Toward mastery of microstructural degrees of freedom in engineering design

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Having “The Microstructural Frontier” theme for the present MMM conference, it is fitting to examine the means for using microstructural information as an integral part of the design-materials-manufacturing enterprise. During the 1980’s and early 1990’s process-modeling frameworks introduced formal linkages between manufacturing and engineering design systems. Extensions of these now treat primarily empirical or mean-field representations of microstructure influences. Common design practices optimize materials structure, as represented via spatiotemporal fields of continuum state variables gleaned from process models of selected manufacturing operations (i.e. casting, forming, etc.) Selectively, those continuum methods are coupled to microstructure evolution and performance models, but only for mean-field representations. Thus, the methods implicitly represent materials structure, or treat it in only a homogenized fashion. Looking further, computational linkages between materials structure descriptions and manufacturing processes or, between materials structure descriptions and engineering performance are more tenuous, even from an implicit perspective. The MMM challenge is to devise schemes for explicitly and objectively operating with microstructural degrees of freedom while minimizing needs for measured information.

In this work we describe a growing software environment that permits objective and quantitative descriptions of hierarchical materials microstructure information and, management of its linkages to both materials performance simulations and experimental validation tools. The environment, which is called “DREAM.3D” [1], is an open source software base that evolved from more than a decade of community wide efforts toward mastering the machine representation of microstructure information. Recent and current developments show the multi-scale applicability of the framework and its formal ties to destructive and non-destructive materials characterization. Further, selected linkages to simulations at multiple scales are also shown. These and future prospects for MMM are discussed.

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Image Based Crystal Plasticity FE Models for Predicting Fatigue in Polycrystalline
Metals and Alloys: Addressing the ICMSE Initiative

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The Integrated Computational Materials Science & Engineering or ICMSE initiative entails integration of information across length and time scales for relevant materials phenomena and enables concurrent analysis of manufacturing, design, and materials. Computational Mechanics plays an important role in this integration. This talk will present various ICMSE approaches in the development of a microstructure based modeling of fatigue crack initiation in polycrystalline alloys. The model implements crystal plasticity theory with explicit grain structures and the mechanical response of polycrystalline aggregates are deduced from the behavior of constituent crystal grains. These calculations provide a platform for the implementation of physics-based crack evolution criterion that accounts for the effects of microstructural inhomogeneity. Systematic development of a crystal plasticity-based fatigue crack nucleation model is conducted. The presentation will also discuss a wavelet transformation based multi-time scaling (WATMUS) algorithm for accelerated crystal plasticity finite element simulations. The WATMUS algorithm does not require any scale-separation and naturally transforms the coarse time scale response into a monotonic cycle scale without the requirement of sub-cycle resolution. The method significantly enhances computational efficiency in comparison with conventional single time scale integration methods. Adaptivity conditions are also developed for this algorithm to improve accuracy and efficiency. Finally the talk will discuss an approach to evaluate coupled crystal plasticity-damage evolution relations based on molecular dynamics simulations of a crystalline material with an embedded crack.
Impact of Spatially Non-Random Solute on the Strength of Aluminum Alloys

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For many aluminum alloys natural aging leads to solute redistribution and solute clustering. The significance of this process on yield strength is well illustrated by alloy AA6111 where the yield strength increase can be >200% upon room temperature aging [1]. The microstructural evolution during this period is complex as the composition, size, shape and spatial distribution of the resulting solute clusters is difficult to define (fig. 1). How one should physically incorporate detailed information coming from atomic scale measurements into mean-field engineering models for yield strength becomes a question since such models do not, by definition, naturally include effects arising from distributions in obstacle size, strength and spatial distribution.

Motivated by a desire to predict the macroscopic yield strength during low temperature aging of aluminum alloys, we have examined the influence of obstacle strength and spatial distribution in the glide plane using meso-scale two-dimensional areal glide models [2,3]. We have also investigated an addition law appropriate for obtaining the macroscopic yield strength when a set of two or more obstacles (e.g. solute, clusters, precipitates and dislocations) is present on the glide plane [3]. Such meso-scale models require ad-hoc assumptions to be made about the correlation between an obstacle and its strength. To investigate this further, particularly for the case of solute clusters, we have performed fully atomistic molecular dynamics/molecular statics simulations to investigate how a dislocation samples different spatially distributed sets of solute atoms for model alloy systems. The challenges and successes of integrating the approaches used in this work will be discussed.

(a)  Mg  Si  Cu  

(b) 

Figure 1: a) The early stages of cluster formation in AA6111 held at 180°C for 4 minutes [1] b) Prediction from an areal glide model of the effect of obstacle clustering in the glide plane on the normalized critical resolved shear stress for dislocation motion [2].

Hierarchical crystal plasticity model for nickel-based superalloys: sub-grain microstructures to polycrystalline aggregates

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A hierarchical crystal plasticity model for Ni-based superalloys is developed for three scales in this study. In order to establish a hierarchical constitutive model, behaviors at different length scales have to be formulated to capture desired phenomena corresponding to the application. Such formulations include all dominated mechanisms. APB-shearing and Micro-twinning are two activated mechanisms in this temperature ranges. In the lowest scale, explicit dependencies on sub-grain scale morphological characteristics are attributed. An essential ingredient for this development is a sub-grain scale crystal plasticity FEM model scale for micromechanical RVE analysis with explicit depiction of the $\gamma - \gamma'$ morphology. The model numerically implements a size-dependent dislocation density-based crystal plasticity model with a representation of APB shearing of $\gamma'$ precipitates by $\gamma$ - matrix dislocations. It is computationally expensive to incorporate the explicit models of the $\gamma - \gamma'$ microstructure in a crystal plasticity based model to simulate the response of the crystalline microstructure of these alloys. Thus to retrieve the morphology features into the next scale, the lowest scale model is homogenized as a function of various microstructural parameters and the activation-based homogenized model is used at the next level (i.e., single crystal grain scale) of crystal plasticity model. In the next ascending scale, a polycrystalline microstructure of Ni-based superalloys is modeling using the homogenized CPFE model for single crystal scale analysis. Different grain features are incorporated to simulate the polycrystalline microstructure by augmentation and incorporation of the homogenized activation energy-based crystal plasticity constitutive model for this scale. The results of each scale are compared with experimental data at corresponding scales with good agreement.
Vi(CA)$_2$T – Virtual Cement & Concrete Aging Analysis Toolbox

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For managing the long term operation of nuclear power plants and preparing the construction of new ones, the assessment of the aging of cement and concrete materials play a significant role. It permits electricity utilities to control civil works’ degradation and optimize their maintenance in order to ensure plants’ safety. At EDF, the biggest nuclear operator in the world (owner of 73 reactors in UK and France, joint-owner of 5 reactors in USA), this assessment primarily relies on an extensive set of periodic monitoring data and experimental tests. EDF approach being turned towards continuous improvement of safety, EDF research and development service (EDF R&D) is currently developing, in a combined effort with EDF engineering services, a numerical tool aimed at predicting cementitious materials ageing, called Vi(CA)$_2$T (Virtual Cement and Concrete Ageing Analysis Toolbox). This contribution presents the version 2.1 of this tool suite.

To be predictive and to avoid relying on both empirical models and a huge database of tests, Vi(CA)$_2$T takes advantage of recent progresses in physics-based material modelling. More precisely, it is made up of

- a physico-chemical computation module to predict the evolution with respect to time of cement phases’ volume fractions,
- mechanical computation modules in order to estimate the evolution of material parameters like Young modulus, compression strength and creep.

In the physico-chemical computation, hydration kinetics are predicted based on the laws of Avrami [1] and of Fuji & Kondo [2]. The effect of silica fume is also taken into account. The mechanical computations are based on mean field micromechanical models developed in literature [3, 4] and at EDF R&D [5, 6]. In the objective of building a professional tool suite for engineering services, the development of Vi(CA)$_2$T considers the user experience as a first priority. Usage is very simple: the user needs to enter only cement and concrete formulations and the computation results are available within less than 60 seconds.

Prospects for version 3 include the estimation of transport properties, such as resistivity or permeabilities. As these properties are expected to be highly dependent on the composite morphology, this might require to switch to full field (3D) micromechanical tools.

Decoding Cement Hydrate: Hierarchical Modeling from Electrons to Microstructures

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Despite the omnipresence of concrete as the world’s dominating manufacturing material, which accounts for 5-10% of the total anthropogenic CO₂ emissions worldwide, the interplay between structure, morphology and chemical composition of its smallest building block, Calcium-Silicate-Hydrate (C-S-H), is essentially unexplored. Together these characteristics of this “liquid stone” gel define cement hydrate and enable modulation of its physical and mechanical properties with the ultimate goal of reducing concrete environmental footprint. Here, we propose a bottom-up multi-scale approach developed with the focus of unraveling the hierarchical structure of C-S-H, which is the principal source of strength and durability in all Portland cement concretes (Figure 1). First, by using statistical mechanics coupled to a combinatorial defect optimization approach, we decode the basic molecular structure of hundreds of amorphous C-S-H gels, corresponding to different chemical compositions. By allowing for short silica chains distributed as monomers, dimers, and pentamers, these C-S-H archetypes of molecular descriptions of interacting CaO, SiO₂, and H₂O units provide not only realistic values of calcium to silicon (C/S) ratios but the densities, which are computed by a unique combination of grand canonical Monte Carlo simulation of water adsorption and molecular dynamics at 300 K. We found that the C-S-H gel structure includes glass-like short-range order features at large C/S, and crystalline features of the mineral tobermorite at low C/S. Second, we show that upon applying strain-controlled tension to the decoded C-S-H polymorphs, rupture occurs mostly around the silica-rich and defected regions. These weak regions enable identifying particle boundaries for various C-S-H particles, which together form the C-S-H microstructure. The latter is modeled using meso-scale Monte-Carlo simulations with inter-particle interactions based on parameters directly obtained from partial atomic charges computed by ab-initio calculations. Finally, we probe the mechanical stiffness, strength, and matrix morphology of the microstructural model, and compare the results with experimentally measured properties of C-S-H. In view of this MMM conference theme on “Microstructural Frontiers”, this bottom-up approach, motivated by combinatorial atomistic modeling, introduces innovative paradigms for acknowledge-based modulation of the cement chemistry at the micro scale to answer the global needs for greening construction materials.

FTMP-based Continuum Description of 4D Discrete Dislocation Systems

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A sophisticated method for expressing three-dimensionally evolving discrete dislocation ensembles is proposed based on Field Theory of Multiscale Plasticity (FTMP)[1] coupled with a working hypothesis called flow-evolutionary law[2]. The law can be visualized by “duality diagram,” where the spatial trace of the incompatibility tensor for the targeted system is plotted against fluctuation part of the elastic strain energy. Collapsing walls made of mixed dislocation networks, screw networks, and that mimicking lath wall, are simulated by using dislocation dynamics, respectively. The duality diagram representation for them is demonstrated to provide a number of valuable pieces of information characterizing the evolutionary aspects of the system. It visually tells us how the targeted system tries to store/release the strain energy, resulting in the configurational changes, while the ratios at each point on the diagram, referred to as duality coefficient \( \kappa \), can quantitatively capture the “stability/instability” of the system, as summarized in Fig.1, where the standard deviation of the dislocation segments from the original configurations is used for characterizing the degree of collapse of the walls. The mixed walls tend to yield larger slope than the lath wall, implying less stability characteristics, whereas the lath wall is regarded as most stable among others as the smaller slope result

![Screw Wall, Mixed: N=0, Mixed: N=100]

**Figure 1:** Quantitative evaluation of collapsing dislocation walls by duality coefficient, i.e., ratio of incompatibility to fluctuating strain energy, in terms of structural stability/instability, comparing three distinct cases.

Hot-working Multiscale Simulations Using Multi-phase-field Finite Element Dynamic Recrystallization Model

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During hot-working of low-to-medium stacking fault energy material, dynamic recrystallization (DRX) with plastic deformation and recrystallization occurs. Therefore, in order to evaluate macroscopic mechanical behaviors during hot-working of the DRX material, it is important to take the microstructure evolution into account.

In our previous study [1], we have developed a hot-working multiscale model where macroscopic mechanical behaviors are evaluated by elastic-plastic large deformation finite element (FE) simulations and microstructure evolutions are simulated by multi-phase-field (MPF) method [2]. We call the model as multi-phase-field finite element dynamic recrystallization (MPFFE-DRX) model.

In this study, we show realistic hot-working simulations using the MPFFE-DRX model. Figure 1 shows a compression simulation of truncated cone with 16 mm height. The simulation was performed as an axisymmetric problem with 100 triangular elements. Although not shown here, the microstructure evolutions are simulated in every triangular element using MPF. The detail results will be presented in the conference.

![Compression simulation of truncated cone using MPFFE-DRX model.](image)

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