Modeling of a Ni-based superalloy: From micro-pillar compression tests to polycrystalline models

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A microstructure based crystal plasticity (CP) model is developed to simulate the elasto-visco-plastic behavior of Inconel 718 grains containing γ' and γ'' precipitates and δ phase. The CP model is an elasto-visco-plastic physically inspired model [1] that accounts for the effect of temperature, softening due to cyclic loading and tension-compression strength differential (when present) at the grain level.

The parameters defining the CP behavior were fitted from tests at the microscale on grains of wrought and cast materials with different contents of γ' and γ'' and δ. The testing at the grain level consisted first on the identification of grain orientations using EBSD and then micromechanical testing at different temperatures by micro-pillar fabrication inside a grain and uniaxial compression. Tests were made using several pillar diameters, strain rates and temperatures. In addition, testing of small polycrystalline samples inside the SEM were done to complement the crystallite characterization. The resulting CP parameters where finally linked with the corresponding microstructure.

The CP plasticity model was finally used to simulate the elastic-plastic and creep behavior of polycrystalline alloys at different temperatures. The polycrystalline behavior was obtained by the finite element simulation of a periodic representative volume element (RVE) of the microstructure [2]. The RVE contained information about grain size, shape and orientation distribution. The resulting behavior was compared with macroscopic tests of alloys with different microstructures to verify the validity of the model.

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Simulating the brittle-ductile transition using discrete dislocation plasticity

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At a given strain rate, metals fracture at low temperatures in a brittle manner characterized by little or no plasticity. As the temperature is raised dislocation nucleation and motion occurs in the highly stressed region surrounding the crack-tip and the material exhibits a more ductile fracture behavior. The dislocations generate a back stress on the crack-tip which acts to shield the crack causing an increase in the fracture toughness. The temperature at which this brittle-ductile transition occurs increases with increasing strain rate. We have studied the relation between applied deformation, governed by the applied loading rate, and dislocation plasticity and crack-tip shielding, where the time scale is determined by Frank-Read source nucleation time and dislocation drag coefficient. Micro-cantilever bending was simulated in plane strain with a discrete dislocation plasticity (DDP) model utilizing cohesive elements to model the crack propagation. The micro-cantilever DDP simulations will be presented and compared to corresponding experiments to investigate rate and size effects in the brittle-ductile transition.

Mesoscale modeling of dislocation mechanisms and the effect of nano-sized carbide morphology on the strengthening of advanced lightweight high-Mn steels

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The development of high performance lightweight steels for structural applications in the automotive industry is currently one of the main targets of steel industries. The FeMnAlC system is a promising low density steel grade that offers a combination of outstanding mechanical properties and specific weight reduction. The addition of Al promotes the precipitation of $L'1_2$ ordered $(Fe, Mn)_3AlC$ carbides, the so-called κ-carbides. In the austenitic FeMnAlC steels, κ-carbides are nano-sized cuboidal precipitates that control the dislocation assisted plasticity of these materials. It is thus important to understand the interaction mechanisms between dislocations and κ-carbides and to investigate the influence of precipitates morphology that arises from spinodal decomposition on the mechanical behaviour. Here we provide new insights into κ-carbide strengthened high-Mn steels by employing TEM observations [1] and simulating comparable microstructure using discrete dislocation dynamics (DDD) simulations. The DDD simulations of this study are based on the previous model developed for cuboidal γ' strengthened Ni base superalloys [2]. To investigate the effect of the κ-carbides morphology we established a similar particles arrangement as indicated by TEM images, concerning particle size and position along <100> directions. In order to get more insight into the bowing of dislocations into the channels between the particles and the subsequent mechanical response theirs size and geometry are varied at a fixed κ-carbide fraction. In connection with TEM observations this gives us the opportunity to understand how the geometrical arrangement of these particles induces the plastic deformation of these materials. This provides new guidelines in the alloy design of advanced lightweight steels based on the underlying dislocation mechanisms at different κ-carbide geometrical arrangements.

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Mechanisms of Plastic Deformation of Polycrystalline Sodium Chloride at room temperature and at 350ºC :2D and 3D observations and modeling

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Synthetized sodium chloride polycrystals have been deformed at room temperature and at 350°C by uniaxial compression a) in a Scanning Electron Microscope, b) for 3D Xray analysis (absorption) on a synchrotron beam line. 2D and 3D markers have allowed the use of Digital Image Correlation to compute the strain fields through an ad-hoc software (CMV). For large grained samples, both intracrystalline plasticity (CP) and grain boundary sliding (GBS) are recorded from the start of the permanent deformation and at both temperature. There is some indication that the orientation of the boundary with respect to the applied uniaxial loading plays a critical part for GBS, as well as the relative crystalline orientations as measured by EBSD (Electron Back Scattered Diffraction). GBS is also found on the samples deformed at high temperature, even though CP is easier in this case than at room temperature. Studies on halite single crystals have indeed determined that this ionic crystal, with a centered cubic lattice, may deform plastically on three potential families of slip systems, which have in common the <110> directions associated to the {110}, {100} and {111} planes respectively. The initial critical shear stresses (CSS) are very different for each family of systems with a strong temperature and strain rate dependence. At room temperature, it is generally recognized that the {110}<110> systems have the lowest CSS. They do not however provide enough independent systems to accommodate any local strain state, so that systems with higher initial CSS or other plastic deformation mechanisms have to be activated as well. At a higher temperature, the initial critical shear stresses of the different families decrease and tend to a common value, which should provide enough active slip systems to accommodate any plastic strain. However, GBS is still a component of the material response.

If direct observations or DIC computations may give some clues about the local activity of slip planes, they are not sufficient to get a complete description of CP. An approach is then to use crystal plasticity finite element methods (CP-FEM) with a careful selection and assessment of the underlying assumptions. Three main hypotheses are reviewed: the choice of a 3D structure based on 2D observations, the boundary conditions and the constitutive equations at the single crystal level. For this last part, we compare results from the literature with experiments that we have performed on single crystals. We thus identify and improve the hardening model used in the computations. Classical CP-FEM models do not account for GBS but allow the estimate of normal or tangential stresses along perfect grain boundaries. In a first step, we use these results to analyze regions where GBS has been observed. In a second step, we enrich the classical model by adding a specific behavior in the vicinity of boundaries allowing some localized displacements.

A massively parallel level-set approach for the modelling of 3D anisotropic grain growth in polycrystalline materials

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Microstructure evolution during heat treatment is of primary relevance because the properties of metallic materials are determined basically by their microstructure. During heat treatment, mainly three phenomena are triggered that modify the microstructure: recovery, recrystallization and grain growth. Grain growth is the enlargement of the crystallites of a polycrystal that takes place in order to minimize the free energy of the system. This phenomenon is controlled by the motion of grain boundaries, which in turn is driven by the local curvature of the grain boundaries and influenced by the mobility and energy of the grain boundaries and their junctions. In the present contribution, we present a model based on the level-set approach that is capable to consider all the factors that affect grain boundary migration and thus, grain growth. A statistically relevant 3D polycrystal was simulated and compared to theoretical expressions for the growth of 3D grains for validation of the model.

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The work is related to my PhD studies, which I would like to present preferentially in the form of an oral talk.

Investigations of the effect of grain boundaries shape modeling in three-dimensional actual polycrystalline aggregates

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The aim of the present study is to investigate the consequences of assumptions on the grain boundaries shape provided in the simulations of polycrystalline aggregates.

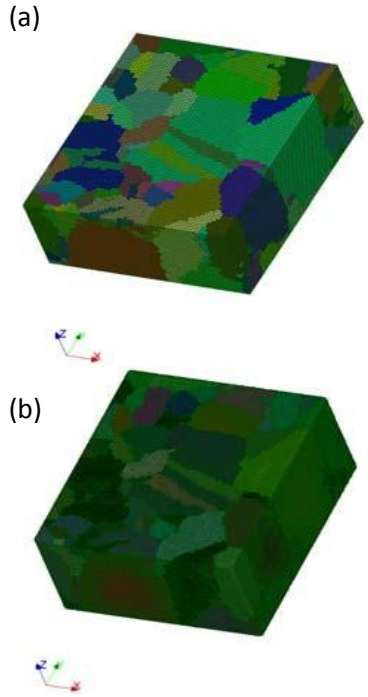

Figure 1: Polycrystalline aggregate made of 130 grains meshed with (a) hexahedron elements and (b) tetrahedron elements based on a Laplacian smoothing applied to grain boundaries.

The framework of this study is the fatigue crack initiation in ductile alloys like austenitic stainless steels that is mainly due to the occurrence of localized deformation in persistent slip bands (PSB) [1]. The study is made on a 316 stainless steel where PSB is classically related to microstructural features such as grain boundaries and neighborhood of the crystallographic grain orientations [2].

To determine the role of the grain boundaries shape on the behavior of polycrystal aggregates, a crystal plasticity model was used to describe the constitutive behavior of each grain in the finite element model of a 3D microstructure submitted to cyclic loadings. From the same initial 3D EBSD map, three polycrystals meshes were generated with different assumptions on the modeling of the shape of grain boundary shape: (i) a mesh based on EBSD measurement points considered as voxels and mesh with hexahedron elements (Fig. 1.a), (ii) a mesh based on a marching cube algorithm and, (iii) a mesh where the microstructure generated by the marching cube algorithm was smoothed with a Laplacian smoothing (Fig. 1.b). A statistical analyze of the FE results is carried out to highlight influences of grain boundaries shape on the local stress and local strain fields and on the macroscopic behavior of the material.

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Microstructure-sensitive modeling of void nucleation in polycrystalline materials

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We present the implementation of a model for void nucleation in a Fast-Fourier Transform (FFT)-based elasto-viscoplastic formulation. The latter produces full-field solutions for the stress and strain in voxelized polycrystalline microstructures[1]. Utilizing the knowledge of which voxel belongs to which grain, the local first order Cartesian moments of the grain structure are used to calculate the grain boundary normal vectors of the voxelized microstructure. [The first order moments are equivalent to the gradient of the grain character within the volume of calculation and the direction of the maximum gradient is the surface normal.] Combining these, the grain boundary tractions can be calculated. We identify "traction hotspots", i.e. regions with tractions that are significantly above the mean, and use them to predict void nucleation sites in copper polycrystal. The proposed methodology can be separately implemented in a dilatational FFT-based model that simulates porosity evolution. The results are compared to both experiments and molecular dynamics (MD) simulations to improve the accuracy of the model[2]. The MD model provides additional insight into other factors to incorporate beyond grain boundary tractions, and with the experiment results used to confirm the models' predictions. There are two paths of the experimental comparison. One path is to compare morphologic trends in the traction hotspots to the experimentally measured morphological trends of voided grain boundaries. The other path utilizes near field high- energy diffraction microscopy (nf-HEDM) to obtain microstructure images of a copper polycrystal before and after shock loading is applied. Traction hotspots derived from the pre-shocked state are then compared to void locations in the post-shocked state.

A second aspect is to use some of these techniques to characterize experimental data obtained from nf-HEDM. Normally, the samples are characterized by the local crystallographic orientation at about 1 micron resolution. Currently, grains are identified by thresh-holding differences in the misorientation angle between neighboring voxels. As above, it is difficult to characterize the grain boundary normal from these voxelized images. The first order moment technique above can be used to define interfaces by looking at the maximum in the gradients; only here it is applied to either the misorientation angle or the quaternion vector that describes the crystallographic orientation. This same analysis can be applied to the simulations, ignoring the grain identities and focusing only on the local orientation, and achieves similar results. Because the grain boundaries and their normals are defined analytically, the results of the simulation and experiment can be directly compared even though they come from meshes with differing resolutions.

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Synergies between experiments and simulations: mapping and modelling of $LiFePO_4$ electrodes

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Electrochemical systems are difficult to analyze, both experimentally or by modeling, because of the complex interplay of electrochemistry, thermodynamics, and transport (diffusion and phase transformations). The interpretation of experimental data is challenging due to the involvement of multiple materials (e.g., electrolyte, electrode particles, and conducting additives). Thus, the combination of experiments and simulations is essential in elucidating the processes underlying experimentally observed phenomena.

This collaborative work is based on an in situ energy dispersive X-ray diffraction (EDXRD) that is used to measure the inhomogeneous electrochemical reaction of $LiFePO_4$ particles within a coin cell. Profiles of the state of charge in two dimensions are obtained throughout the process. To understand the evolution of the state of charge during the discharge process, we simulate the dynamics using a cell-scale model parameterized with experimental measurements. We use simulations to extract the effective material parameters and use the results to hypothesize their changes from a cycle to another. These hypotheses then inspire additional simulations at microstructure-level and experiments, which will be discussed.

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