Simulation analysis of stress and strain partitioning in dual phase steel based on real microstructures

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The mechanical response of alloys consisting of multiple phases is governed by microscopic strain and stress partitioning among the various phases, crystals and subgrains. Yet, due to the limitations that are inherent in the experimental characterization of the stress-strain partitioning that takes place at the micro-scale, microstructure optimization of such alloys is typically based on the averaged macro-scale response (e.g. engineering stress-strain curve). To strengthen the connection between microstructure and mechanical properties, a novel methodology is introduced in this work that enables the joint simulation and experimental based analysis of the deformation- induced evolution of heterogeneous materials with multiphase microstructures.

This is achieved through a combined numerical-experimental approach, i.e. relying on crystal plasticity (CP) simulations and in-situ deformation experiments both initiated from the same electron backscatter diffraction (EBSD) mapped representative microstructural area of interest. 2D full-field crystal plasticity simulations are run employing a recently developed spectral solver suitable for high-phase contrast materials [1, 2] implemented in the crystal plasticity simulationkit DAMASK [3]. The model is created directly from high resolution EBSD based crystal structure, phase, and orientation maps. The individual phase properties are obtained by additional inverse CP simulations of nanoindentation experiments carried out on the original microstructure [4]. The simulated local strains are compared to experimental results obtained by a recently developed, digital image correlation-based, high-resolution, 2D strain mapping methodology [5].

The methodology is 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. Obtained strain maps reveal significant strain heterogeneity arising from martensite dispersion, ferrite grain size, and defect densities effects; and early damage nucleation at notch-like irregularities in martensitic zones that cause high stress triaxiality. Deviations between simulations and experiments can be explained in terms of known limitations of the involved techniques. The presented integrated engineering approach provides a high dimensional set of micro-mechanical output information that can enhance the understanding and further development of complex bulk multiphase alloys.

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[4] C. Zambaldi, Y. Yang, T. R. Bieler, D. Raabe: Journal of Materials Research 27 (2012), 356-367
[5] see talk by C. Tasan in Symposium A

Resolving the evolution of pore structures in 304-L laser welds

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The failure of partial-penetration Nd:YAG laser welds in 304-L stainless steel have been investigated through the direct incorporation of pore structures at the specimen level. Micro-computed tomography (μCT) is employed to characterize multiple weld schedules and develop idealized representations of the size, shape, and spacing of the pores. Pore growth and the subsequent necking are natural outcomes of the simulation.

The large deformations between pores require a robust mapping scheme for the remeshing and mapping of internal state variables [1]. We employ higher-order tetrahedral elements to resolve strong gradients and ease the burden of discretizing complex and evolving pore structures.

Through our ability to idealize, resolve, and evolve pore structures, we can investigate the performance of candidate weld schedules.

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Understanding how oxidized grain boundaries fail:
A combined experimental and crystal plasticity finite element approach

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Stress Corrosion Cracking (SCC) of Alloy 600 in the primary loop of Pressurized Water Reactors (PWRs) represents one of the most challenging forms of materials failure the nuclear industry has faced. Over the last decades many mechanisms have been proposed to explain this complex localized sub-mode of corrosion but experimental evidence in favour of one of them is still unavailable. Although Alloy 600 is known to suffer from cracking along grain boundaries (intergranular SCC) under PWR primary water conditions, information about the stress necessary to induce cracking and the link between the specific grain boundary (GB) microstructure, degree of oxidation and deformation behaviour is still unknown.

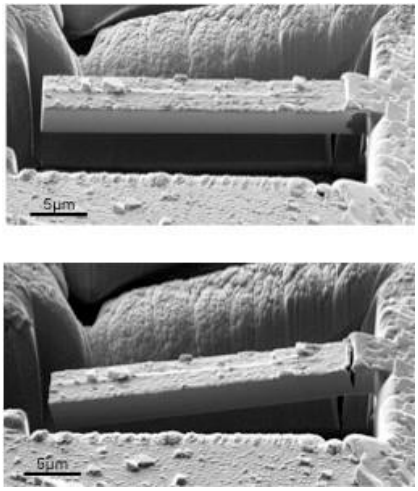

Figure 1: SEM images of a FIB-machined cantilever, before (top) and after (bottom) the micromechanical test. The bottom image shows how the oxidized portion failed (intergranular) along the grain boundary after testing.

A novel approach, combining extensive experimental work and modelling through the crystal plasticity finite element method (CPFEM), now enables the quantification of the stress necessary to fail individual oxidized GBs. This approach involves the micromechanical testing of cantilevers containing the GB of interest (Figure 1), to obtain information about the elastic modulus, yield stress and fracture toughness, as well as a detailed characterization of the fracture region via 3D FIB-Slicing and (S)TEM to correlate the measured mechanical response to the specific (3D) microstructure and degree of oxidation. Selected Area Diffraction (SAD) is used to identify grain orientations and active slip directions. With this information, a realistic crystal plasticity model of the cantilever is built, employing a user element (UEL) for Abaqus [1]. Previous work [1-2] has highlighted the dependence of local stress and slip accumulation on grain orientation. In this work we are able to incorporate the crystallographic orientations and sample geometry into our model very accurately

We also use cohesive contact to simulate the fracture of the metal/oxide interface, allowing our model to reproduce the different fracture modes observed in experiments, and the interaction between plasticity and fracture. We aim to use our calibrated model to predict the fracture behaviour of different types of GBs, including variations in misorientation and carbide coverage. This could reveal which oxidized GBs are harder to fracture, which is relevant to the field of GB engineering.

The authors want to thank INSS (Japan) and EDF (France) for the provision and autoclaving of the samples. EDF is further acknowledged for the financial support of this work.

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Cyclic deformation experiments and plasticity modeling of three Ti microstructures

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The performance of titanium alloys is strongly dependent on their microstructure formed during thermo-mechanical processing. Accurate modelling of the microstructure-sensitive deformation for titanium alloys is crucial for future materials design and development. The current state-of-the-art for modelling polycrystalline deformation is through the crystal plasticity finite element method (CPFEM). In the present work, a crystal plasticity framework based on a Kocks-type of flow rule has been calibrated to data acquired from cyclic deformation experiments performed on three different titanium microstructures: 1) Ti-64 in a beta-annealed condition; 2) Ti-18 in a solution-treated, age hardened (STA) condition; 3) Ti-18 with a beta-annealed, slow-cooled, age-hardened treatment (BASCA).

The crystal plasticity model employs physically based parameters to determine the simulated mechanical response, many of the parameter values have been obtained from materials characterization as well as from literature sources. The remaining parameters have been estimated such that the simulated macroscopic stress-strain response closely agrees with the experimental results. The robustness of all the calibrated model parameter sets were evaluated by comparing simulation results to additional experimental data. The simulated plasticity model was able to accurately capture the stress-strain response of each microstructure while maintaining the relative strength trends presented in the literature for the estimated parameters (see Fig. 1) [1].

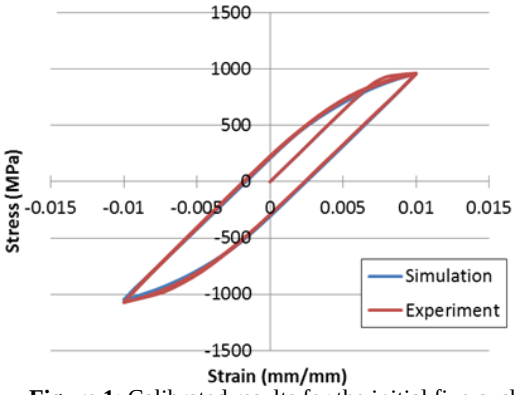

Figure 1: Calibrated results for the initial five cycles of loading of the Ti-64 β-annealed microstructure at room temperature with fully reversed, ε_a=1%, and $5x10^{-4}$ s^{-1} loading. [1]

The present work demonstrates the process of model development and calibration necessary to simulate the cumulative deformation mechanisms which cooperatively produce the observed experimental results. These calibrated models have great potential for future utilization in microstructure sensitive studies which can expedite the materials design process by identifying ideal microstructure morphologies for specific applications.

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The Deformation Induced Martensitic Transformation of Metastable Austenite

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Metastable austenitic steels are valued for their high strength and uniform elongation. This unusual combination of properties arises from the progressive transformation of the microstructure from austenite to α′-martensite during deformation. Unsurprisingly, the success of any model for the bulk mechanical response is tied to successfully modelling the dependence of martensitic transformation on deformation. Lacking a fundamental understanding of the processes that control nucleation and growth of the martensite phase in this case, models must rely on empirical descriptions of the transformation kinetics. Recent work on the role of stress and plastic strain on crystallographic variant selection has raised the question of the relative importance of plasticity versus local stress state in governing the transformation kinetics[1-3]. In this work, we have attempted to study a simplified situation by examining the martensitic γ to α′-BCC transformation via molecular dynamics and molecular statics simulation using an empirical potential that mimics many of the characteristics of pure Fe. These results are examined in conjunction with experimental work on the martensitic transformation in γ-Fe precipitates in model alloys as well as the martensitic transformation in stainless steels. In particular, the role of local stress state is emphasized in the process of nucleation. The resulting orientation relationship between a confining FCC matrix and martensite is discussed in terms of the pathway followed during the γ to α′-BCC martensitic transformation.

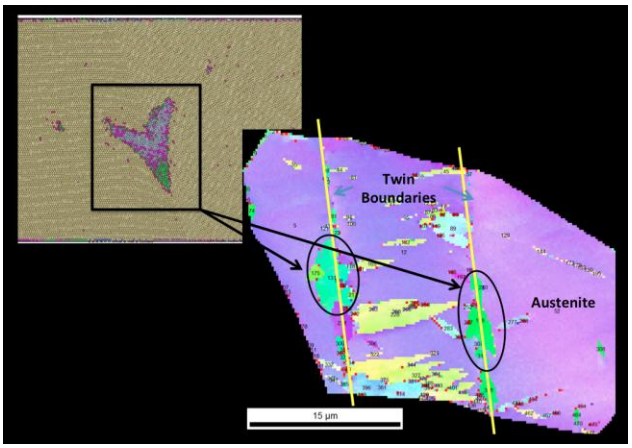

Figure 1: Comparison of the morphology and crystallography of martensite formed during deformation at a twin boundary in an FCC matrix by molecular dynamics simulation (top, left) and experimentally (by EBSD) at annealing twin boundaries in a metastable austenitic stainless steel (bottom right).

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Microstructure based continuum modeling of highly anisotropic metals

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We present our methods for incorporating deformation physics and microstructure evolution into continuum level simulations of highly anisotropic metals. This involves a combination of modeling efforts and experimental validation at length scales ranging from the micro-scale to continuum level.

Our micro-scale constitutive law accounts for a dislocation- based hardening law for multiple slip systems and experimentally characterized twinning modes at the grain level. We incorporate the micro- scale deformation laws into a viscoplastic self-consistent (VPSC) polycrystal homogenization scheme that is calibrated with mechanical tests and experimental measures of texture and twin volume fraction evolution. These experiments include compression and tension tests in multiple orientations for three different starting textures. We included strain rate and temperature effects through thermally-activated recovery, dislocation substructure formation, and slip-twin interactions that are calibrated to experiments at multiple strain rates and temperatures. The VPSC based polycrystal model is implemented into an implicit finite element (FE) framework. In this approach, a finite element integration point represents a polycrystal material point and the meso-scale mechanical response of each integration point is obtained by the mean-field VPSC homogenization scheme. We demonstrate the accuracy of the FE-VPSC model by analyzing the mechanical response and microstructure evolution of α-uranium samples under simple compression/tension and four-point bending tests. Predictions of the FE-VPSC simulations compare favorably with experimental measurements of geometrical changes and microstructure evolution. The model accurately captures the tension–compression asymmetry of the material associated with twinning, as well as the rigidity of the material response along the hard-to- deform crystallographic orientations. We apply this method to predict strain heterogeneities that occur during rolling and forming operations of α-uranium parts.

Strain Gradient Crystal Plasticity Modelling – An Efficient Approach to Capture Experimental and Discrete Dislocation Dynamics Observations?

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Size effects are commonly observed in the elastic-plastic deformation of micro-specimen in experiments, e.g. in tensile tests (for a recent work see e.g. [1]). One major contribution to this phenomenon in the mechanical response stems from the resistance of grain boundaries against plastic flow [2].

It is shown that this experimentally observed behavior can be reasonably captured with a single-crystal strain gradient plasticity theory for small deformations. This theory is extended by a grain boundary yield criterion [3]. For numerical efficiency the use of an equivalent plastic strain and its gradient are emphasized.

The theory is implemented in weak sense with Finite Elements. Tensile test simulation results of oligocrystals are shown. Further comparison to an experiment and a comparison to Discrete Dislocation Dynamics (DDD) simulations are presented.

Discussion of the latter comparisons and an outline of further possible refinement of the theory at hand conclude the talk.

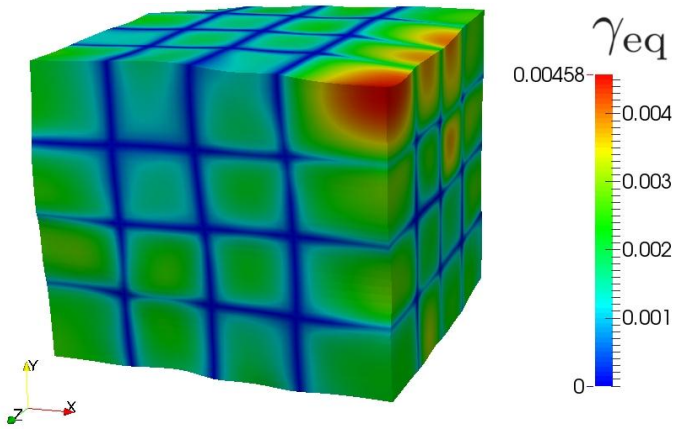

Figure 1: 64-grain tensile test simulation, equivalent plastic strain field distribution at the the onset of plastic deformation

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Intermittent and heterogeneous plasticity in hcp alloys: correlations between experimental results and multiscale models

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Zirconium and titanium alloys exhibit, in a wide domain of temperatures and strain rates, a strongly heterogeneous spacio-temporal distribution of plasticity at scales that vary across the domain and also with their microstructure, their texture, the amount of plastic strain and the load path. Various slip systems are observed to generate arrays of dislocations including pile-ups, tangles and subgrains.

Throughout the temperature and strain rate domain where negative strain rate sensitivity and its associated strain localization phenomena are observed, Ti base alloys exhibit two radically different *eigen-modes* of plasticity: 1- the *friction mode* that leads to intermittent plasticity in strain localization bands that are usually mobile. 2 – the *solute drag mode* of plasticity akin to creep and that can eventually lead to complete « arrest » due to the cumulative effects of strain- and time- hardening.

Creep bifurcation phenomena, observed as prevailing in the lower temperature part of the domain, can adequately be modeled by simply combining KEMC equations with FEM. When bifurcation takes place "within the structure" (test piece, part in service), the contrast in flow stress level of neighboring zones increases and results in local accumulation of damage and finally enforces fracture. These detrimental strain localization phenomena are enhanced when the structure is exposed to "Fatigue with dwell time" or "creep-fatigue" mode.

The shortcoming of this simple approach lies in the formation of strain rate bands, the size, distribution and velocities of which are not observed experimentally. The spacial distribution of strain localization in hcp structures appears to be strongly dependent on grain orientations and local combinations of plastically compatible grain associations. A polycrystalline model was therefore developed which includes "a" basal, prismatic and pyramidal slip systems, "c+a" pyramidal slip systems, realistic values of their CRSS and their potential strain and time hardening abilities. The results compare well with the experimental observations of tensile curves exhibiting Portevin-Lechâtelier serrations and the corresponding distribution of grain orientation sensitive strain and strain rate localizations. This model also provides detail information regarding the strain burst patterns eventually leading to creep arrest.

Grain-scale Experimental Validation of Crystal Plasticity Finite Element Simulations of Tantalum Oligocrystals

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Quantitative comparison of experiments and simulations of polycrystalline deformation behavior at the grain scale is challenging due to the heterogeneous subsurface grain morphology. To mitigate this effect of unknown subsurface microstructure, we used tantalum tensile specimens with a pseudo-two-dimensional grain structure with grain sizes on the order of millimeters. The deformation of tantalum oligocrystals (less than 20 grains in the gage section) was characterized using various experimental techniques and quantitatively compared with predictions using a novel BCC crystal plasticity finite element (CP-FE) model.

An experimental technique combining in-situ electron backscatter diffraction (EBSD), high-resolution digital image correlation (HR-DIC), and profilometry, was used to map intergranular crystal rotation, surface strain fields and out-of-plane topographic distortion, respectively, at various applied strains. The CP-FE predictions of deformation agreed reasonably well with experimental measurements. Possible causes of localized disagreements and the influence of model parameters will also be discussed, such as the mesh dependence, the assignment of initial crystal orientations and the choice of the slip planes and hardening laws.

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