch creep testing

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The need to increase plant efficiency has led to wide-spread usage of new creep strength enhanced ferritic steels which can be exposed to higher temperatures over extended service time intervals (e.g. boiler tubes of power plants). Modified ferritic/martensitic P91 steels that are preferred in power plant applications due their superior high temperature properties like lower thermal expansion coefficient, higher thermal conductivity and improved creep and oxidation resistance still require attention as regards the welding process and the long-term strength of their weldments, in particular, the susceptibility to creep cracking inside the Heat Affected Zone (HAZ) adjacent to the base metal that is referred to as Type IV cracking. Therefore, it is necessary to formulate constitutive material models to adequately describe the material response under various loading conditions, and to establish numerical procedures to predict the material behaviour.

A constitutive model coupling thermoplastic behaviour and creep damage is developed and implemented into Abaqus software for predicting the creep performance of P91 steel during Small Punch (SP) creep testing, a miniaturised test method capable of probing the individual zones of weldments. The numerical results are compared with experimental ones obtained under different test loads at a constant temperature of 600°C. There is good agreement observed between the experimental and the numerical deflection□time curves for the different creep stages and the creep rupture times. The predicted damage also compares well with the experiments.

PREDICTION OF CREEP-RUPTURE PROPERTIES FOR AUSTENITIC STAINLESS STEELS UNDER GONE NEUTRON IRRADIATION

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The paper presents the physical and mechanical model that allows predicting fracture of materials subjected to neutron irradiation under creep. The model is based on the equations of void nucleation and growth on grain boundaries that were proposed earlier. The equations are developed for the case of neutron irradiation of a material. The constitutive equations describing viscoplastic deformation of a material with regard to void evolution are formulated. The criterion of microplastic collapse of a unit cell is used as a fracture criterion. The creep-rupture strength and ductility of austenitic materials in the initial and irradiated conditions with different neutron flux levels are predicted on the basis of the model. The calculated results are compared with the available experimental data.

In-service corrosion-hydrogen degradation of structural steels and its experimental modeling

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Technical expertise of the integrity of long-term operated structures should take into account both detection of defects and evaluation of degradation of relevant materials properties. This problem is of particular importance for structures that operate in corrosive environments. The in-service degradation of mechanical, corrosion and corrosion-mechanical properties of structural steels operating in corrosive environments is considered in the paper. This study considers in particular the corrosion environment as a source of metal hydrogenation and subsequent acceleration material degradation.

In-service degradation of structural steels under ambient and elevated temperatures is considered. The important role of hydrogen in-bulk material degradation is demonstrated. Experimentally shown that hydrogen rises creep rate in power steels, evidently, due accelerating diffusion processes, like temperature increase. On this base and using Larson-Miller approach the method of a prediction of hydrogen effect on creep rate is proposed.

The different mechanisms of material degradation are considered: deformation strengthening, deformation aging (Cottrell atmosphere formation) and dissipated damaging, and connected with it the specific of a change of the mechanical properties.

Since the long-term in-service properties degradation consisted mainly in a decrease of the brittle fracture toughness, the tests under the embrittling conditions (notched or pre-cracked specimens, impact loading, preliminary hydrogenation and low temperature) provide high sensitivity to in-bulk material degradation.

The two in-laboratory methods of simulation of in-service steel degradation are considered. The first one is intended for elevated temperatures and consists in high speed thermocycling of specimen in hydrogen atmosphere from working to ambient temperatures, using a possibility to fix a huge hydrogen concentration at low temperature. The second one is intend for ambient temperature and consists in preliminary hydrogenation of specimen by electrolytic charging, holding of specimen up to 30 days under static stresses that corresponds to service conditions and heating of specimen at 250 °C for hydrogen desorption and deformation aging.

The fact that some electrochemical parameters are very sensitive to in-service degradations of steels is used by a new electrochemical NDT method for prediction of mechanical properties degradation, which is based on the built correlations between electrochemical and mechanical characteristics. In this connection the special problem should be resolved: a choose of electrolyte which satisfies the high method sensitivity.

Advanced Materials for Future Nuclear Energy Technologies

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Future energy technologies will place increasing demands on materials performance with respect to extremes in stress, strain, temperature, pressure, chemical reactivity and radiation flux. Understanding how these extreme environments affect the physical and chemical processes that occur in the bulk material and at its surface will enable the design of materials with greatly enhanced performance. First part of this talk will introduce nuclear fusion reactors as a potential source of sustainable energy and the material related challenges in realizing this energy source. Second part will focus on the challenges related to tungsten alloys and review their behavior under extreme irradiation environments. Microstructure refinement via surface deformation will be demonstrated as a way to increase irradiation damage resistance of tungsten.

Integrated experimental-numerical analysis of microstructural strain and stress evolution in bulk nanostructured alloys

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Microscopic strain and stress partitioning among the present phases govern the macroscopic mechanical response of multi-phase alloys. However, these phenomena are challenging to probe due to the multiple scales involved, dynamic nature of the deformation process, and lack of dedicated methodologies. The challenge is even more enhanced for multi-phase alloys with features smaller than micrometer scale.

A novel approach is introduced in this work that strengthens the connection between microstructure and mechanical properties in such alloys. To this end, numerical simulations and experiment analyses are carried out in an integrated manner to investigate the microstructural deformation mechanisms in multiphase microstructures.

For the experiments, a novel, in-situ SEM imaging and digital image correlation (DIC) based methodology is developed that allows concurrent microstructure and strain mapping at sub-micron resolution. Strain mapping is achieved by the application of a layer of nanoparticles on the sample surface (as the DIC pattern) that are selectively imaged during deformation. Concurrent microstructure mapping is achieved by optimization of imaging conditions to minimize the interference of the DIC pattern nanoparticles.

For the simulations, the electron backscatter diffraction (EBSD) map of the undeformed state of the same in-situ investigated microstructural patch is used to create the model. 2D full-field crystal plasticity simulations are run employing a recently developed spectral solver suitable for high-phase contrast materials implemented in the crystal plasticity simulation-kit DAMASK. The individual phase properties are obtained by additional inverse CP simulations of nanoindentation experiments carried out on the original microstructure.

The methodology will be demonstrated here on the example of martensite-ferrite dual phase (DP) steel, for which promising correlation between the simulations and experiments is achieved, despite the complex micro-mechanics of this material.

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Void Coalescence through Internal Necking

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Coalescence of voids through internal necking is ubiquitous in metal alloys. In a recent study, Thomason's criterion for the onset of void coalescence through internal necking [1] is extended to include the effect of shear loads, by performing plastic limit load analyses in a finite element (FE) framework [2]. Limit load analysis in a standard FE framework requires applying a large load step with no geometry update. This means that the equilibrium equations are solved in the initial (undeformed) configuration, i.e., the void growth phase is bypassed and void coalescence occurs in the initial configuration. The aim of the present study is to investigate the effects of void growth and void shape changes on internal necking. For this purpose, three dimensional voided unit cell calculations are performed for a large range of different stress triaxialities and void sizes/shapes. The predictive capacities of the original Thomason's criterion as well as of its modified/extended versions are critically assessed through comparison with the FE results in terms of the best agreement for the mesoscopic strain of the unit cell at the onset of void coalescence. The modified criteria given in [2] provide accurate predictions in comparison with the FE calculations.

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Crystal plasticity constitutive modeling calibration of polycrystalline IN718 superalloy grains based on microcompresion tests

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A phenomenological crystal plasticity (CP) model was developed to simulate the elasto-plastic behaviour of IN718 grains. A polycrystalline sample of IN718 was used for this investigation with an average grain size of 150 µm. The microstructural characterization revealed that the sample was mainly composed of γ phase, with negligible contents (<1 vol. %) of δ phase particles at the grain boundaries and MC carbides. The micro-compression tests were carried out in single-crystal orientations, by machining single-crystal micropillars inside individual grains using a focused ion beam (FIB) system and compressing them using a flat punch inside an instrumented nanoindentation system. Different micropillar compression tests were performed to quantify the effects of pillar diameter, strain rate and pillar orientation.

The parameters of the CP model were fitted from the micro-compresion tests results. A finite element (FE) model of the micropillar was used to perform a sensitivity analysis of the different geometrical parameters in order to better understand the experimental testing results for the fitting of the CP model. The calibration of the CP model was done by considering only the plastic contribution of the experimental stress-strain curves, avoiding the initial tip-micropillar misalignments and the local plastic flow prior to pillar yield. The resulting CP model was finally evaluated by comparing the simulation of other independent micro-compression tests with the corresponding experimental result and the agreement was remarkable in all the cases.

The CP model was applied then in a 'Representative Volume Element' of the polycristalline IN718 through a periodic Voxel-type polycristalline FE model. The mechanical behaviour of the polycristalline FE model (based on single crystal properties) was compared in the end with the macroscopic response of this material. This model represents the basis to develop a realistic polycristalline FE CP model of IN718.

Material Tests of the Polyurethane by Using the Digital Image Correlation Measurement Method

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The material properties and the stress relaxation characteristics of the polyurethane (PU) material are determined by using Digital Image Correlation (DIC) measurement method. Tests are performed for two different strain levels by two different strain rates. Specimens are stretched up to 20% and 30% engineering strain level by 100 mm/min and 500 mm/min displacement speeds. Extensometers are generally used to measure the strain values of PU materials. However the accuracy level of the extensometers is very low compared to DIC. The strain levels involved in the experiments are also high for strain gages which are useful for low strain values. However with the DIC system, it is also possible to measure true strain values and thickness reduction values of the specimens. The DIC system includes two 4 M cameras, controller and a computer. The Aramis software is used to process the images to determine the true strain and stress values. Tests are performed on a 10 kN machine and images which are processed with the Aramis system to determine the major, minor strains and the thickness reductions. Specimens are left for stress relaxation for two hours following the load application at two different strain rates. During the relaxation period, load values are measured by the load cell of the tensile test machine, and true stress versus time curves are determined utilizing the true strain values measured by the DIC system. Finally, Prony series with 5 terms of the true stress versus time curves are determined by the MSC Marc software to be used in the stress analysis of the PU material.

Intersonic Delamination in Curved-Thick Composite Laminates under Quasi-Static Loading

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In aerospace industries, new advances in composite manufacturing technology enable to produce principle structural elements as composite materials in complex shapes. However, Interlaminar Normal Stresses (ILNS) are induced once a moderately thick laminate takes highly curved geometry such as an “L” shape. ILNS promotes mode-I type of delamination propagation which is the weakest fracture mode for conventional composite laminates. This is a problem that has recently risen to the forefront in in-service new composite civil aircrafts. This study presents on experimental and computational investigation of dynamic delamination in a 12-layered Graphite/Epoxy woven fabric L-shaped laminates under quasi-static loading. The delamination initiation and propagation processes were captured using a million fps high speed camera which revealed intersonic crack tip speeds around 2500m/s. The experiment is modeled using cohesive zone modeling by implementing a rate-dependent bilinear cohesive model into ABAQUS/Explicit. The numerical results are in good agreement with the experimental results including shear wave speeds, load-displacement curves and fracture pattern. Shear Mach waves fronts, follower reflecting waves, train of pulses in normal stresses and vortex like particle velocity patterns are observed in the simulations.

Crystal plasticity phase transformation model for metastable austenitic stainless steel

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Transformation induced plasticity (TRIP) has a large contribution in providing high strength with high ductility to metastable austenitic stainless steels. Metastable austenite (a softer phase) transforms into martensite (hard phase) during the deformation of the steel. This enhances the strain hardening behaviour and postpones the necking phenomenon. We have proposed a precise micromechanical model to describe the mechanical behaviour of this steel which can also be extended for TRIP steels in future. Our efforts to model the deformation behaviour of this steel include the prediction of phase transformation and its influence on mechanical properties of the steel. To account for inhomogeneous plastic deformation (caused by grain boundaries and phase transformation) strain gradient effects have been added to the model. The non-local crystal plasticity (CP) model takes into account both, isotropic and kinematic work hardening, provided by geometrically necessary dislocations (GNDs). The main feature of our phase transformation model is the separate treatment of strain induced nucleation and stress assisted growth of martensite. An explicit relation between martensite nucleation and plastic deformation has been considered. Stress assisted growth can also occur before the yield stress of austenite is reached, depending on the thermodynamic driving force provided by elastic deformation. We have applied this model to a realistic microstructure (obtained from EBSD orientation maps) to study the influence of phase transformation, grain boundaries and internal stress (provided by GNDs) on the deformation behaviour of the steel. Our results also reveal the importance of internal stresses occurring during the deformation for the global mechanical behavior.

An inverse optimization strategy to determine single crystal mechanical behavior from polycrystal tests: application to Mg alloys

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An inverse optimization strategy was developed to determine the single crystal properties from experimental results of the mechanical behavior of polycrystals. The polycrystal behavior was obtained by means of the finite element simulation of a representative volume element (RVE) of the microstructure in which the dominant slip and twinning systems were in the constitutive equation of each grain included (basal, prismatic, pyramidal slip and extension twinning). This work is based on the crystal plasticity model developed in [1] and implemented as a UMAT in the finite element code ABAQUS. Kalidindi's model was used for the twinning [2] mechanism and a power-law was chosen to lead the elasto-viscoplastic flow (so in plastic slip rate as on twinning volume rate). The inverse problem was solved by means of the Levenberg-Marquardt method [3, 4], which provided an excellent fit to the experimental results. This method is based on minimizing an objective function $O(\boldsymbol{\beta})$ (1) that depends on the comparison between the experimental curves (**y**) and the numerical curves $f(\boldsymbol{\beta})$. These last ones are obtained by the finite element analysis of the RVE with a set of parameters $\boldsymbol{\beta}$ which define the single crystal behavior for the boundary conditions considered.

$$O(\boldsymbol{\beta}) = \sum_{i=1}^{n} \left| y_i - f(x_i, \boldsymbol{\beta}) \right| = \left\| \mathbf{y} - \mathbf{f}(\boldsymbol{\beta}) \right\| \qquad (1)$$

The iterative optimization process followed a hierarchical scheme in which simple representative volume elements were initially used, followed by more realistic ones to reach the final optimum solution, leading to important reductions in computer time (Fig. 1).

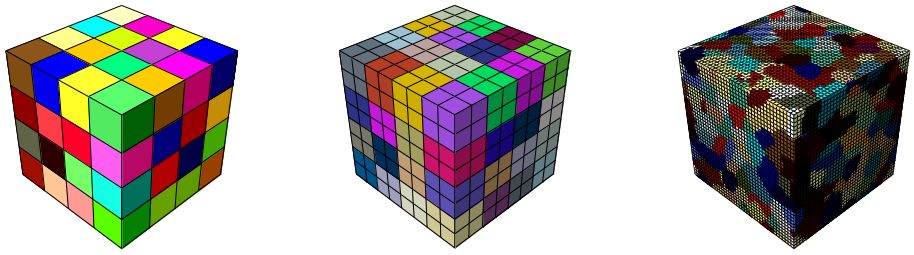
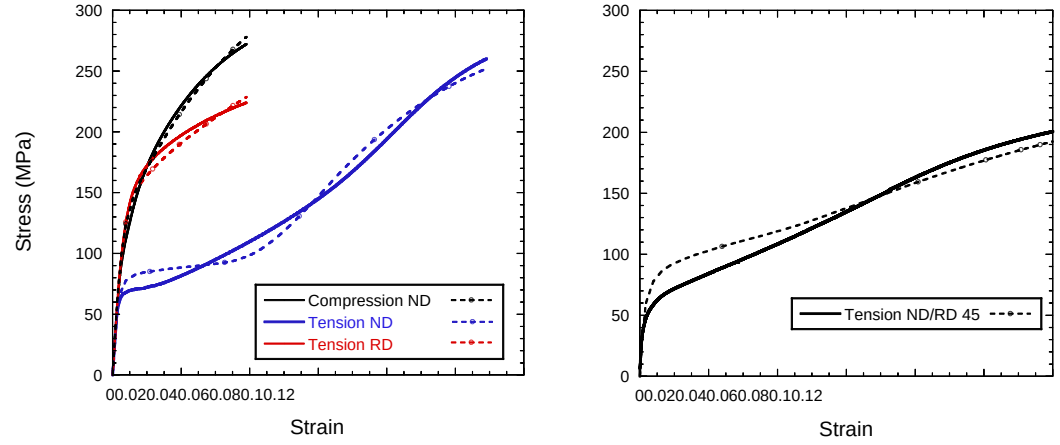


Figure 1. Different RVEs of the polycrystal microstructure

The new strategy was applied to identify the initial and saturation critical resolved shear stresses and the hardening modulus of the active slip systems and extension twinning in a textured AZ31 Mg alloy [4] and in the MN10 and MN11 rare earths Mg alloys.

The AZ31 adjust was very precise (Figure 2a) and the results were in general agreement with the data in the literature ($CRSS_{twinning} > CRSS_{basal}$) (Table 1) but also showed some differences. They were partially explained because of the higher accuracy of the new optimization strategy but it was also shown that the number of independent experimental stress-strain curves used as input is critical to reach an accurate solution to the inverse optimization problem. It was concluded that at least three independent stress-strain curves are necessary to determine the single crystal behavior from polycrystal tests in the case of highly textured Mg alloys. Furthermore, this allows to predict other independent load cases with precision (Figure 2b).

By reference to the MN10 and MN11 values obtained from the optimization, the CRSSs changed as the volume fraction of rare earths increased, from pure Mg to MN10 and MN11 (0-0.5 and 1 % respectively) (Table 1). The method showed that the CRSSs of basal and twinning modes increase while the CRSSs of pyramidal and prismatic systems decrease respect pure Mg values of reference [6]. In parallel, the ratio of CRSS of twinning respect basal was reduced producing a promotion of twinning in every direction. All these changes were more pronounced on MN11, with a higher content of rare earths. In this case the macroscopic behavior was almost isotropic and the values obtained for the CRSSs were very similar for all the systems.



Figures 2a and 2b. Adjusted and predicted curves on AZ31

	System	Mg	AZ31	MN10	MN11
τ_{crit} (MPa)	Basal	1.75	23	12	40
	twinning	3.5	35	24	42
	Prismatic	25	80	65	46
	Pyramidal c+a	40	88	75	50

Table 1. Fitted CRSS on the Mg alloys AZ31, MN10 and MN11

The procedure developed has a great potential because it will allow to determine the influence that the alloying elements have on the crystal behavior or the effect of other material parameters (temperature, strain rate, grain size, etc.) by a simple comparison of the adjusted microscopic properties under different scenarios.

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An enhanced Mori-Tanaka Homogenization Scheme for Incremental, Non-Linear Rate-Independent Plasticity

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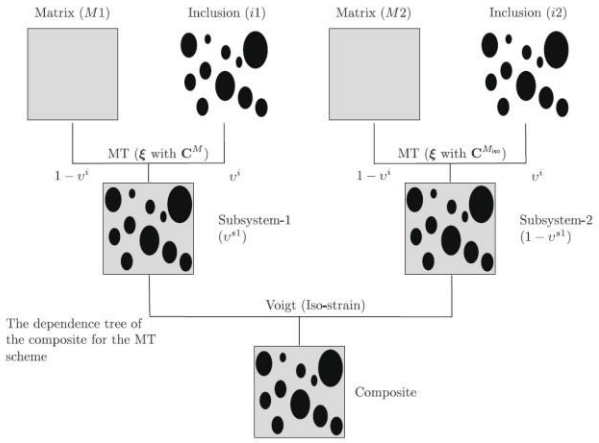

Fig. 1. Schematic diagram showing the dependence tree for the enhanced Mori–Tanaka (MT) based homogenization model [1].

Recently, a method has been developed to extend the Mori-Tanaka mean-field homogenization scheme to the non-linear material's response range for composite materials made of an elasto-plastic matrix containing elastic particles [1]. The key idea in this method is to perform multi-step homogenization with two subsystems as shown in Fig. 1. For subsystem-1 (volume fraction υ^{s1}), the tangent operator of the matrix material, C^M, is used to calculate the Eshelby tensor ξ. *CM* is a fourth order anisotropic tensor, even if the matrix material is isotropic. In order to calculate the Eshelby tensor for subsystem-2 (volume fraction 1-υ^{s1}), the isotropic part of the tangent operator of the matrix material, $C^{M\text{iso}}$, is used. Numerical simulations show that using only subsystem-1 leads to stiffer results, and subsystem-2 to more compliant results when compared to finite element calculations in terms of the overall stress/strain behavior of the composite. Therefore, the overall response of the composite is obtained by combining the two subsystems through an iso-strain (Voigt) homogenization. Now, the volume fraction υ^{s1} can be fine-tuned with respect to the FE calculations (as well as to experiments) in order to obtain the best agreement in terms of both the overall and the per-phase response. In this study, the proposed method is extended for composites where both the inclusions and the matrix are elasto-plastic. An extensive parametric study is performed and the variation of υ^{s1} with mechanical properties of both phases is investigated. The capabilities and the limitations the proposed method are critically addressed for a wide range of elasto-plastic materials.

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ACKNOWLEDGEMENTS

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Comparison of dislocation-based model of recovery and cross-correlation based EBSD measurements in single crystals

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Subgrain growth during recovery has been investigated using simulations of two-dimensional discrete dislocation dynamics on a hexagonal lattice having three symmetric slip planes [1]. To account for elevated temperature (i) dislocation climb was allowed and (ii) a Langevin type thermal noise was added to the force acting on the dislocations. The growth exponent and the subgrain structure were examined.

Cross-correlation based analysis of electron backscatter diffraction (EBSD) patterns is often carried out to map plastic strain variations in deformed polycrystalline samples [2]. Firstly, the effects of sample surface preparation methods were investigated including Ar ion polishing and traditional electropolishing treatments. Then the distortion maps of the specimen are computed with the cross-correlation technique. This method is capable of detecting changes of the crystal orientation to higher accuracy, than the commercial software provided for standard EBSD devices that analyze each EBSD pattern individually.

In this work the simulation and experimental results were compared to characterize the evolution of dislocation structures and corresponding distortion fields in highly deformed Cu single crystals during low temperature annealing.

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Effect of Size on Nanoindentation and Compression of □-Fe Single-Crystal Nanoparticles: A Molecular Dynamics Study

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Using Molecular Dynamics (MD) simulations, we investigate how the mechanical properties of □-Fe (a BCC metal) nanoparticles depend on their size. Nanoparticles of various sizes were constructed based on the Winterbottom (Wulff) construction. The nanoparticles were either indented or compressed and their mechanical response, as well as the underlining dislocation mechanisms during the deformation, was simulated.

In contrast with our previous observations in FCC metals [1], we did not observe an indentation size effect. A detailed analysis revealed that ½<111> edge dislocations were nucleated on the (110) plane on the interface between the indenter and nanoparticle. However, these were pinned on both ends to the contact area with the indenter. As the indenter is further lowered into the nanoparticle, one or both edges of the dislocations are unpinned from their nucleation site and the edge dislocation glides towards the lateral facets. Examining several particle sizes and aspect ratios, as well as thin films, we show that this mechanism, which is different than that reported in FCC metals, is size independent.

Under compression, the nanoparticles yielded at size dependent compressive stresses, which can be described by a power-law. The plastic yield is followed by a hardening stage, which is also size dependent. The yield point corresponds to the nucleation of ½<111>{110} edge dislocations at the top vertices of the upper facet. The edge dislocations extend on their glide plane into the particle until reaching the substrate or intersecting with other nucleation dislocations.. The stress needed to nucleate the dislocation at the vertices is size dependent due to the stress gradients in the nanoparticle. At the hardening stage, new dislocations are nucleated at the upper vertices on the same planes, resulting in a pile-up which is responsible to the hardening. At a certain compressive stress, the pile-up vanishes, leading to a large plastic deformation in the nanoparticle. The compressive stress at which the pile-up vanishes corresponds to the number of dislocations that accumulate in the pile-up, which in turn depends on the nanoparticle's size.

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Nanoindentation study of iron nanoparticles produced by solid state dewetting

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We employed the nanoindenting atomic force microscopy (AFM) for studying mechanical response of submicron Fe particles produced by solid-state dewetting of 25 nm-thick Fe film on sapphire. The particles were strongly faceted, with the {011} top facet parallel to the substrate. These crystals were indented by a sharp diamond tip in the AFM and exhibited elastic behavior up to very high stresses, followed by an abrupt displacement burst (pop-in). The hardness of the particles was calculated employing a method based on the work of indentation, and the resulting values were compared with the hardness of coarse grain polycrystalline Fe. The majority of the particles showed significantly higher values of hardness than the bulk, and analysis of the data revealed that particles become harder as their aspect ratio decreases. A simple model of particles hardening based on back-stress from dislocation pile-ups at the Fe-sapphire interface was proposed.

ω phase accommodated nano-twinning mechanism in Gum Metal: an *ab initio* study

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Gum Metal is a recently developed Ti-Nb-based alloy with exceptional mechanical properties. More interestingly, it is claimed to exhibit dislocation-free plasticity. A unique deformation micro-mechanism termed as the "giant fault mechanism" is proposed to be active in this material, however, this claim is disputed in various recent studies reporting presence of different deformation mechanisms (i.e. slip, stress-induced martensite and twinning). Our investigations reveal that the addition of oxygen to this system modifies the dominant deformation mechanism from stress-induced martensitic transformation and {332}<113> macro-twinning mechanisms (for low oxygen contents) to ω phase accommodated {211}<111> nano-twinning mechanism (for the Gum Metal composition). In the present work we theoretically investigate the local transition mechanism of the β phase to the ω phase along the {211}<111> twin boundary. Our results based on *ab initio* energetics calculations and linear elastic inclusion theory indicate that the elastic strain energy play a minor role in the β to ω transition, and an energy barrier exists on the energetic pathway. It is shown that the energy barrier can be overcome by the {211}<111> shear stress, explaining why {211}<111> twinning induces the local formation of ω phase along the twin boundary. The ω phase in turn represses the propagation of the twin along its transverse direction and confines the twin in nano dimensions.

Velocity relaxation in 3D dislocation system

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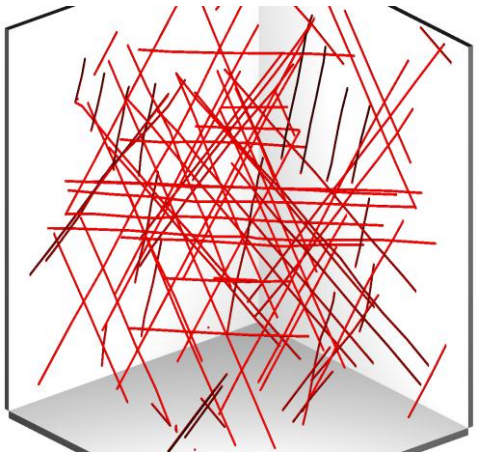
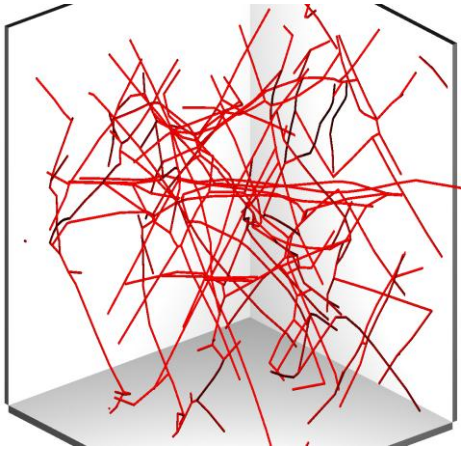
Plasticity in crystalline materials is due to motion of crystal defects known as dislocations. Dislocations create an anisotropic stress field around themselves which can be quite complex giving rise to rich variety of possible interactions. These interactions generate a complex free energy landscape which can trap the dislocations to metastable states. One commonly used method to initiate dislocation systems in simulations is to position the dislocations randomly. This random configuration however is not in equilibrium and the systems starts to relax toward its free energy minimum. In order to model realistic physical systems the details of this relaxation are important.

Simulations of simplified 2D dislocation models [1] have shown that the velocity relaxation follows a power-law in time which is typical of frustrated glass-like systems.

Random initial configuration



Relaxed configuration



Here 3D discrete dislocation dynamics (DDD) code ParaDis [1] is used in order to simulate velocity relaxation of dislocations in Aluminum. 3D DDD is a method where three dimensional dislocation segments are modeled as straight lines connected by discretization points. The stress field is obtained from linear elasticity theory. The code is modified so that it calculates the average normal component of the segment velocity.

Our result's show that velocity relaxes as a power-law in time also in three dimension. This leads to the conclusion that when simulating realistic systems one should relax the initial configuration to an equilibrium state before external stress is applied.

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MEMS-BASED MICRO TENSILE TESTING DEVICE

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A microtensile test device for the determination of elastic modulus and fracture strength of silicon nanowires (SiNW) is designed. Uniaxial deformation of SiNW is induced by an electrostatic comb-drive actuator and the displacements are measured by a differential capacitive sensor. SiNW is fabricated between the actuator and the sensor monolithically. A code is generated and utilized for the optimization of the device geometry. The overall performance of the device is analyzed via finite element analysis. N type SOI wafers having 10μm device silicon layer and 2μm BOX layer are used for fabrication. Fabrication of devices is in progress.

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Modeling of Spherulite Microstructures in Semicrystalline Polymers

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

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

Modeling Slip-Twin Interactions in High-Manganese Austenitic Steels

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High manganese austenitic steels (HMnAS) attained interest for decades due to their applicability in different industries, such as automotive, defense, railroad and mining. These steels having high strength, ductility, toughness and large strain hardening capacity, in addition to their outstanding wear resistance become important. Many studies had been conducted so far to be able to maximize their performance and fully understand the underlying reasons of the rapid strain hardening of HMnAS.

Previous studies showed that simultaneously active different micro-deformation mechanisms exemplifying slip, twinning, phase transformation, stacking fault and dynamic strain aging, are responsible for their significant strain hardening capacity. Temperature, strain rate and chemical composition are important parameters determining which one of the given deformation mechanisms will dominate the deformation. In HMnAS not only slip and twinning are activated simultaneously during large portion of the deformation, but also they interact with each other providing further strain hardening. During plastic deformation, if twinning is the dominant deformation mechanism, secondary or tertiary twin systems may also be active besides primary twinning system. Additional involvement of the grain boundaries, twinned regions and interstitial interactions provide additional complexity to micro-deformation process.

In the current study; to understand the exact cause of the rapid strain hardening in HMnAS, high-velocity compression tests with different velocities at different temperatures were practiced. Three different steels named as Hadfield, X-IP and TWIP (TWinning Induced Plasticity) were tested. Formation of vast amount of nano-twins within the already developed twins was discovered in Hadfield steel sample. Nano-twins inside twinned regions had been reported before; however they were visible only via detailed microstructural analysis. To the best of authors' knowledge; in the current study, massive nano-twins found within pre-formed twins were visible on the sample surface. They were easily examined even via confocal microscopy. On the other hand no nano-twin formation inside primary or secondary twins is captured on TWIP or X-IP steels.

A visco-plastic self-consistent (VPSC) crystal plasticity approach is utilized for prediction of macroscopic response behavior of materials making use of their microscopic deformation mechanisms and textures. This algorithm models the plastic deformation of the material under external strains and stresses considering reorientation and the shape change of the grains. However, VPSC does not incorporate the specific problems of high manganese austenitic steels. For instance massive twinning activity, the effect of high angle grain boundaries on dislocation-grain boundary interactions or the effect of high density dislocation walls were not included in the algorithm. Consequently, formulations solving the incomplete strain hardening equations were proposed and added to VPSC for modeling the high manganese austenitic steels. In the light of new experimental results, significant role of twinning in the low strains and twin-slip interactions were modelled utilizing VPSC. Modified algorithms were successful predicting the texture evolutions and deformation responses.

Micromechanical modeling of strength of tempered martensite

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Keywords: Martensite laths, Orientation relationships, Crystal Plasticity modeling, homogenization

Tempered martensite is known for its complex hierarchical microstructure consisting of laths, subblocks, blocks and packets that all have special crystallographic orientation relationships [1-2]. This type of microstructure is a key in determining the micromechanical behavior of martensitic steels.

This work mainly focuses on the simplified representation and homogenization of the hierarchical microstructure of tempered martensite. The crystallographic orientations are described based on the generally observed Kurdjumov-Sachs orientation relationship. We applied local and non-local crystal plasticity finite element formulations [3-4] to predict the yield onset and plastic deformation of martensitic microstructures on the basis of single crystalline regions within the sub-blocks or blocks.

With this micromechanical model of martensite the anisotropy in the material response to multiaxial mechanical loading with respect to the orientation of the microstructural units is investigated. The global mechanical behavior of the micromechanical models is represented by yield curves and stressstrain plots and it is found that larger misorientations between microstructural units and more complex microstructures lead to a more isotropic global mechanical behavior, but at the same time cause larger internal stresses from which cracks or other defects might originate.

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TEMPERATURE DEPENDENT CRYSTAL PLASTICITY MODEL FOR THE PREDICTION THE MECHANICAL PROPERTIES OF NANO-TI

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Computational homogenization by means of the finite element analysis of a representative volume element of the microstructure is used to simulate the deformation of nanostructured Ti. The behavior of each grain is taken into account using single crystal plasticity (CP) models which include the microscopic mechanisms of plastic deformation by slip along basal, prismatic and pyramidal systems. Pure empirical CP models and physically motivated ones are used to model the effect of temperature on the mechanical response.

An inverse analysis technique was used to obtain the effect of temperature on the deformation of nano-Ti produced by ECAP-C and drawing. The inverse analysis was done by the adaptation of a Levenberg-Marquardt optimization method and aims to obtain the grain behavior from macroscopic compression tests performed under different temperatures. The results of the polycrystalline model combined with the optimization method and the compression tests led to the evolution of the slip on the different active slip systems. It was observed that the evolution of the activities of the different slip systems changed non-proportionally with the temperature and the systems with the highest CRSS at room temperature reduced their resistance at high temperature at almost the same value as the soft ones.

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A variational approach to gradient plasticity based on non-convex plasticity energies

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Incremental energy minimization represents a powerful mathematical tool, which was applied to fracture mechanics, damage and many other problems. In the present work it is used in the context of gradient plasticity for describing the evolution of the deformation in materials whose energy is given by the sum of three terms: an elastic bulk energy, a dissipative cohesive energy, and a non-local gradient term. In the one dimensional setting, the model was successfully applied to the study of plastic slip patterning, and to analyze the response of bars to tensile loadings. It has been recently extended to two dimensional crystal plasticity, and some preliminary numerical results are presented and discussed.

Graded, ultrafine-grained, ferrite/martensite dual phase steel

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By microstructure refinement, ferrite/martensite dual phase (DP) steel is reported to achieve higher strength without sacrificing uniform ductility. In order to further increase its ductility without sacrifice of strength, we studied the effect of introducing microstructure gradients at the macroscopic scale. To this end, DP steel samples with ultrafine-grained (UFG) middle layer sandwiched between coarse-grained (CG) outer layers are produced employing a hot/cold deformation simulator. The strain partitioning at the micro-scale is investigated by means of in-situ deformation experiments and associated novel high resolution correlative strain and microstructure mapping methodology.

Results of the uniaxial tensile tests reveal that the DP steel with ultrafine-grained (UFG) middle layer and coarse-grained (CG) outer layers exhibits doubled ductility for the same ultimate tensile strength, compared to the monolithic UFG DP steel. Preliminary numerical analyses reveals that the enhanced ductility is arising due to the stress state difference between UFG and CG layer which leads to internal compressive stresses and hinders damage nucleation and macroscopic localization.

Modeling deformation and fracture in Ni nanowires at various temperatures using Cleri-Rosato potential

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The mechanical properties of Nickel nanowires have been studied at different temperatures using molecular dynamics simulations. Molecular Dynamics (MD) simulations have been carried out on pure Nickel (Ni) crystal with face-centered cubic (FCC) lattice upon application of uniaxial tension at nanolevel with a speed of 20 m/s. The deformation corresponds to the direction <001>. To the calculated block of crystal - free boundary conditions are applied in the directions <100>, <010>. A many-body interatomic potential for Ni within the second-moment approximation of the tight-binding model (the Cleri and Rosato potentials) was employed to carry out three dimensional molecular dynamics simulations. MD simulation used to investigate the effect of temperature of Ni nanowire on the nature of deformation and fracture. Temperature effect on the extension property of metal nanowire is discussed in detail. The mechanical strengths and the mechanical strain of the nanowires decrease linearly with the increasing temperature. The feature of deformation energy can be divided into four regions: quasi-elastic, plastic, flow and failure. Experiments have shown that when the temperature increases the yielding stress decreases, the first stage of deformation was narrowed, and the second stage was widened. The results showed that breaking position depended on temperature. The simulation results at nanoscale play an important role on the mechanical behaviors of nanostructures.

Compatibility concept: A way to make the continuum plasticity size dependent

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Galileo possibly was the first person who performed cantilever beam bending experiment and discovered that one cannot simply double or triple the dimensions of a beam, and expect it to carry double or triple the load. This observation is what we today know as the "*scaling laws*" in continuum mechanics. Recently, however, lots of small-scale experiments confirm signifiant changes in the material behaviors compared to their conventional counterparts [1]. In crystalline metals, this size effect may attributed to the defects distribution (e.g. dislocation) which give rise to enhanced strengthening and hardening responses as the characteristic micro-structural sizes (e.g. grain size, dislocation spacing) become comparable to the specimen size. Similar observation could be expected on the response of such miniaturized specimens under cyclic loading. For example, one may observe dramatic changes in the asymmetry of the stress-strain response with a reduction in the specimen size. While the conventional continuum plasticity phenomenologically incorporates the kinematic hardening, it does not address the size dependent asymmetry of the stress-strain response.

In this work, a recently developed non-local continuum plasticity framework [2] will be utilized to investigate size-dependent cyclic response of single crystalline micro-beams. The continuum plasticity is enriched to include the meso-scale information of the dislocation kinematics and kinetics via revisiting the strain (and lattice curvature) compatibility equation. Accordingly, a three-dimensional internal stress tensor (a.k.a. back-stress) evolves due to the non-homogeneous distribution of the excess dislocation density and corresponding image effects from the free surfaces. This internal stress appears as additional resolved shear stresses in the crystallographic visco-plastic constitutive law for individual slip systems.

The results exhibit a strengthening-like behavior under monotonic loading and exhibits a length-scale dependent asymmetry under cyclic loading. Various size-dependent hardening mechanisms and their contribution on overall response will be discussed. Furthermore, the reversible plastic deformation mechanism associated to the structural rearrangement of excess dislocations will be discussed. This may explain the absence of cyclic hardening in micron scale in contrast to its bulk counterparts. A comparison with experimental results [3] suggests that the length-scale for internal stresses, described as a correlation length-scale, should increase with decreasing specimen thickness.

This observation is rationalized by associating the internal length-scale with the average slip-plane spacing, which may increase with decreasing specimen size due to paucity of dislocation sources [4].

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Crystal Structure and Physicochemical Properties of Two Supramolecular Compounds: $(C_4H_8NH_2)_4[Mo_8O_{26}]$ and $(NH_4)Na_2[As^{III}Mo_6O_{21}(O_2CCH_2NH_3)_3]8H_2O$

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Two inorganic–organic hybrid supramolecular compounds based on polyoxometalates formulated as $(C_4H_8NH_2)_4[Mo_8O_{26}]$ (1) and $(NH_4)Na_2[As^{III}Mo_6O_{21}(O_2CCH_2NH_3)_3].8H_2O$ (2) have been synthesized by conventional solution method and characterized by infrared, UV–Vis and single-crystal X-ray diffraction analyses. Thermal analysis was performed to study their thermal stability. The atomic arrangement in compound (1) can be described as inorganic layers built by $[Mo_8O_{26}]^{4-}$, pyrrolidinium cations are embedded into layers. The ascinating structural feature of compound (2) is that the glycine molecules are bounded to two edge-sharing Mo centers via their carboxylate functionality leading to functionalized heteropolymolybdate $[As^{III}Mo_6O_{21}(O_2CCH_2NH_3)_3]^{3-}$, extensive net hydrogen bonds between cations and anions contribute to the crystal packing. The electrochemical behavior of compound (2) has been studied.

Modeling of initiation circumstances for IASCC; research the effects of irradiation on stress corrosion damage

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IASCC has not been observed globally in PWR internal structures, however, its appearance can be expected in the future. Some of the cracks occurred in the baffle bolts have been attributed for IASCC. Furthermore, IASCC cracks were found in internal structural elements of the active zone of the reactor (such as the coating of the control rod). This shows that IASCC is an assumed aging process for reactor internal structures, which should be taken into account during the long time operation.

The aim of the research is to compare the effect of the caused processes due to irradiation and heat treatment, as well as forming on the stress corrosion crack propagation in case of 08H18N10T/08H18N12T austenitic stainless steel and to prove that the effect of the irradiation assisted embrittlement can be modelled using suitable heat treatments, which allows the laboratory tests in non-active environment. The main structural material used for WWER 440 for RVI is titanium stabilized austenitic stainless steel 08Ch18N10T (equivalent to A-321).

As a result of cold forming, austenite hardens, its toughness and deformation capability decrease, its strength increases, so that the cold plastic deformation has the same effect as the radiation in macroscopic scale. The heat treatment and pre-forming simulation method can be combined with ion radiation which can approximate the effects of neutron radiation in the surface layer quite well. The ion radiation does not activate the surface, but because of the different physical processes, calculations need to check the extent of the destruction.

Greater than a few tenths of dpa irradiation in case of reactor internal structural materials already increases the yield stress and tensile strength, while regarding the formability (ductility) characteristics are reduced. Beyond the change of strength properties the irradiation effects on the fracture toughness, as well.

Based on the performed tests it can be concluded that combining heat treatment and forming processes with ion radiation on the surface layer, the segregation processes - especially intergranular - due to neutron radiation and their effects on the steel toughness and stress corrosion susceptibility can be modelled in qualitative way (Chromium carbide segregation is observed using TEM); the state of the material in corrosion point of view is equivalent to irradiation damaged material or can be transformed using appropriate calibration procedure.

The influence of addition elements (Ti, B, Zr) on properties mechanical and corrosion resistance of intermetallic alloy FeAl-B2

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Abstract- The FeAl alloys have been the subject of extensive research in 60 but because of their excessive fragility, the use of doping by alloying elements has given hope to the family of alloy and impetus to the search.

In the context of the present work we studied alloys developed on the basis of the intermetallic Fe-Al40 in an arc furnace with adding alloying elements (Ti, B, Zr). The objectives of this study been to seek to improve the mechanical strength of the alloy to ambient temperature, and the corrosion resistance.

The microstructures of alloys produced were examined by the Optical microscope (OM) and scanning electron microscope (SEM). The different phases present in the material were identified by X-ray diffraction (XRD). Numbers hardnesses were determined by Vickers hardness test (HV) and measures Vickers microhardness. The electrochemical studies were performed in using potentiodynamic polarization curves and the electrochemical impedance spectroscopy (EIS).

Microstructural observations indicated the presence of precipitates which result from the introduction of B and Zr. Adding Boron in alloy FeAlTi decreased hardness, but the combined effect of the (Ti, B, Zr) leads to a low temperature hardening. It was observed that all elements added to the binary alloy FeAl improved the corrosion resistance, but the alloy presented FeAlTiB best features of protection against corrosion.

Distribution of the electric field according to the evolution of the discharge in a system point plane with insulating barrier

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The facilities high and middle tensions include mixed structures the most often, combining at least two phases of insulation: solid/liquid or solid/gaz. This type of insulation is in several equipments as the cutouts, the cables, the transformers and the airlines.

At the time of the setting in service of the devices electric in them make part, these insulating structures can be submitted to different types of constraints and more especially to the electric constraints. And in presence of a field electric, various phenomena can take birth in the volume of these materials or in surface. Indeed, when the electric field passes a certain value so-called doorstep, the discharges volume or surface can be generated and drive to the destruction of the insulating structure (following a straining of the insulating structure or to a bypassing of the strong insulator) or even to the stake out of order of the system.

In this work we examine the influence of the position of the insulating barrier and the length of the electric discharge on the electric field distribution, and we study the influence of these parameters on the relative theoretical efficiency to the distribution of the electric field in the system point plane. For this, we use the method of the elements ended up for the calculations the slant of the FEMM code, partner in the Matlab programming language.

A micromechanical-based model for the ductile cohesive-volumetric damage

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KEYWORDS: Micromechanics, Plasticity, Cohesive Zone Models, Homogenization

For numerical purposes, the cohesive-volumetric finite element method has gained much popularity in crack and damage simulations. A micromechanical-based damage model is here proposed for such ductile "cohesive-volumetric" media. The proposed model defines theoretical and practical criteria for the calibration of cohesive zone models (CZMs) in these simulations.

The studied medium is made of a hardening matrix (Hencky plasticity) containing penny-shaped cohesive inclusions (traction-separation laws). The spatial distribution of the cohesive inclusions can fit a prescribed finite element discretization. The overall elasto-plastic and damageable behavior is derived using a non-linear homogenization technique (variational approach of P. P. Castañeda, [1]). The proposed model: i/ can be applied whatever the shape of the cohesive law contrary to what is proposed in the literature, and ii/ has the capacity to exhibit the influence of the triaxiality loading rate on the overall ductile damage properties.

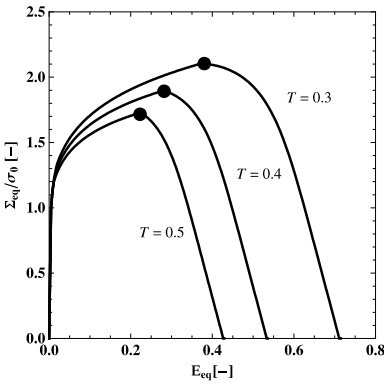

Figure 1. Effect of the triaxiality loading rate, T, on the overall behavior: normalized overall stress vs overall strain

For the case of a perfect-plastic bulk medium, a closed-form expression of the macroscopic potential is obtained. And whatever the volumetric plastic behavior, direct relationships between the local cohesive parameters and the overall material properties are developed. These relationships depend on: 1/ the mesh size and morphology, 2/ the applied triaxiality loading rate and 3/ the macroscopic material properties (maximal stress, failure energy, etc). More particularly, it is shown that the cohesive parameters are triaxiality-dependent. This dependency is consistent with previous results available in the literature and based on numerical or experimental studies (e.g. [2]).

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Phase transforming metals as fillers in soft polymeric matrices

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KEYWORDS: shape memory alloy, dynamic thermo-mechanical analysis

The inherent vibration of dynamical mechanical systems is unwanted, as this vibration could damage the system itself and also effect the surrounding severely. Therefore, many vibration absorbing, isolating and damping strategies are developed and presented in the literature (e.g., [1]). The main difference is, basically, in the location where the vibration canceling is introduced [1]. Vibration damping is mainly introduced in small mechanical oscillating devices and elastomers are the materials of choice (e.g., natural rubber, butyl rubber, etc.) [2]. Fillers are commonly incorporated in elastomers in order to tailor their behavior for the operating state. Carbon black and silica, among others, are frequently used as fillers. Magnetically polarizable particles have also been introduced to an elastomeric material due to the capability to change the material's behavior continuously, rapidly and reversible in an external field [3]. Active fillers in an elastomeric matrix have the advantage of being interactive to an external physical field, such as a magnetic field. Another approach could be the herein presented incorporation of shape memory alloys (SMA) to an elastomeric matrix. SMA's behavior can be temperature, mechanical loading and magnetic field dependent [4]. Filled in an elastomer, the inherent hysteretic behavior of the elastomer can be changed (reinforcement), however also the hysteretic behavior of SMA could be exploited. Preliminary experiments with SMA wires showed, that the stiffness of the composite is increased, as expected, but also the damping capability is improved. To get a better understanding of the composite, each constituent of the composite should be characterized. The objective of the presented poster is to demonstrate the dynamic thermo-mechanical behavior of SMA. Three different NiTi alloys have therefore been examined in uniaxial tension at various temperatures and loading frequencies. The storage and the loss modulus are evaluated. In addition to the dynamic thermo-mechanic analyses (DTMA), DSC measurements are performed to determine the characteristic phase transition temperatures.

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Effects of strain gradients on texture evolution in nano-indentation experiments: A numerical study

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Nano-indentation is a well-established experimental method to characterize the material's mechanical behaviour at small scales. However, its complexity such as the heterogeneity of the deformation field, anisotropy, size effects, complicated boundary and kinematic boundary conditions challenges the understanding of the deformation mechanisms in the indentation zone. Consequently, numerical simulation techniques are frequently used to study the underlying mechanics in indentation experiments. For instance, deformation-induced lattice rotations below an indent have attracted attention as there exists a close connection between crystallographic shear, the main mechanism governing the deformation, and the resulting lattice spin [1].

In this study, a three-dimensional enhanced modeling of strain-gradient crystal-plasticity (EMSGCP) finite element model of nano-indentation for Ti-15V-3Al-3Sn-3Cr was developed to demonstrate the influence of strain gradients on the crystalline reorientation and the deformation patterns. In EMSGCP theory, the initial microstructure of samples determining a value of critical resolved shear stress (CRSS) of slip systems was described in terms of geometrically necessary dislocations (GNDs) in addition to statistically stored dislocations (SSDs). The incipient strain gradients were correlated with the sample's surface-to-volume ratio. Appropriate material parameters were obtained by calibrating a developed three-dimensional finite-element model with the data from experiments.

This study demonstrates that there exists a strong connection between the patterns of lattice spins and the indents' pile-up profiles. Also the activity of the slip systems and their relative contributions to the overall plastic slip can be predicted more accurately using the EMSGCP theory compared to a conventional crystal plasticity theory.

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Multi-Scale Heat Treatment Simulation of a Pressure Die Casting Die

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Today there is an increasing trend to substitute traditional steel sheet structures with large size die casted light metals components in order to reduce the overall weight of the car body. Not only the high casting temperatures necessary to cast these large dies cause high thermal loads on the die but also the strength of the "Hot work tool steels" drops exponentially at those temperature levels. As a result, a premature failure of the dies is often observed in the industry. The second important aspect which significantly affects the higher costs of producing large size die casted light metal component is the possible cracking of the die casting dies during the heat treatment and the final finishing process after the heat treatment. Concerning these two aspects the simulation of high temperature mechanical properties and the simulation of the heat treatment process at macroscopic level to predict the possible cracking and distortions become essential for the tooling industry.

For this purpose precipitation simulations of the hot work tool steel X40CrMoV5-1 during two different tempering temperatures are conducted with MatCalc. The simulated microstructure delivers the necessary microstructure parameters for the prediction of yield stress, flow curve and the creep-parameters from physical based models which are the decisive parameters to simulate the stress relaxation during tempering. The predicted material properties are compared and verified with the experimental findings. These material parameters are used as an input for the following FEM simulation of the heat treatment of a pressure die casting die in Abaqus.

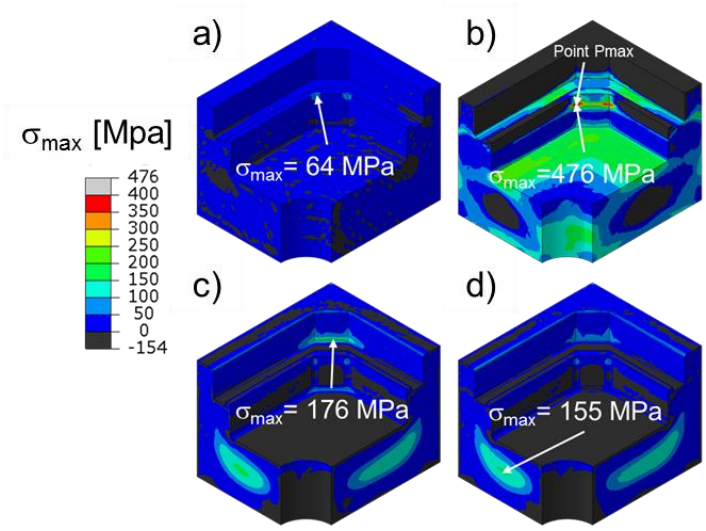

Figure 1: Distribution of principal stress maximum (σ_{max}) (a) after austenitization, (b) after quenching, (c) after the first tempering step, (d) after the second tempering step

LITHIUM MOTION IN CRYSTAL FRAMEWORKS OF SOME COBALT PHOSPHATES: A BOND-VALENCE-SUM INVESTIGATION

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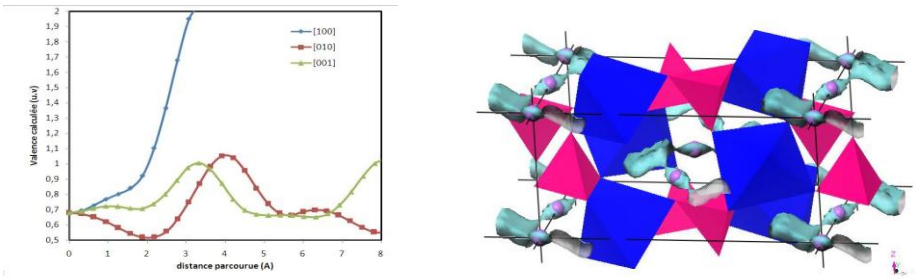
The concept of bond valence sum usually used to validate crystal structures was generalized to simulate cations conduction in many crystal compounds and successfully gived a correlation between ionic conduction and crystal structures, e.g. sodium in Nasicon conductors [1].

Bond valence sum f(x, y, z) is calculated for a grid of points (x, y, z) taking into account that the starting positions for lithium are the crystallographic positions determined by X-ray diffraction analysis and that the free motion occurred along initial migration directions such as those of tunnels towards crystallographic sites, following the lowest bond valence sum f(x, y, z). Points in this valence map with the lowest f values correspond to stable positions; the highest values are associated with bottlenecks. This model is applied here to predict the lithium motion in the crystal bulk of many cobalt phosphates such as in $LiCo_2P_3O_{10}$ [2] and the olivine-like $LiCoPO_4$ [3].



(a) (b)

The BVS versus the covered distance (a) and the simulated lithium pathways (b) in $LiCoPO_4$.

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Challenges in the robust prediction of long term stress relaxation at high temperatures. Results from the European Creep Collaborative Committee round robin.

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Data assessments, materials modelling and development as well as recommendations for model selection have been a main objective of the European Creep Collaborative Committee ECCC. The poster presentation describes the latest inter-comparison round robin on modelling long term relaxation. The bolting steel 1Cr-0.5Mo-0.25V steel tested by NIMS, Japan has been assessed by a number of ECCC assessors striving to define models capable of predicting the relaxation in the full data range, i.e. in both strain (0.1-0.25% total strain) and temperature (450-550°C). The assessors use methods of their own preference for interpolation, extrapolation and calculation of prediction errors for a full data set and a heavily culled data set. The used methods include 3 types of forward creep models, classical relaxation models, parametric (Time-Temperature-Parameter curve families) solutions and entirely new modelling approaches. The results show that there are large differences especially in the ability to robustly predict beyond the range of data. The different success of these models particularly on extrapolation has highlighted the great importance of post assessment testing such as those advocated by ECCC.

Computational modeling of c-axis compression of magnesium single crystal using gradient-enhanced crystal plasticity

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A finite-deformation strain gradient crystal plasticity model is implemented in a three-dimensional finite element framework in order to investigate the deformation behavior and the size-dependent hardening response of magnesium single crystals. The potential-based and thermodynamically consistent material model is formulated in a non-local and non-linear inelastic context in which dislocation densities are introduced via strain gradients. With regard to the uniaxial compression of single crystal micropillars, the model is able to predict the discrete dislocation glide in terms of a band-shaped slip zone. Moreover, the presence of strain gradients leads to an additional energetic-like hardening effect which results in an increase of the macroscopic strength with decreasing crystal size as reported in several experimental investigations. In this regard, two different pillar sample sizes at the micron scale with (0001) orientation are taken into account in order to show the observed scale effect. As experiments have shown, the crystallographic orientation leads to the activation of pyramidal {11-22} <11-23> slip systems since the loading axis coincides with the vertical c-axis of the lattice. A comparison between numerical results and corresponding experimental data is presented.

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Modeling creep resistant and less dissipative composite structures

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This study presents an integrated micromechanical model-FE framework to obtain the effective thermomechanical response and micro-macro field variables during the coupled heat conduction and quasi-static thermoviscoelastic deformation of a particulate composite that takes into account the dissipation of energy from the viscoelastic constituents. The purpose is to use this micro-macro scale framework for analyzing response of viscoelastic composite structures subjected to a coupled mechanical and thermal effect and at the same time recognizing different nonlinear response of the constituents. This can lead to rigorous design of composite structures without the need of expensive computational costs. Schapery's nonlinear thermo-viscoelastic constitutive model with stress and temperature dependent material properties is used for each constituent. The constitutive model for the heat flux follows classical Fourier's law with a temperature dependent thermal conductivity. A micromechanical model for predicting the effective nonlinear thermal- and mechanical properties of viscoelastic composites reinforced with solid spherical particles is developed. Simplified micromechanical relations are formulated in terms of incremental average field quantities, i.e., stress, strain, heat flux and temperature gradient, in the subcells of the micromechanical model. A time integration algorithm for simultaneously solving the equations that govern heat conduction and thermoviscoelastic deformations of isotropic materials is developed. The algorithm is then incorporated within each sub-cell of the micromechanical model together with the macroscopic energy equation to determine the effective coupled thermoviscoelastic response of the particulate composite. The integrated micromechanical-FE framework is used to analyze coupled heat conduction and deformations of viscoelastic composite structures. It was established that the fully coupled thermoviscoelastic analyses should be performed when analyzing the viscoelastic composites under cyclic loading for a longer period of time. Our analyses forecast a better design for creep resistant and less dissipative structures using particulate composites and functionally graded materials. The dissipation effect is important when the composite structures are subjected to cyclic mechanical loading over a relatively long period of time, which will be useful in determining fatigue life of composite structures.

A variational approach to gradient plasticity based on non-convex plasticity energies

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Incremental energy minimization represents a powerful mathematical tool, which was applied to fracture mechanics, damage and many other problems. In the present work it is used in the context of gradient plasticity for describing the evolution of the deformation in materials whose energy is given by the sum of three terms: an elastic bulk energy, a dissipative cohesive energy, and a non-local gradient term. In the one dimensional setting, the model was successfully applied to the study of plastic slip patterning, and to analyse the response of bars to tensile loadings. It has been recently extended to two-dimensional crystal plasticity, and some preliminary numerical results are presented and discussed.

High temperature crack growth models of Grade 91 steel specimens and comparison with material properties in RCC-MRx

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KEYWORDS: Grade 91 steel; Fatigue crack growth; Creep crack growth; Defect assessment; Sodium-cooled fast reactor

In defect assessment or leak before break analysis under creep-fatigue loading, crack growth models are necessary. French design code of RCC-MRx provides fatigue crack growth model and creep crack growth model for Mod.9Cr-1Mo steel (ASME Grade 91) steel in Section III Tome 6. In this study, crack growth models were derived from a number of crack growth tests for Gr.91 steel specimens under separate creep loading and fatigue loading at elevated temperature. The fatigue crack growth data were obtained from two specimen types; one is standard CT specimen with half inch (12.7mm) thickness and the other is round bar single edge crack tension specimen. The creep crack growth test data were obtained for standard CT specimen with half inch thickness. The data were compared with those of the RCC-MRx which are based on standard CT specimen with 1 inch (25.4mm) thickness and the conservatism of the crack growth models in RCC-MRx were reviewed. Other material properties including tensile strengths and creep strain rules were compared. Technical issues on material properties in current version of RCC-MRx 2012 edition for Grade 91 steel associated with defect assessment at elevated temperature were raised and discussed.

The study of Fe∑5(310) and Fe∑3(111) with V impurities by multiscale simulation method

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KEYWORDS: Fe grain boundary; V impurity; Density functional theory; Molecular dynamics

Fe∑5(310) and Fe∑3(111) with V impurities are studied by using Density Functional Theory(DFT) method and Molecular Dynamics (MD) method. The defect formation energies, impurity segregation energies and the strength energies of the grain boundaries with the different configurations are obtained both by DFT method and by MD method. The results are analyzed based on the brittlement and enhancement mechanisms of the impurities described by Rice Wang. Molecular dynamics tensile tests (MDTT) are performed to get the further understand of the effects of impurity V on the grain boundaries.

Plastic deformation behavior of single crystalline irregular honeycombs: a crystal plasticity study

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This study is inspired by the recent development of metallic foams, especially single crystalline gold foams. Currently, most of the modeling studies at continuum scale on metallic foams are focused on the cellular structures, based on isotropic models. In this study, we consider the effect of the initial orientations on the deformation behavior of the single crystalline irregular honeycombs. The interplay of the cellular structure and the crystallographic orientation will be presented and discussed.

Direct Multiscale modeling of powder pressing and sintering

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Direct Multiscale modeling (DMM) is a numerical approach aimed at consolidation modeling of powder-based materials. “Multiscale” means the method performs numerical analysis of the consolidation processes simultaneously at both the mesostructure scale of powder particles and the macroscopic scale of the consolidating component. “Direct” indicates the main specific feature of the method: the results of mesoscopic calculations are directly used for the prediction of the macroscopic behavior through homogenization and extrapolation procedures without an intermediate stage of formulation of analytical constitutive equations.

Mesoscopic structure of consolidating component is defined through the set of mesoscopic unit cells of material corresponding to the different control points in the macroscopic volume of the component. During calculations two-scaled finite-element numerical procedure follows both mesoscopic structure evolution in unit cells and macroscopic shape change of the component. Though sometimes cumbersome, this approach is convenient for the solution of macroscopically non-homogeneous problems with complex mesostructure evolution. For the powder pressing they include prediction of damage development and strain-hardening of powder components, analysis of residual stresses after component ejection from die. Kinetics of sintering substantially depends on mesostructure coarsening, damage and anisotropy development that can be different in different elements of initially non-homogeneous or constrained sintered components. Recently, DMM has been successfully implemented as a subroutine in commercial software.

Post-polymerization shrinkage of resin-based dental composite materials

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KEYWORDS: Polymerization, Post-polymerization contraction, dental composite materials.

Polymerization is a process of reacting monomer molecules together in a chemical reaction to form polymer chains. In dentistry, polymerization of composites is enhanced using halogen or LED lamps. In clinical practice, most common issues occurring due to the effects of polymerization shrinkage are marginal discoloration, secondary carries and micro-cracks between the composite and tooth tissue. Following the most intensive shrinkage during polymerization, polymerization shrinkage may continue over the next 48 hours. This phenomenon is referred to as post-polymerization shrinkage. Its occurrence is caused by an increased concentration of free radicals, which continue with their movement after the light is turned off. Increased concentration of free radicals is caused by breaking of double bonds. Released radicals are sufficient for the polymerization to continue, i.e. for composite material shrinkage to occur. The aim of this paper was to analyze different methods used for monitoring of the occurrence of post-polymerization shrinkage in dental composite materials. An additional goal of this paper was to explain the phenomena that happen in composite materials leading to post-polymerization shrinkage, as well as to determine to what extent the material deforms over time.

Methods typically used for strain analysis of specimens after polymerization include the TMA method (Thermo mechanical analyzer), CEA 06-032UW120 (electrical resistance polyamide-backed strain gauges). During the experiment, the dependence of specimen strain (%) from time (shrinking and expanding of the specimen) was monitored.

CIVIL STRUCTURAL HEALTH MONITROING USING PIEZOELECTRIC TRANSEDUCER

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KEYWORDS: Piezoelectric ceramic, dielectric material, health monitoring, damage detection, civil infrastructure.

Lead-Zirconium-Titanium Oxide [Pb(Zr1-xTix)O3)] is widely known as piezoelectric ceramic patch. It is light weight, low-cost, small size and has good dynamic performance, high elastic modulus, high rigidity, brittleness and low tensile strength. Besides, it exhibits large range of linearity, fast response, long term stability and high energy conversion efficiency (Sirohi and Chopra, 2000a). On the other hand piezopolymers are characterized by low charge characteristics and low stiffness. Due to their flexibility, they can be formed into thin sheets and can be adhered to any curved surfaces. However, piezopolymers are more sensitive to mechanical loads over a larger range, which renders them to be better sensors. The advent of commercially available low cost piezoceramics has opened new opportunities for dynamic structural identification using embedded active sensors. Embedded active sensors are small piezoelectric (PZT) ceramic patch that can be permanently attached to the structure. Recently the study of smart materials to apply to civil engineering has become a major issue. To list some of these studies, health monitoring of members, self-repairing, actuating structural members are of interest. These aim to make the structures more highly characterized by using new technology and to make structural performance higher by using smart materials. This paper aims to highlight the applications of piezoelectric ceramic materials in the field of civil infrastructure i.e. damage detection, monitoring, critical load evaluation on structure, vibration control, predictive life estimation and bio cell characterization etc.

Micromechanical Model for Cocciopesto Mortars Based on Experimental Observations

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Masonry has been traditionally used for the construction of load-bearing elements and the craft was perfected mainly during the Roman and Byzantine periods, when masons started to modify mortars with various admixtures. It was found that lime mortars containing crushed bricks, known as *cocciopesto*, exhibited superior durability and resistance to mechanical loading. Therefore, millions of tourists can nowadays appreciate the ancient masonry structures, containing cocciopesto in their bed joints, in spite of their considerable age and fierce earthquakes they were often subjected to.

Despite the enormous value of those structures, there is no comprehensive study focused on the mechanical interaction of crushed bricks with other phases in the cocciopesto mortars, explaining the superior mechanical performance. The existing works deal mainly with their chemistry and focus on the morphology of individual phases.

The purpose of this work is to propose a simple micromechanical model to predict the key mechanical parameters of cocciopesto mortars. The model is built on outcomes of microscopy observations and macroscopic tests, from which we came to the conclusion that the formation of shrinkage-induced cracks between closely packed aggregates presents the key factor governing the mechanical response Therefore, a two-scale description is developed, in which the shrinkage-induced cracks are introduced into the homogenized medium collectively representing the lime matrix, aggregates, and pores. Assuming that the matrix is the only phase responding in a non-linear manner, the overall response is estimated by the incremental Mori-Tanaka scheme, leading to computationally efficient predictions of mortar stiffness, tensile and compressive strength, and fracture energy in tension.

The model predictions are found to be in a good agreement with results of a comprehensive experimental study and clearly explain the advantages of compliant aggregates, such as crushed bricks, over stiff sand particles. In addition, since the model utilizes parameters with a clear geometrical or physical meaning, it has proved itself as a suitable design tool for modern cocciopesto mortars, optimized with respect to the requirements of the public authorities in relation to the preservation of cultural heritage.

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Non-Local Sandwich Beam Theory for Micro- and Macro-Structural Stresses

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This paper presents the developments of the non-local sandwich beam theory that can be used to assess the global response of the beam in terms of displacements and stresses. When these responses are computed, the microstructural effects are accounted for, thus the microstructure period is seen in these responses. The theory utilizes homogenization-localization and modified couple stress beam theory developed by Reddy. The homogenization considers all steps of the derivation of the prevailing differential equations from displacements through strains and stresses to external loading. This enables accurate localization process that recovers the microstructural effects from the homogenized solution for beam bending and them couples to global response. This allows the prediction of the local failure within the beam. The theory is presented as well as some case studies that are supported by experiments: the shortest beams have only four unit cell along their length, while in the longest we approach the situation where the unit cell length is infinitely small in comparison to the beam characteristic length. The presented theory can be utilized to deformations and predict stresses accurately within all cases between these two extreme situations. It also converges to the physically correct solutions in case of infinite and zero shear stiffness; especially the limit of zero shear stiffness is important as there the traditional Timoshenko beam theory fails to predict the response correctly. This case can occur for instance when there is plastic hinge formation within the unit cells of the sandwich beam. Present theory can be extended to different microstructures and further to plates. The benefit of the present methods is that it is analytic which enables identification of the physical parameters. It is also relatively fast that enables fast structural analyses.

Effects of high temperatures on the residual behavior of concrete

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KEYWORDS: Ordinary Concrete, high temperatures, heating and cooling, residual compressive strength, residual modulus of elasticity, loss of residual mass.

Knowledge of the behavior of concrete and residual (after heating) is an issue of great interest for the evaluation of safety in civil engineering constructions. Several studies have focused on the behavior of concrete at high temperatures but little research has focused on the residual behavior of concrete. At the viewpoint of engineer and researcher, it is the latter behavior that determine the stability or otherwise of the structure after being subjected to high temperatures. In this paper, an experimental study was conducted to understand the behavior at high temperature of the Tunisian residual concrete. The tests ATG / DTA were used to determine the various physico- chemical processes occurring within the cement paste. Two speed of temperature rise (0.5 ° C / min and 10 ° C / min) was applied these two gears have shown the presence of a kinetic, To take this into account, bearing temperature (corresponding to the peak temperatures obtained during tests TGA / DTA) with three different durations (4h, 8h and 24 h) were applied in order to study the effect of the heating time on the properties of the concrete, These cycles of heating and cooling are interested in the study of mechanical properties (residual compressive strength and modulus of elasticity residual) and physical (loss of residual mass , permeability) on concrete specimens of dimensions 10x30 cm. .Compression tests have shown that the different properties of conventional concrete decrease with temperature. Moreover, more the heating stage is longer more the reduction is important.

Crystal plasticity with asymmetric stress-strain state measures

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One of the issues in the construction of multilevel models based on crystal plasticity is the validity of using symmetric measures of stress and strain state at mesolevel (level of crystallite). For example, using symmetric orientation tensors for intragranular slip systems leads to implicitly introduction in the model of slip systems [1], which are absent in the real material. Furthermore, using of symmetric stress-strain measures in elastic-plastic models leads to non-uniqueness solutions due selecting the active slip systems while stress state in the vertex of the yield surface: on the basis of additional hypotheses only 5 active slip systems selected from 6 (or 8) on which the Schmid law is hold; note that in the case of a special orientation of crystallites all slip systems are equal [2].

Two-level elastoviscoplastic and elastoplastic models for bcc-polycrystalline is proposed [3]. Crystallite lattice rotations determined with regard to incompatibility of dislocation sliding in neighboring crystallites. The consistency conditions of constitutive relations at the different scale levels are used for model levels connection.

Modelling of various loadings (tension, compression, shear) of representative volume of copper showed that (even when using a symmetric tensor of elastic properties crystallite) for elastoplastic models calculation results with symmetric stress-strain measures are different due to different choices of active slip systems that leads to a difference in the accumulated displacements and rotations of the lattice of the crystallites (elastoviscoplastic models give an unambiguous result). The using of asymmetric stress-strain measures in elastoplastic models allow to avoid this ambiguity.

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Integranular cracking in polycrystalline aggregates using cohesive zone approach

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Understanding and controlling early damage initiation and evolution are amongst the most important challenges in nuclear power plants, occurring in ferritic, austenitic steels and nickel based alloys. In this work a meso-scale approach to modeling initiation and evolution of early intergranular cracking is presented. This damage mechanism is present in a number of nuclear power plant components and depends on the material (e.g. composition, heat treatment, microstructure), environment and load. Finite element modeling is used to explicitly model microstructure-both the grains and the grain boundaries. Spatial Voronoi tessellation is used to obtain the grain topology. In addition, measured topology of a 0.4mm stainless steel wire is used. Anisotropic elasticity and crystal plasticity are used as constitutive laws for the grains. Grain boundaries are modeled using the cohesive zone approach. Different modelling assumptions/parameters are evaluated against the numerical stability criteria. The biggest positive contribution to numerical stability is the use of cohesive-type contact instead of cohesive elements. A small amount of viscous regularization should be also used along with the addition of a small amount of viscous forces to the global equilibrium equations. Two cases of grain boundary damage initiation are explored: (1) initiation due to normal separation and (2) initiation due to a combination of normal and shear separation. The second criterion significantly decreases the ductility of an aggregate and slightly improves the numerical stability. In addition, an application of strain gradient crystal plasticity study on a 2D polycrystalline aggregate obtained with Voronoi tessellation is presented with a demonstration of length scale effect.

Coalescence of Primary Voids in the Presence of a Secondary Population

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Many metallic alloys contain a secondary population of voids with a relatively small average void size, besides the primary family of void with larger void sizes. The aim of the present study is to extend the coalescence criterion of Thomason for primary voids [1], to incorporate the effect of secondary voids. For this purpose, finite element based limit load analyses are performed on cubic unit cells containing two populations of voids, as shown in Fig. 1. The unit cell is subjected to an axisymmetric stress state with a predominant stress component ($\Sigma_{22} > \Sigma_{11} = \Sigma_{33}$) with the remaining Σ_{ij} being zero. The matrix of the unit cell is modeled as an elastic-perfectly plastic material obeying J_2 flow theory. The effects of parameters such as the relative volume fractions of the primary and secondary voids, the aspect ratio of the primary voids, and the number of the secondary voids sitting on the ligament, on the critical stress at the onset of void coalescence, Σ_{22}^{c}, are investigated. The results show that the extended version of the Thomason criterion proposed in this study is able to accurately predict the onset of void coalescence between primary voids in the presence of secondary voids.

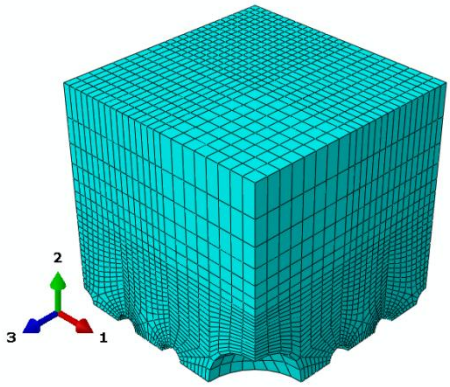

Fig. 1: Finite element mesh for the 1/8 of the cubic unit cell. The unit cell contains a primary (spheroidal) void at the center, and the ligaments between adjacent primary voids carry a layer of secondary (spherical) voids.

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A mesoscopic stochastic model for micron-scale plasticity

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Plastic deformation of micron-scale single crystalline specimens is accumulated by large intermittent strain bursts (dislocation avalanches) [1]. The size of these bursts is power law distributed, with a cut-off depending on the external shear stress (driving force). It has been proposed that at a critical stress value the cut-off tends to infinity, showing analogy with continuous phase transitions. This phenomenon is often investigated numerically in a depinning transition framework [2–4].

In this presentation we investigate the statistical properties of strain bursts with a cellular automaton model where the yield point is a local quantity and it is randomly distributed in space representing the quenched disorder of the media. As a consequence, deformation is also a local quantity which is increasing when the local stress exceed the local yield point. The elementary deformation is an Eshelby's inclusion where the interaction is long-range with strong anisotropy. As the external shear stress is increasing avalanches appear which size become larger and larger. Contrary to previous models, bursts are also allowed in the opposite direction of the external force due to the nonpositiveness of the interaction kernel.

This model gives an effective method to investigate the properties of avalanches, e.g.

- the effect of the specimen size on the size distribution of bursts and which is in agreement with recent DDD simulations [5]
- the connection between the external stress and the value of the cut-off of the power-law distribution
- the effect of the chosen flow stress distribution on the spatial correlation of avalanches
- the effect of the stress kernel of the Eshelby's inclusionon the shapes and the spatial correlation of the avalanches.

After investigating which parameters of this model influence the statistical properties of the plastic response, the differences and similarities between the results of this model and experimental measurements, 2D discrete dislocation models and other mesoscopic models are noted. The quantities that contradict the depinning transition framework are highlighted.

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