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14. ABSTRACT This project has made major developments in two areas that are of significant importance in modeling deformation and fatigue behavior of polycrystalline metals and alloys. The work has developed significant collaboration with researchers at AFRL and has received acclaim within the Air Force materials community. A book edited by the PI and D. Dimiduk is a result of this collaboration. The products developed include: (i) 3D Polycrystalline Microstructure Reconstruction from FIB Generated Serial Sections for FE Analysis: This work develops a robust CAD-based methodology for simulating 3D microstructures of polycrystalline metals and alloys from orientation microscopy images of material sections. This is followed by discretization into a 3D tetrahedral mesh for finite element (FE) analysis. (ii) Dual-Time Scale Finite Element Model for Simulating Cyclic Deformation and Fatigue Crack Nucleation in Polycrystalline Alloys: A major focus of this research is simulating fatigue crack initiation. A dual-time scale crystal plasticity finite element model is developed. A novel wavelet decomposition based multi-time scale methodology is proposed, which significantly reduces the computational time till crack initiation.					
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COMPUTATIONAL MODELING SYSTEM FOR DEFORMATION AND FAILURE IN POLYCRYSTALLINE METALS

A Proposal to

THE AIR FORCE OFFICE OF SCIENTIFIC RESEARCH

RESEARCH AREA: Metallic Materials, Aerospace and Materials Sciences Directorate

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PROJECT SUMMARY

The proposed research entitled '*Computational Modeling System for Deformation and Failure in Polycrystalline Metals*' will develop an integrated system of experimentally validated computational models, for simulating the deformation and failure behavior of polycrystalline metals and alloys. The system will consist of *computational models and software* for: (a) 3D microstructure reconstruction and characterization of morphological and crystallographic information, (b) image-based microstructural computational models incorporating crystal plasticity and fracture laws, and (c) a multi-time scaling time integration algorithms for cyclic deformation, to investigate the effect of material microstructure on deformation behavior and fatigue life. The computational system is expected to assist engineers, especially in the aircraft engine industry, in their product design for enhanced performance and reliability.

It is well known that the development of such an integrated system is a necessary, yet challenging undertaking. Conventional commercial Finite Element Method (FEM) codes have a number of shortcomings when modeling real materials due to lack of certain key aspects, such as efficiency, accuracy in the presence high gradients and discontinuities, numerical stability, etc. Important advances are needed in computational tools and methodologies to overcome these shortcomings. The PI has gained considerable research experience in the development of advanced micromechanical computational models for material characterization and modeling that can effectively address some of these problems for polycrystalline and poly-phase materials. An important component of the development of any computational model is its validation with experiments. Collaborations of the PI with Dr. M.J. Mills (OSU), Dr. D. Dimiduk (AFRL/MLLM) and Dr. M. Uchic (AFRL/MLLM) in his current research [1,2], have provided this indispensable component to add robustness to the models. The proposed research will involve collaborations with Drs. Mills, Fraser of OSU, and Drs. Dimiduk, Uchic and Parthasarathy of AFRL/MLLM, for insight and validation of the computational systems to be developed. The research partners have complimentary strengths that will contribute towards the comprehension and overall goals of this research. The proposed program will complement ongoing research thrusts in the Materials Directorate at AFRL and at OSU under the *Science and Technology Workforce for the 21st Century (STW-21)* cooperative agreement program between OSU and AFRL.

Computational models will be developed in the proposed program to incorporate accurate microstructural morphology and crystallographic information for analyzing structure-sensitive deformation and fatigue behavior. Primary focus will be on aerospace metals and alloys, e.g. IN-100, Ti-6242 and Ti-6Al-4V, with a motivation to improve performance and reliability of aerospace engine materials. A comprehensive approach will be pursued, coupling the following elements:

- (i) Reconstruction of 2D and 3D microstructural models with real morphological features and crystallographic orientations from quantitative metallography combining focused ion beam (FIB) and electron back-scatter detector (EBSD) in orientation imaging microscopy, microstructural characterization, and statistical methods.
- (ii) Development of experimentally validated finite deformation rate-dependent crystal plasticity models with size effects, for analyzing deformation and creep in polycrystalline aggregates.
- (iii) Development of an experimentally validated cohesive zone model for inter and intra-granular fracture initiation and growth for fatigue crack modeling.
- (iv) Development of a *stable, accurate and efficient* image-based micromechanical finite element model, for crystal plasticity and damage, incorporating real morphological and crystallographic features. A novelty of this model would be in the powerful adaptive techniques for automatically changing the element resolution and topology with evolving strain localization and damage.
- (v) Development of multi-scaling algorithms in the time domain for compression and localization in cyclic deformation analysis.

In summary, the proposed research will develop experimentally validated *innovative high fidelity computational tools* to provide improved predictive capabilities for fatigue failure analysis in materials with aerospace applications. The program is expected to advance the state of the art in analysis methodology for high confidence in component performance and life calculations.

1. STATEMENT OF OBJECTIVES

Following the Air Force's thrusts in advanced military, aerospace and space exploration systems, the proposed research is aimed at developing an integrated system of *computational models and predictive tools* that can be utilized to enhancing performance and reliability of polycrystalline metals and alloys used in aerospace applications. These materials, e.g. IN-100 or Ti-6242 and Ti-6Al-4V are used in aircraft engine components. Understanding the role of material microstructure, at the length scale of grains and polycrystalline aggregates, on the deformation and failure characteristics of the material is critical to the reliable design of components for high performance applications. Such an understanding requires an analysis framework that can predict inhomogeneities in time-dependent plastic flow under fatigue and creep conditions. Naturally, that sets a requirement for representing the real microstructure and defects, within the plasticity analysis tools. A robust design methodology must also link variabilities involved at all length scales that can affect the components in service performance.

Developing advanced computational tools to unravel these complex relations will be the objective of the proposed research. Most of the current efforts in this area employ commercial FEM codes like ABAQUS [3]. Many of these implementations suffer from severe limitations in efficiency, accuracy and resolution in regions of high gradients, as well as numerical stability, for modeling real materials. The PI has been involved in the development of advanced micromechanical computational models for material characterization and analysis of deformation and failure in poly-phase and polycrystalline materials. This experience will be utilized in the proposed research to develop numerically stable and robust, *image-based micromechanical computational models* of plasticity and damage, incorporating real morphological and crystallographic features. The goal will be to investigate/predict the dependence of cyclic deformation behavior and fatigue crack evolution, on the material microstructure. The model development will be intricately coupled with experimental validation, for which the material system will concentrate on Titanium and Nickel alloys with hcp and fcc crystalline structure respectively. The program will complement ongoing research thrusts on materials development and structural design at the Materials Directorate of AFRL/MLLM under the leadership of Dr. D. Dimiduk. Ongoing collaborations with Professors M.J. Mills and H. L. Fraser at OSU and Drs. D. Dimiduk, T.A. Parthasarathy and M. Uchic at AFRL/MLLM will be augmented under the auspices of this research program. A comprehensive approach will entail the following activities.

- i. *Construction of 2D and 3D Microstructural Models*: This task will create computer models of the material microstructure, incorporating morphological features like grain geometry and neighbor description, and crystallographic orientations. Quantitative metallography, combining focused ion beam (FIB) techniques for material sectioning and electron back-scatter detector (EBSD) in orientation imaging microscopy (OIM), will provide the necessary microstructural information and data. Such experimental activity is already in progress at OSU and AFRL facilities under the existing *Science and Technology Workforce for the 21st Century (STW-21)* cooperative agreement between AFRL and OSU. Subsequently, microstructural characterization, statistical and stereological methods and computational algorithms will be explored for effective 3D construction.
- ii. *Development of Experimentally Validated Constitutive and Damage Models*: In this task, finite deformation rate-dependent crystal plasticity models with size effects will be developed, for analyzing cyclic deformation and creep in polycrystalline aggregates. In addition, special cohesive zone models with traction-displacement laws will be developed for inter and intra-granular fracture initiation and growth during cyclic deformation and fatigue cracking. The models will be validated with experiments for plastic deformation and creep in polycrystalline aggregates and evolution of fatigue fracture. This research will be integrated with ongoing experimental research programs at OSU (Mills, Fraser) and AFRL/MLLM (Dimiduk, Parthasarathy, Uchic) on state of the art mechanical testing and material characterization.

- iii. *Development of Adaptive Image based Micromechanical Computational Models:* This task will build novel finite elements models that evolve from the material microstructure and have special characteristics of numerical stability, accuracy and resolution and efficiency, for highly non-homogeneous fields. In particular, a grain-based finite element model (*GBFEM*) manifesting the material crystalline structure and morphology will be developed using computational micromechanics for finite deformation rate-dependent crystal plasticity and microstructural damage evolution. Adaptivity of the computational domain is a necessary feature to enhance efficiency, especially in the presence of evolving localized deformation and cracking. GBFEM will be endowed with *adaptive* capabilities to identify and impart preferential resolutions to these regions by local enrichment. It will also admit changing topology due to the onset and growth of microcracks through adaptive introduction of cohesive zone models of fracture. Time stepping algorithms, currently used in commercial codes for the simulation of cyclic deformation during fatigue, have serious limitations with respect to the number of cycles that can be simulated. An adaptive multi-time scaling methodology is currently being developed by the PI to overcome this limitation through homogenization and localization of computations in the time domain [4]. This multi-time scaling methodology will be incorporated in the computational modeling framework. Finally, to facilitate large scale computing of real materials, the models will be coupled with high performance computing tools, incorporating parallel structure with dynamic load balancing strategies.

In summary, this research will introduce new directions and advance the state of the art in computational modeling methodologies that can provide an improved level of understanding of the factors that cause fatigue failure in metallic materials.

2. MOTIVATION AND SIGNIFICANCE

Advanced military aerospace systems like the Joint Strike Fighter, unmanned missile technologies, future military aircrafts as well as improved space access systems, are thrust areas of priority at the Air Force [4]. Major goals of these programs are to drastically reduce hardware and support costs, improve reliability, expand reusability and to enhance thrust-to-weight performance. Improved materials having high specific properties, e.g. low weight, high stiffness, fatigue strength, and fracture toughness at a range of service temperatures are essential for achieving these lofty structural-efficiency goals. The need for the proposed research is derived from these thrusts to improve space and aero-propulsion systems.

Progressive developments in advanced materials have contributed tremendously to the enhancements in aerospace applications, especially in the thrust-to-weight ratio of aero-gas turbine engines. This has mainly been possible through the introduction of titanium and nickel based alloys like super-alloy IN-100 and Ti-6242 and Ti-6Al-4V, which have provided enabling technology for enhanced performance and reliability. The design and development of lightweight, high temperature-creep resistant aerospace engine components like fan blades, high-pressure compressors and high-pressure turbines (figure 1a) have benefited significantly from these materials. Their contribution is vital, not only in terms of desirable properties, but also improved reliability. Continuing growth of the aerospace industry demands further research and development of advanced materials having heterogeneous or graded microstructures, such as the dual-microstructure turbine disks. The proposed research is motivated by the need for rational design procedures to select '*optimal material microstructures*' that will enhance the material's mechanical behavior and failure characteristics.

Aerospace components are exposed to cyclic loading conditions due to start up and shut down processes or load reversals during service. In many cases, this results in their fatigue or time dependent fracture.

Fatigue failure in the microstructure primarily evolves in three stages, viz. (i) crack nucleation due to inhomogeneous plastic flow or grain boundary failure, (ii) subsequent crack growth of difficult to predict microstructurally small cracks, by cyclic stresses at a rate dictated by plasticity, stress range and environment, and (iii) coalescence of cracks into the faster crack propagation regime. The phenomena of high-cycle and low-cycle fatigue have been traditionally characterized using macroscopic parameters like applied stresses, cyclic frequency, loading waveform, hold time etc., as well as statistical distributions of fatigue life and fatigue strength [6-11]. Fatigue design by total life approaches includes the stress-life or S-N approach where the stress amplitude versus life is determined, and the strain-life approach e.g. the Coffin-Manson rule, where the number of cycles to failure is determined as a function of plastic strain. Predicting the time to initiate a fatigue crack and propagate it to failure has been the prime objective of these models. In the stress-life approach, the applied stresses are nominally elastic and the number of cycles to failure is large as in high cycle fatigue, while in the strain-life approach components undergo significant plastic straining and crack propagation. The total life approaches have been adjusted for notch effects using fatigue strength reduction and for variable amplitude fatigue e.g. in the Palmgren-Miner rule of cumulative damage. In all cases, microstructural effects are represented only by shifts in such data curves after extensive testing.

Alternatively, the defect or damage tolerant approaches determine fatigue life as the number of cycles to propagate a crack from a certain initial size to a critical size. These are determined from threshold stress intensity, fracture toughness, limit load, allowable strain or allowable compliance. The models assume the presence of a flaw in the structure and predict life, using laws like the Paris law [12]. Fatigue crack advance has been conventionally based on linear elastic fracture mechanics analysis related to the concepts of similitude, in which, stress intensity factors uniquely characterize fatigue crack growth. A number of studies on fatigue behavior of commercial alloys [13,14] have demonstrated the influence of deformation, damage mechanisms, creep, oxidation and microstructural instabilities on cyclic life. Creep-fatigue life predictions models have been developed where the interaction between creep and fatigue has been accounted for by a frequency factor [15], strain range partitioning [16], and damage functions based on hysteresis energy [17]. Although these models have worked well for specific alloys under specific test conditions, a lack of underlying physics and microstructure based considerations plague their portability to other materials and load conditions.

The advanced materials used in many aerospace components have complex multi-colony, multi-phase polycrystalline aggregates (figure 1b). The mechanical behavior and fatigue failure response are intricately governed by microstructural features that include morphological and crystallographic characteristics, e.g. shape, size and location of phases in the colony structure, relative colony size and locations, crystal orientations and misorientations, grain boundary geometry etc (figure 1c). These intrinsic attributes alone would be complex enough, however even further complexity derives from these features interacting with extrinsic defects and design features. In the recent years, detailed micromechanical models have been used to understand damage mechanisms leading to fatigue failure and to throw light on the stochastic nature of fatigue phenomena. However, morphological and crystallographic heterogeneities yielding anisotropic properties and localized non-homogeneous deformation impose severe challenges to these computational models. While some computational models of heterogeneous materials have predicted the stress-strain behavior with reasonable accuracy [13,14] their competence in predicting microstructural variability and effects on ductility and fatigue failure is far from mature. Crystal plasticity theories with explicit grain structures are effective in predicting localized cyclic plastic strains [15]. But their use in accurate damage prediction by inter- and trans-granular and grain boundary decohesion is a difficult task, due to interactions of grain orientations, micro-damage, strain localization and other factors. Studies on deformation modeling [16] have established that preferred grain orientations due to crystal rotation facilitate slip transmittal across grain boundaries and are a dominant cause for material flow anisotropy leading to failure. Metallographic analyses indicate that aside from texture, highly non-homogeneous deformation at inter- and intra-granular levels can

significantly affect the macroscopic softening and failure process [17]. Experimental studies [18] suggest that the growth of crystallographic micro-slip bands along active slip systems of plastic flow is a likely mechanism for localized instability. These micro-bands originate from plastic flow concentration along preferred slip directions and from compatibility requirements between interacting grains. They continue to grow across grain boundaries due to grain structure instability and eventually manifest as macroscopic shear bands. The interaction of microscopic shear bands with transverse grain boundaries also leads to grain boundary micro-cracking, which grow in size and merge to cause fracture.

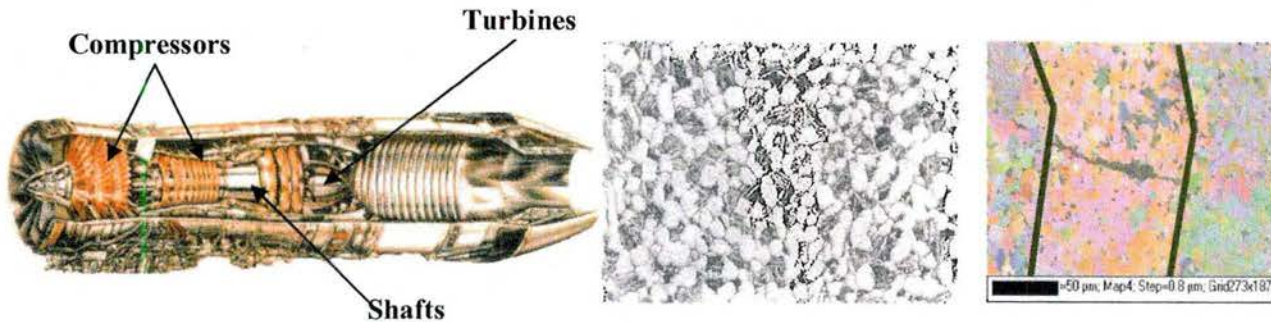


Figure 1: (a) A gas turbine engine, (b) optical micrograph α/β forged Ti-6242 alloy used in the compressor rotor, (c) fatigue crack growth in OIM image.

The difficulties are further compounded by the diversity of mechanical testing conditions. While simple testing conditions, e.g. uniaxial tension-compression tests at constant load amplitudes [19,20,21] have helped in identifying mechanisms of crack evolution processes, their unambiguous extrapolation to various materials is questionable.

In facing up to the challenges faced in the accurate and efficient analysis and design of advanced materials in aerospace components, the proposed research will launch a research program to develop an experimentally-validated computational simulator for predicting material behavior and failure characteristics. Microstructural image-based adaptive computational tools will be developed for a better understanding of the role of material microstructure on mechanical behavior. The models will involve polycrystalline plasticity for multiple phases and crack growth laws. Multi-time scaling facilities will be developed to enable simulation of large number of cycles to failure. This research is expected to provide novel tools and superior technology for better utilization of advanced materials in Air Force and space applications.

3. BACKGROUND & PRIOR RESEARCH OF THE PI IN RELATED AREAS

In his past and current research, the PI has been involved in development of *image-based multiple scale computational models* for mechanical behavior and failure analysis of heterogeneous poly-phase and polycrystalline materials, and for their microstructural characterization. Some of this research in related fields is summarized below.

3.1 Quantitative Metallography and Material Characterization of Polyphase Microstructure

3D microstructures were constructed for characterization and modeling by serial sectioning of particle-reinforced composite (Al-SiC and Al-Si systems) microstructures in [22,23,24]. The 3-D microstructure models were computationally constructed by sequentially stacking a series of scanning electron/optical micrographs (figure 2).

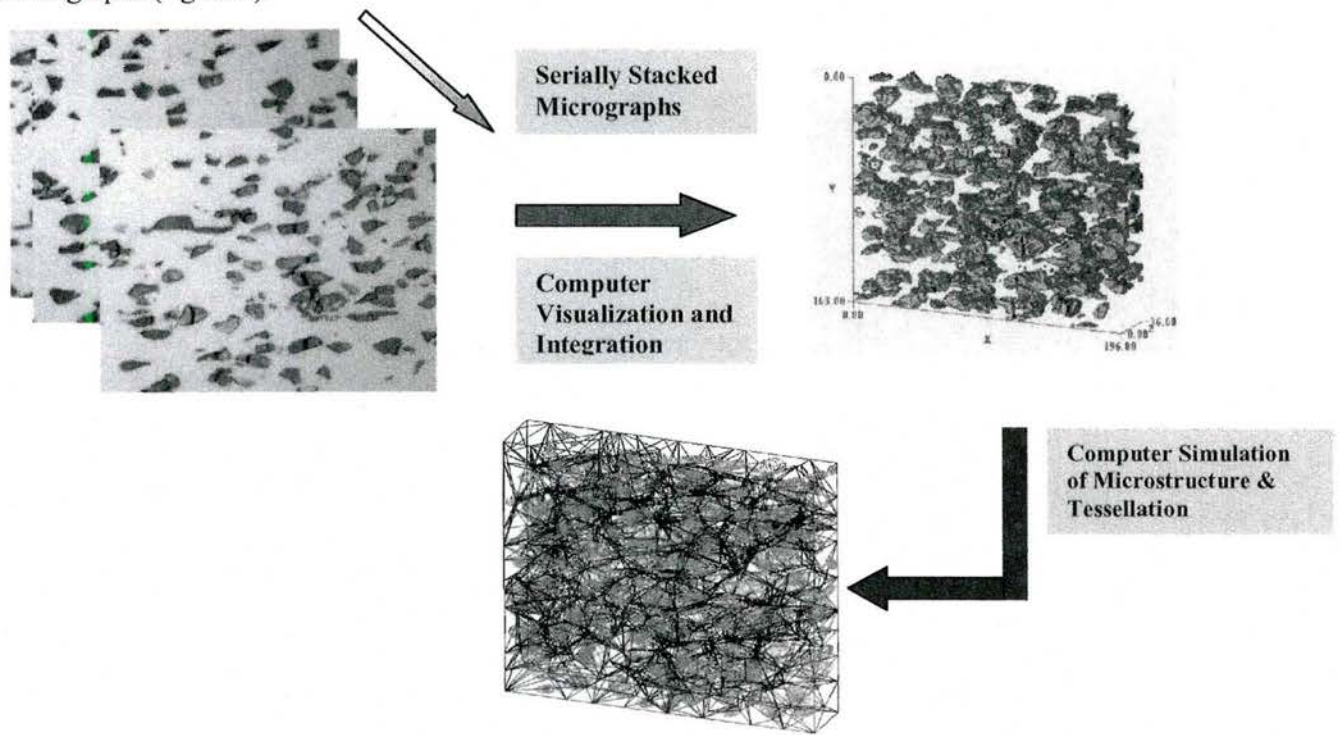


Figure 2: Microstructure for SiC particle reinforced aluminum alloy: (a) a Parallel section micrographs obtained by serial sectioning; (b) computer image created by serially stacking micrographs; (c) simulated equivalent microstructure tessellated into a Voronoi mesh.

The microstructures were tessellated into a network of 2-D and 3-D Voronoi cells (figure 2c). Methods of image analysis have been developed using spatial analysis techniques such as tessellations, and statistical functions like spatial correlation, intensity, and distribution functions. Microstructures were characterized to investigate the role of morphology on the initiation and propagation of damage. Statistical analyses were conducted with marked correlation functions to establish optimal sizes of the microstructural representative volume elements or RVE's.

3.2 Microstructural Characterization of Polycrystalline Microstructures using FIB/EBSD Systems

In this recent work on the STW21 project [2], a new technique utilizing an automated approach of combining a Focused Ion Beam (FIB) and Electron Back-Scatter Detector (EBSD) has been implemented for the collection of 3-D orientation data that can be used to accurately model grain and sub-grain particle structures. The process is capable of sectioning a sample with inter-slice thicknesses as low as 50 nanometers and capturing an orientation map of each slice (see figure 3a). Reconstruction of the 3-D orientation data involves combining or “stacking” the 2-D slices obtained by the FIB-EBSD process (figures 3b and c). A special interactive program called *Micro-Mesher* is developed in this work, which uses the orientation data and information to define microstructural features such as grains and second phase particles. Grain boundaries are typically tortuous and have local position and orientation fluctuations. *Micro-Mesher* approximates these spatially complex boundaries with line segments by using an error-per-unit-length algorithm as set by the user (figure 3b). Important microstructural statistics like size, number of neighboring grains, orientations and misorientations, second phase particles size and inter particle spacing, that are used to define and characterize the 3-D microstructure are also calculated by *Micro-Mesher*. The 3-D statistical information gained from this process improves the ability to accurately characterize the microstructure [2].

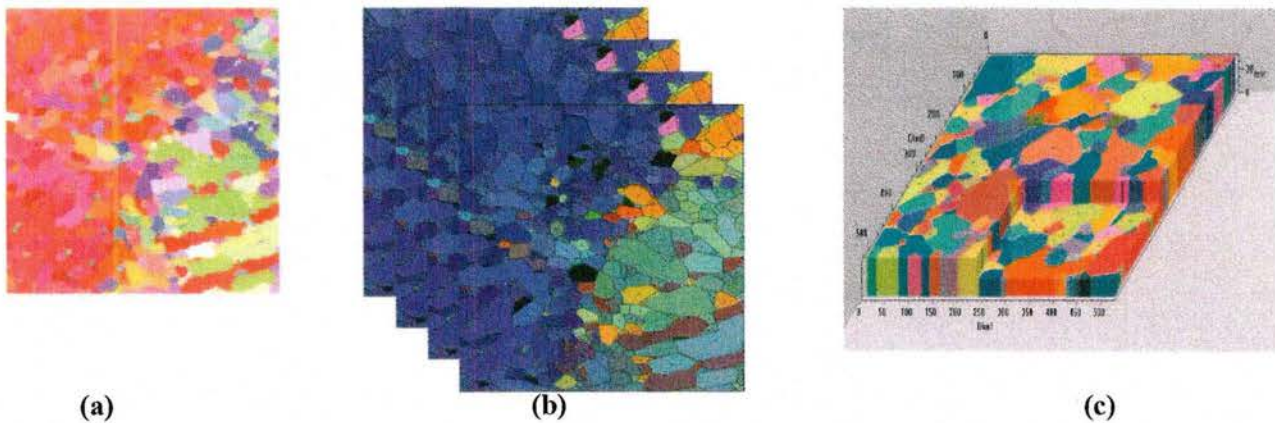


Figure 3: (a) A focused ion beam grain image of a Ti-6242 microstructure from an OIM scan (b) Grain map after approximation by *Micro-Mesher* and sequential stacking, and (c) a 3D computer image created by serially stacking micrographs.

3.3 The Voronoi Cell Finite Element Model (VCFEM) for Micromechanical Modeling

Accurate micro-mechanical modeling of failure in complex heterogeneous microstructures requires very high-resolution models. A powerful Voronoi Cell Finite Element Method (VCFEM) has been developed in [25-30] for accurate *image-based modeling* of non-uniform heterogeneous microstructures. Morphological arbitrariness in dispersion, shape and size of heterogeneities, as acquired from actual micrographs (figure 2c and 3a), are readily modeled by this method. The VCFE model naturally evolves by tessellation of the microstructure into a network of multi-sided Voronoi polygons (figure 4a). Each Voronoi cell with embedded heterogeneities (particle, fiber, void, crack etc.) represents the region of contiguity for the heterogeneity, and is treated as an element in VCFEM. VCFEM elements can be considerably larger than conventional FEM elements and incorporate a special hybrid FEM formulation. Incorporation of known functional forms from analytical micromechanics substantially enhances its convergence. A high level of accuracy and efficiency has been achieved with VCFEM. It can also provide an excellent link between quantitative metallography and mechanical response [28,29]. Successful applications of 2D-small deformation VCFEM have been made in thermo-elastic problems [27], elastic-plastic problems of composite and porous materials [23,25] and damage initiation by particle cracking and interfacial debonding [28,29,30]. An adaptive *VCFEM* has been developed in [25] where optimal

improvement is achieved by adaptive enrichment of the displacement and stress fields. In figure 3c, the stress in a fiber-reinforced composite microstructure by the VCFEM model (figure 4a) is compared with those obtained by a high resolution FEM (figure 4b). Grain level anisotropy and texture and accurate representations of the grain structure are still unresolved issues with this method that will be addressed in the proposed effort.

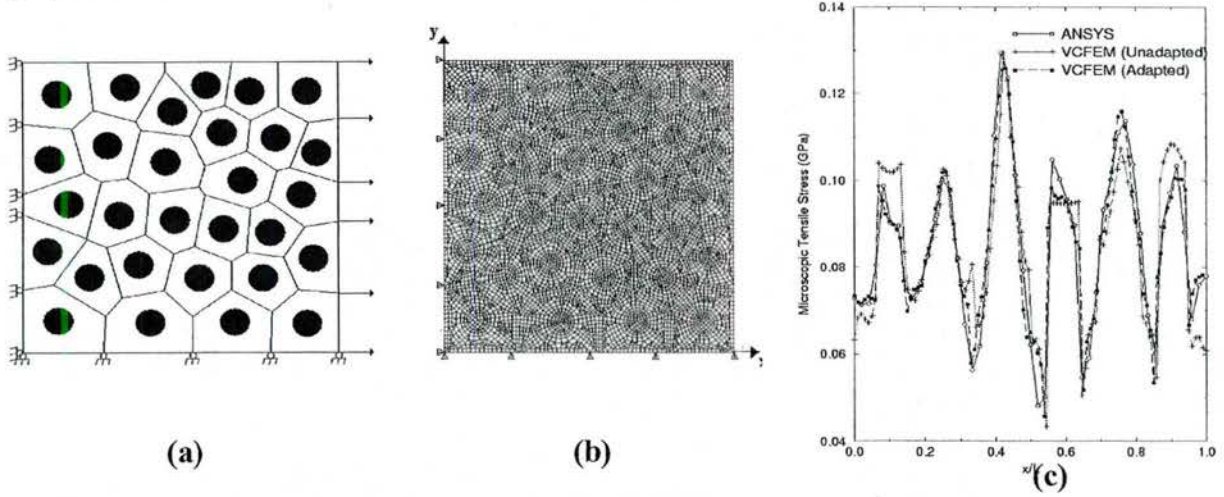


Figure 4: (a) VCFEM mesh; (b) a conventional FEM (ANSYS) mesh for a composite microstructure with dispersed inclusions; (c) Microscopic stress variation by VCFEM and a high resolution ANSYS mesh.

3.4 The Voronoi Cell Finite Element Model for Microstructural Damage Modeling by Interfacial Debonding, Particle Fragmentation and Matrix Cracking in Composite Microstructures

The initiation and growth of damage by interfacial decohesion in fiber-polymer matrix composites is analyzed in [30]. The VCFEM model is augmented with cohesive zone constitutive relations to model the progress of interfacial debonding. Interfacial traction increases with separation to a maximum and subsequently subsides to zero traction, signaling debonding in cohesive zone models. A combined experimental-computational study is conducted with polymer matrix composite specimens with excellent agreement is obtained between experiments and the simulations. Numerical simulations of various multiple-fibers microstructures with different morphologies (dispersions, volume fractions and size distributions) are conducted to understand their influence on the decohesion process. Figure 5a shows a typical nonuniform microstructure of a fiber reinforced composite that is tessellated into a Voronoi cell mesh. Figure 5b shows the corresponding debonding pattern at the fiber-matrix interface. The debond-induced damage is found to be very sensitive to the local morphology e.g. inter-fiber spacing. It is shown that the initiation and especially propagation of debonding depends not only on the total cohesive energy, but also on the shape of the traction-displacement curve. The model is used to study the influence of various local morphological parameters on damage evolution by interfacial debonding.

The Voronoi cell FEM has also been developed to adaptively simulate microstructural damage induced by particle fragmentation and subsequent ductile fracture of the matrix. An experimental-computational study was conducted to understand damage phenomenon that causes failure in SiC-reinforced aluminum alloys [28,29,31]. Through a blend of mechanical testing, microstructural characterization and micro-mechanical analysis, quantitative aspects of microstructural morphology that are critical to damage nucleation was investigated. Interrupted testing prior to complete failure of a tensile specimen was conducted to gage the influence of microstructure on the dominant damage path. Various characterization functions were generated and sensitivity analysis was conducted to explore the influence

of morphology on damage. VCFEM was used to model damage initiation by particle cracking and propagation of damage through multiple particle fragmentation into a dominant crack. VCFEM simulations compared excellently with experimental observations as shown in figure 5c and 5d.

The recent extension of VCFEM is in the coupling of damage modes by particle cracking and ductile rupture of the matrix. A void initiation growth-based continuum plasticity model (Gurson-Tvergaard model for porous plasticity) is used to manifest ductile fracture in the matrix. The VCFEM model adaptively evolves in this augmentation to selectively provide high resolution in regions of plastic strain localization and high void concentration. Figure 5e shows the contour plots showing localized plastic strain and ductile fracture in a simulation with particle and matrix cracking.

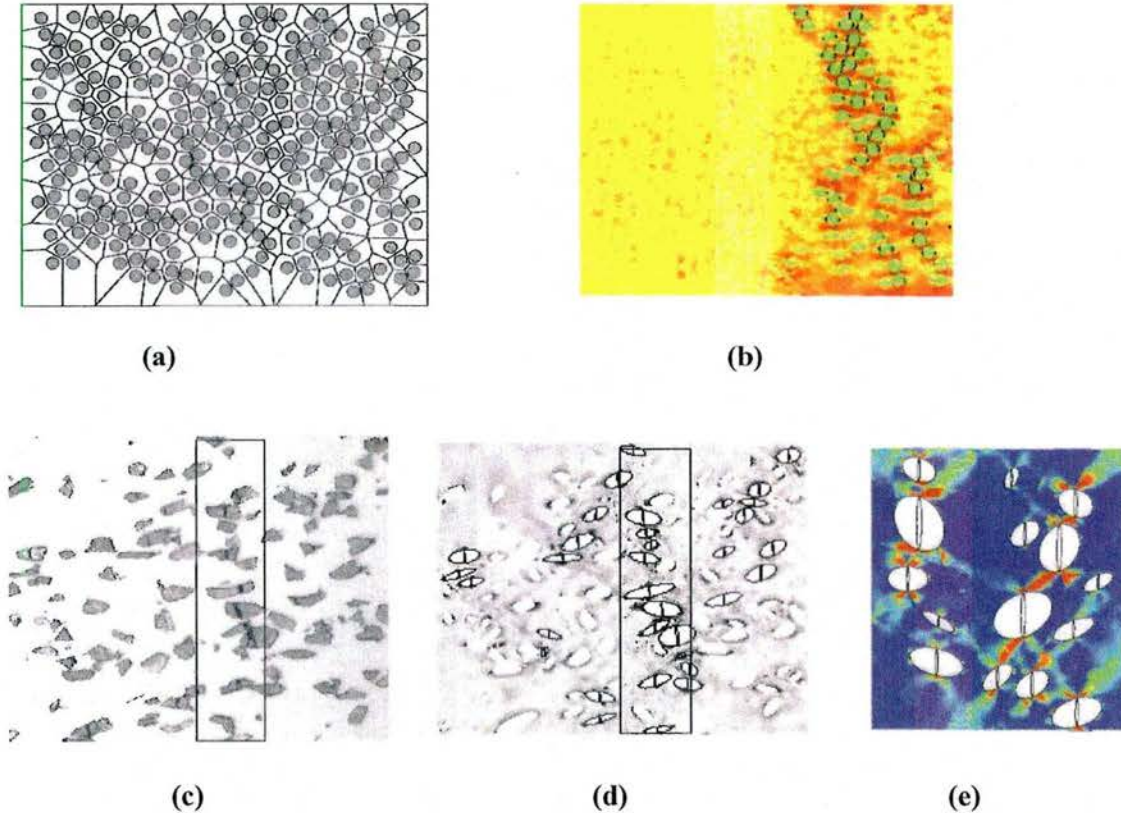


Figure 5: (a) A tessellated mesh of Voronoi cell elements for a nonuniform fiber reinforced polymer matrix composite microstructure, (b) A localized damage path induced by interfacial debonding, (c) Experimental micrograph of an Al-SiC showing cracked particles, (d) VCFEM simulation of the equivalent micrograph showing damage and equivalent plastic strain, (e) Contour plot of plastic strain in a VCFEM microstructural simulation with particle and matrix cracking.

3.5 Multi-Scale Simulations with the Micromechanical Models

Composite structures inherently consist of multiple-scales, e.g. macro, meso and micro-scales. In this effort, an adaptive multi-level computational system has developed for *adaptively* creating a hierarchy of computational sub-domains that provides necessary resolution at different scales [32-37]. Macroscopic analysis is done by conventional finite element method, while the Voronoi cell finite element model is used for meso- and microscopic analyses. *Error indicators* are formulated to regulate element refinement and inter-scale transition from macroscopic regions to microscopic "hotspots" of stress or strain localization. The ultimate goal is to have an automated computational model that will model failure as a multi-scale phenomenon of damage initiation and propagation. The adaptive multi-level model has been

conducted for multi-scale problems in elasticity problems without damage in [32,33] and in structures with evolving damage by interfacial debonding in the microstructure [38,39].

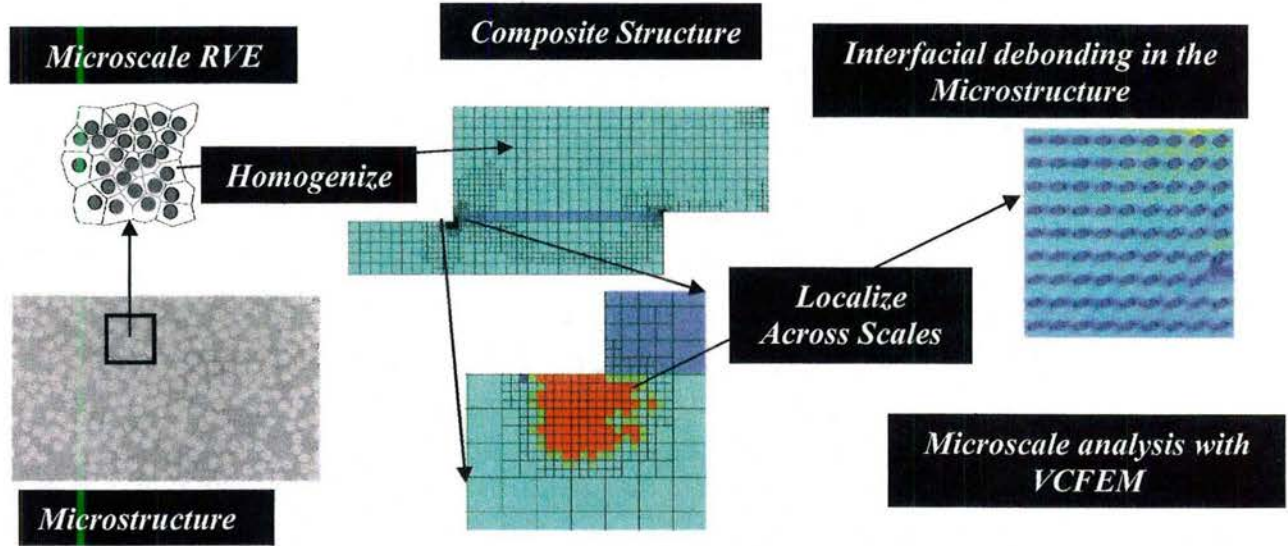


Figure 6: Multi-scale modeling of debonding based failure in a fiber-reinforced bonded joint with a two-way coupled multi-level computational model

3.6 Modeling Creep and Cyclic Deformation in Polycrystalline Ti Alloys and HSLA Steels

The PI has been recently involved in two parallel experimental-computational studies on analysis of creep deformation in polycrystalline Ti-6242 alloys [1] and cyclic deformation in HSLA steels [40,41]. In these studies, a time-dependent crystal plasticity model is incorporated in ABAQUS UMAT [3], to account for large strains, material anisotropy and time-dependent nature of plasticity, integral to creep. The finite element models incorporate crystallographic orientation distributions directly from OIM data. Statistically equivalent orientation distribution is assigned to the finite element model through a special orientation assignment method from OIM images. In this method, sets of Euler angles are generated according to area fraction of orientation distribution function (ODF) values in the OIM, and used to generate the orientation distributions in the computational model as shown in figure 7. A genetic algorithm (GA) based multi-variable optimization method is performed to calibrate crystal plasticity parameters for various slip systems, from a limited set of experimental results.

The study on polycrystals of α -Ti-6Al and α - β Ti-6242 alloys [1] is aimed at gaining an understanding of the role of material microstructure on dwell behavior, through a combination of modeling and experiments. The inelastic deformation by slip in hexagonal closed packed (*hcp*) Ti-alloys is highly anisotropic due to difference in deformation resistances in different slip systems. An important outcome of the study is the understanding of load shedding and local stress rising phenomenon in polycrystalline aggregate of Ti alloys. Creep and dwell cyclic loading can lead to local crack initiation at critical locations within the microstructure with large orientation mismatch. It is observed that the stress concentration is significantly affected by the material rate sensitivity and the peaks increase considerably with time. Considerable local yielding leading to plastic strain is realized in the microstructure, even at macroscopic stress levels lower than the yield stress. Significant local stress concentrations evolve with time in the material microstructure due to compatibility constraint at the interface.

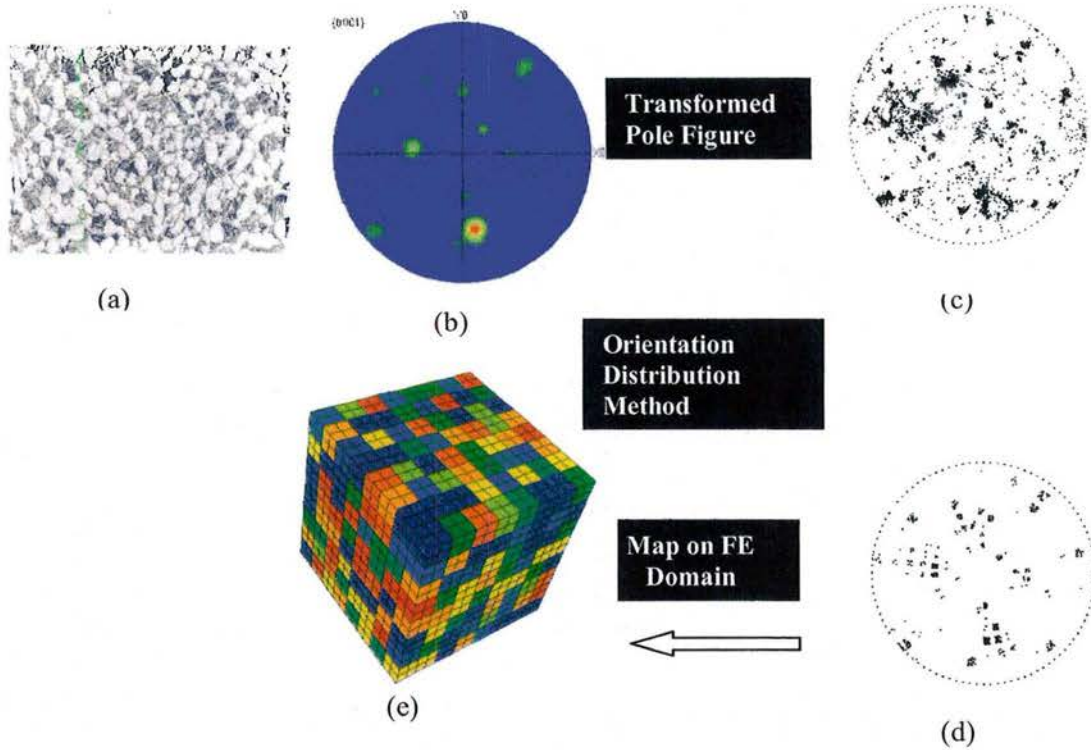


Figure 7: (a) Micrograph of a forged α/β Ti-6242 alloy, (b) contour plot of the experimental (0001) pole figure, (c) transformed experimental pole figure from contour plot to points in the discretized regions of the projected plane, (d) statistically equivalent orientations obtained from the orientation assignment method (e) orientation distribution for the FEM simulations of polycrystalline Ti-6AL.

For the understanding the behavior of *HSLA steels*, a study combining experiments with finite element based simulations is conducted to develop a crystal plasticity model for prediction of the cyclic deformation behavior [40,41]. The experiments involve orientation imaging microscopy (OIM) for microstructural characterization and mechanical testing under uniaxial and stress/strain controlled cyclic loading. The crystal plasticity model for bcc materials uses a thermally activated energy theory for plastic flow, self and latent hardening, kinematic hardening, as well as yield point phenomena. Material parameters are calibrated from experiments using a genetic algorithm based minimization process. The computational model is validated with experiments on stress and strain controlled cyclic loading. The effect of grain orientation distributions and overall loading conditions on the evolution of microstructural parameters is studied. The cyclic stress-strain plots under strain and stress controlled loading are shown in Figure 8.

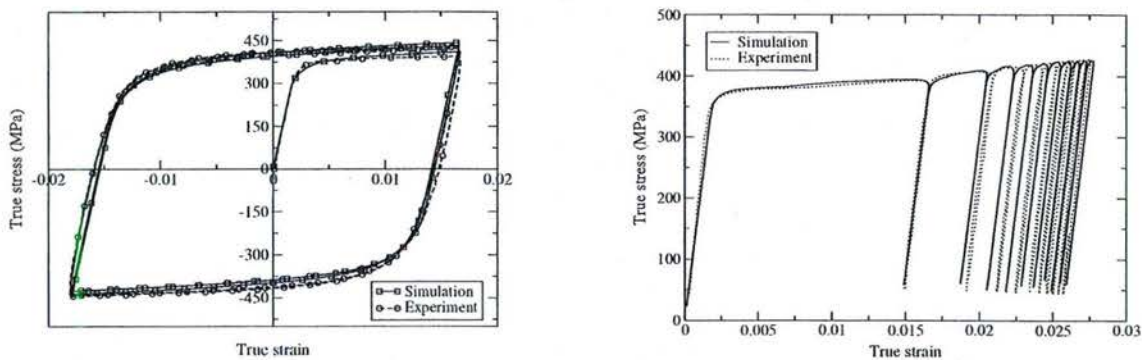


Figure 8: Comparison of experimental and simulated stress-strain plots for (a) strain controlled tests and (b) stress-controlled test.

4. RELATION TO CURRENT STATE OF KNOWLEDGE

Within the framework of modeling plastic deformation, two approaches viz. the continuum and the crystal plasticity approaches, have emerged. Motivated by experimental observations, the continuum approach introduces phenomenological models with scalar or tensor internal variables whose growth is determined by appropriate evolution laws. Various continuum models proposed, include the anisotropic quadratic yield function of Hill [42], yield surface vertex models with deviation from normality [43,44], anisotropic yield criteria with isotropic plasticity equivalent concept [45], and isotropic elastic-viscoplastic models [46,47]. Though popular for their relative simplicity, they do not properly represent underlying physical complexities due to the lack of appropriate length scales. Higher order gradients have also been introduced in expressions for flow stress and yield surfaces to incorporate length scale effects in these continuum theories [46,47]. However they still lack accurate representation of those phenomena, which are strongly affected by evolution and interactions on the microscale.

In the crystallographic approach, the mechanical response of polycrystalline aggregates are deduced from the behavior of constituent crystal grains with specific assumptions about their interaction. For example, the Taylor model [49] assumes that each grain is subject to the same uniform deformation as the entire aggregate. In this model, compatibility is satisfied and equilibrium holds in each grain, but equilibrium is usually violated between grains. Using the principle of maximum work, Bishop and Hill [49] calculated the yield stress based on Taylor's assumption. The Taylor-Bishop-Hill theories have been extensively used to predict textures and stress-strain response in fcc and bcc polycrystalline metals. Though the Taylor model and its derivatives are reasonably effective in predicting gross features of deformation, a number of studies (e.g. [50,51]) have predicted sharper textures than experiments. This is attributed to nonuniform deformations due to grain interactions in real polycrystals [52]. Relaxed constraints methods [53] have been proposed to incorporate intergranular interactions, with relaxation of the requirements of Taylor model. Experiments on large grain sheet materials by Skalli et.al. [54] have shown that full constraint and relaxed constraint models each work well only for some grain orientations. Other important contributions in this area include the work of Iwakuma and Nemat-Nasser [55], who have used Hill's self consistent averaging methods to develop finite rotation-small strain constitutive relations for rate independent and rate dependent crystals. Most of these models have however overlooked the relation between plastic instabilities and the details of microstructural description and intergranular interactions.

Various computational studies have modeled anisotropy and its evolution in large deformation processes with the crystallographic approach (e.g. Havner [56], Mathur et. al. [57], Kalidindi et. al. [58]). A majority of these models are based on variants of the Taylor assumption, thereby trivializing grain interactions and morphological effects like grain shape, size and arrangements. While some models have utilized continuous orientation distribution functions (ODFs) [59], a majority of them do not account for microstructural interactions and morphology, in predicting the onset and growth of plastic localization. The role of grain shape and grain boundaries on localization has been studied by Lemonds et. al. [60] for bicrystals of identical geometry, but of different crystallographic orientations and hardening. They concluded that grain boundaries cause nonuniform deformation and that the formation of shear bands is strongly affected by initial misorientation across the boundary and the difference in latent hardening. Nonuniform deformation behavior of polycrystals with inter-granular interaction has been investigated by Harren and Asaro [50] using finite element models with very large number of elements (element size $\sim 1/100$ grain size). The importance of grain boundaries and triple point junctions in slip activity and deformation nonuniformities is brought out in their research. Similar simulations have also been conducted by Kalidindi et. al. [51] and Beaudoin et. al. [61]. Panchanadeeswaran and Doherty [62] have emphasized the need for incorporation of *actual metallurgical structures*, such as grain size, shape and orientation in models, due to otherwise poor qualitative agreement between texture predictions and experimental measurements. This has also been emphasized by Becker and Richmond [63] in their finite element simulations of TEM micrographs for predicting flow localization and failure in aluminum alloys.

Since polycrystalline deformation is predominantly three-dimensional in nature, it is essential that the microstructural models be developed with detailed 3D information. This requirement poses major challenges to currently available metallography practices. Techniques based on ultrasonics or its variants, such as acoustic microscopy or laser ultrasonics [64,65] rely on good reflection properties and have limited application in metals. While X-ray based computed tomography [66,67] methods are widely used in 3D solid model generation, they are generally deficient in achieving the resolution desired for detailed study of polycrystalline metals. Recently, synchrotron based CT technology has been developed to yield tomographic images with considerably high resolution [68]. However, this method is still not commercially available and is generally quite expensive.

Many metals and their alloys exhibit strong grain size effects due to strong inhomogeneous deformation fields in the grain interior [69]. The conventional homogeneous constitutive models of [51,61] etc. fail to accurately predict the scale dependent behavior. The nonuniform deformation occurs at length scales, which for plastic deformation are associated with the dislocation structures. This causes the plastic flow to be size dependent with an increasing hardening for decreasing grain sizes (Hall Petch effect) [70]. The nonuniform plastic deformations give rise to the development of geometrically necessary dislocation (GND) which are required to preserve crystallographic lattice compatibility and cause short and long range effects on the constitutive behavior. The GND's act as obstacles to the motion of gliding dislocations which carry the plastic deformation, also known as statistically stored dislocations (SSD). Of the total dislocation density, the GND density is defined as the minimum density required to accommodate a given strain gradient and SSD density is the rest [71]. Various strain gradient models have been proposed for capturing size scale effects. Some of these approaches have introduced intrinsic material length scale in plasticity [72,73,74,75,76], while others have related the underlying physics to the generation and distribution of dislocations [77] or to plastic and elastic incompatibilities [78,79,80]. However some of the shortcomings of these models are due to 2D idealizations, considerations of global strain gradient instead of those at the grain level, and global incompatibilities through the curl of the deformation gradient tensor rather than slip system incompatibilities. Additionally, the influences of the GND's in these models are superposed on the hardening or slip resistance, thus ignoring their distinct contributions compared to SSD's. In a more physically based modeling effort, Evers [81] has developed a model where the GND densities are directly related to the gradients of crystallographic slip. In this model, the slip resistance is caused by the short range interaction of all SSDs and GNDs. Furthermore, any heterogeneity in the GND density field also causes a long range influence on crystallographic slip through back stress contribution, since at a length scale that is several orders of magnitude larger than each individual dislocation size, the net effect of the GND densities does not vanish. This physically motivated strain gradient plasticity model shows promise and will be experimented with in the proposed work.

The recent years have seen significant efforts in modeling cyclic plasticity and fatigue with considerations of microstructural stress-strain evolution. On the micro-scale, the state of stress in a polycrystalline aggregate during cyclic loading depends on grain orientation in relation to its neighbors as well as with respect to the loading direction and constitutive properties of the material. Finite element calculations have shown that depending on the loading conditions, significant gradients of stress can arise within a single grain. The variation of stress over grains in a polycrystalline aggregate, at any given location in the continuum depends on the single crystal properties of the material as well as the local crystallographic texture. Dawson and coworkers [82] have investigated the mechanical behavior of aluminum alloy in cyclic loading using crystal plasticity based FEM simulations of crystalline aggregates. Up to 1000 cycles are simulated in their experiments. While initial orientations are assigned by sampling orientation distribution functions from measured crystallographic orientations, grain morphology is not explicitly accounted for. Neutron-diffraction is used to measure residual lattice strains. Their simulations show that under constant amplitude strain cycles, the macroscopic stress decays with increasing cycles with evolving lattice strains. Miller and Dawson [83] have considered a feature based 'digital material' with

statistical description of morphology, lattice orientation, intra-grain lattice misorientation, and material constitutive model in an attempt to deploy accelerated insertion of materials. McDowell and coworkers have incorporated a crystal plasticity model with kinematic hardening in ABAQUS to model cyclic plasticity in high cycle fatigue in Ti-6Al-4V [84]. Random distributions of grains with hcp secondary α and bcc β in a lamellar structure are modeled and the microstructure is subjected to cyclic loading. Simulations of simple components have also been done to consider fretting fatigue.

A number of fatigue models considering the effects of microstructural variations have been considered in the recent years. Chan [85] has formulated fatigue crack growth laws in the power law regime in terms of material properties like yield stress and fatigue ductility and microstructural parameters like dislocation cell size and dislocation barrier spacing. He attributed the lack of strong microstructural influence on the fatigue crack growth due to increasing yield stress and fatigue ductility with decreasing dislocation barrier spacing. A probabilistic treatment of this model has been considered in [86], where randomness in yield stress, fatigue ductility and dislocation barrier spacing have been correlated to the variations in fatigue crack growth rate. The recent research of Chan [87] is extending the above models for describing dislocation structure evolution, fatigue crack initiation and growth and linking various scales. A fatigue crack initiation model is constructed in terms of microstructural parameters like grain size, slip band spacing, inclusion size crack size and notch size. Tryon and Dey [88] has proposed a similar methodology to aid in the design and prediction of reliability of metallic components based on probabilistic microstructural fatigue models. The variation of fatigue life is predicted as a function of the statistical variation of the microstructure of the material.

The proposed research has sufficient uniqueness and the potential to advance the state of the art in the modeling of fatigue failure in real polycrystalline microstructures. The fatigue crack initiation and growth models will directly evolve from finite element simulation of the microstructure. A novel contribution of this research will be in the development of robust computational and constitutive models for prediction of localization and subsequent crack evolution. Adaptivity of computational models to accommodate the material evolution is a necessary tool that has not been applied extensively to this class of problems.

5. OUTLINE OF THE OVERALL APPROACH

The system of computational models and codes to be developed in the proposed research will be an ensemble of tasks that are elaborated below. It is expected, that on completion, the project will be able to deliver a comprehensive set of computational tools that can predict the effect of material microstructure on cyclic deformation and fatigue crack evolution. It is important to note that components of the overall framework will be modular, in that they can be interchanged with more appropriate models as they evolve. This PI's ongoing collaborations with Professors Mills and Fraser at OSU and Drs. Dimiduk, Parthasarathy and Uchic at AFRL/MLLM will be critical in the development and validation of the computational models through results of mechanical testing and quantitative metallography. Letters from these collaborators are attached in the appendix. Major developmental tasks are summarized below.

5.1 Microstructural Computer Model from OIM Data and Characterization

Accurate mapping of polycrystalline microstructures from metallographic observations to the finite element model is essential for reliable prediction of deformation and damage evolution leading to failure. Mean values of characteristic features like phase volume fraction, grain size, shape and orientation distributions are not adequate in this respect, especially with respect to predictions of localization, crack

initiation and growth. A combination of these features set the grain-level kinematics of the material and controls the local driving forces for energy partitioning, defect formation, and ultimately, failure. Capturing details of variabilities of key 3D microstructural features is important to enhance the predictive capability of the computational model. This requirement poses major challenges to currently available metallography practices. In this research, the methods described in section 3.2 and [2] will be advanced to create equivalent 3-D microstructural images from metallographic analyses data as described next.

A. Sectioning-Based 3D Microstructure: The newly developed automated approach of characterizing 3D microstructure using a Dual Beam Focused Ion Beam (FIB)-SEM system will be advanced to create a seamless transition from 3-D orientation data to computer models of model grain and sub-grain structures. The microscope is capable of highly-localized micro-machining and ion imaging using the FIB column, and non-destructive high-resolution imaging and Electron Back-Scatter Diffraction (EBSD) using the SEM column. Serial sectioning of the specimen by the FIB is followed by the EBSD system to determine grain section orientations. The *Micro-Mesher* program has been developed to post-process the OIM data and generate grain boundary structures from differences in grain orientation data [2]. It approximates spatially complex boundaries with line segments with a user prescribed error-per-unit-length algorithm. This program will be refined and tested in this research for a variety of different microstructures. A sequence of the *FIB/EBSD/Micro-Mesher* generated sections (see figure 3b) will be stacked using 3D visualization software like Slicer-Dicer [89] to construct the 3D microstructures. The 2D polycrystalline sections and the 3D computer generated micro-regions will be processed for microstructural characterization. Important microstructural parameters like distributions of grain size and shape, orientation distribution functions (ODF) and other stereological characteristics will be compared for 2D and 3D microstructures.

B. Statistically Equivalent Computed Microstructure: In an alternate approach, an attempt will be made to generate statistically equivalent 3D microstructures from surface OIM data of a representative micro-region. The proposed method will design an algorithm to generate an optimal distribution of points for 3D tessellation of the micro-region, based on these points or seeds (figure 9). The convergence of the optimal point distribution algorithm will be established by comparing the distributions of microstructural parameters on the surface of the tessellated region with that from the surface OIM data. An iterative algorithm will be pursued, till the convergence criteria are satisfactorily met for important distribution functions. This method is expected to be combined with established stereological methods [90-94] which estimate the number density and size of 3D objects from density and size of 2D sections. The PI has compared predictions of some stereological methods with serial sectioning methods to examine their effectiveness in [23,24]. This experience will be put to use in the above method. The experimental method in task A will be used to validate the proposed method in task B.

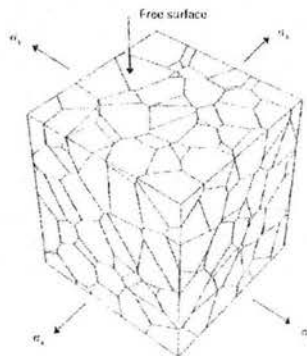


Figure 9: A point based 3D tessellation for generating a statistically equivalent micro-region

5.2 Constitutive Model Development and Validation

This task will focus on the incorporation, development and validation of crystal plasticity constitutive models for specific applications of polycrystalline aggregates, e.g. Nickel base superalloys like Ni₃Al (phases with fcc structure) and Ti alloys Ti-6 Al (hcp) and Ti 6242 (colonies with hcp with bcc phase structure). Both classes of materials may contain more than one phase and are similar in size scale. The Ni grains are essentially equiaxed with particles inside. The Ti grains may have colonies of similarly oriented laths of α (hcp) and β (bcc), with individual laths having different crystallographic orientations. The γ/γ' boundary in Ni is relatively low energy and can be coherent. In Ti the α/β interface has an orientation relation, but is not as low energy as the γ/γ' boundary. Important aspects of this work are discussed below.

A. Framework of the Constitutive Model: The primary aim of this task will be to examine the effectiveness of constitutive models through finite element modeling of single crystal and polycrystalline behavior using crystal plasticity models, implemented in the finite element code ABAQUS through the user interface UMAT. Similar implementation of experimentally validated models has been accomplished by the PI's group in [1,40,41]. Rate dependent crystal plasticity models [95,96,9,98,99,100] relate the plastic shear strain rate $\dot{\gamma}^\alpha$ of each slip systems of the crystal lattice to the effective shear stress τ_{eff}^α and the slip system deformation resistance s^α through a visco-plastic power law relation as,

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left(\frac{|\tau_{eff}^\alpha|}{s^\alpha} \right)^{1/m} \exp \left\{ -\frac{\Delta G^\alpha}{kT} \right\} \text{sign}(\tau^\alpha),$$

where m characterizes the material rate-sensitivity and $\tau_{eff}^\alpha = |\tau^\alpha - \tau_{kin}^\alpha| - s_a^\alpha$ is the resolved effective stress, which is the driving force for the dislocation motion on slip system α , τ_{kin}^α is the resolved back stress; τ^α is the Schmid stress, s_a^α is the part of the critical slip resistance due to the athermal obstacles to slip. ΔG is the activation free energy required to overcome the obstacles to slip without the aid of an applied shear stress; k is the Boltzmann's constant and T is the temperature. The slip system resistance is assumed to evolve as: $\dot{s}^\alpha = \sum_\beta h^{\alpha\beta} |\dot{\gamma}^\beta|$, where $h^{\alpha\beta}$ describes the rate of strain hardening on slip system α due to shearing on the slip system β . Kinematic hardening is essential for modeling cyclic deformation, for which, an evolution law for the slip system back stress has been proposed by Armstrong and Frederick [101] as: $\dot{\tau}_{kin}^\alpha = (\mathbf{w}_n \cdot \mathbf{n}^\alpha) \mathbf{m}^\alpha$, where $\mathbf{w}_n = \sum_\alpha \Omega^\alpha (\mathbf{m}^\alpha \otimes \mathbf{n}^\alpha + \mathbf{n}^\alpha \otimes \mathbf{m}^\alpha)$. The evolution of kinematic hardening completely characterizes reversible non-proportional cyclic stress-strain behavior.

B. Microstructural Finite Element Models of Single and Polycrystals, Colonies etc.: In this task, crystal plasticity parameters will be calibrated from experiments performed by Mills, Dimiduk (see letters) by inverse methods. Explicit models of microstructural regions with constituent phases will be modeled and loaded for specific slip activation in accordance with the experimental studies. For example, in a Ti-6242 colony specimen, lath regions of α (hcp) and β (bcc) phases with the Burger's orientation relation will be modeled in FEM to calibrate slip system parameters for the individual phases (see figure 10). It is computationally exhaustive to use these explicit two-phase models to represent grains/colonies polycrystalline aggregate modeling. Consequently homogenized effective models with reduced degrees of freedom will be developed. In these models, the effect of the explicit phases can be represented by

corresponding slip systems and other averaged parameters like volume fraction. The effective models will be tested for polycrystalline aggregates, constructed from equivalent orientation distributions of those measured via electron-backscattered diffraction (EBSD) techniques. Results of the polycrystalline model will then be compared with experimentally measured constant strain rate and creep tests for different orientations

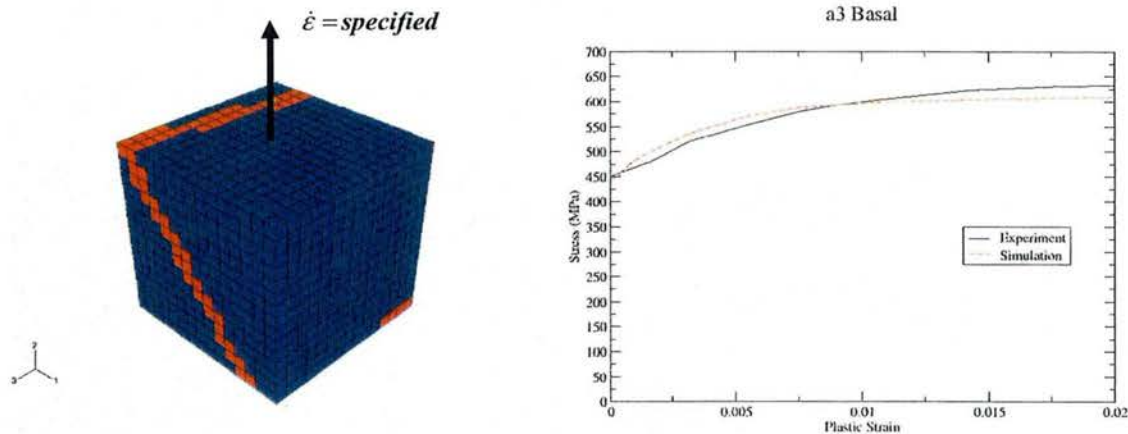


Figure 10: (a) A computational model of transformed β colony showing α and β phases corresponding to a_3 basal loading, (b) a comparison of experiments and simulated results.

C. Tension-Compression Asymmetry: Work by Mills has demonstrated that creep rates in polycrystalline Ti-6242 are significantly larger in tension than in compression. A question to be answered in this research is whether the asymmetry is due to the presence of β in the two phase alloys, or whether the asymmetry is a feature of the α phase of Ti alloys (perhaps due to a non-planar dislocation core configuration). To this end, Mills will be conducting tension and compression testing of single crystals of Ti-6Al. This information will then be used by to develop a more complete description of the deformation of the α phase which may include this asymmetry.

D. Grain Size Effects in Crystal Plasticity Models : Many metals and their alloys e.g. Ti 6242, exhibit strong grain size effects due to strong inhomogeneous deformation fields in the grain interior [69]. There have been few direct measurements of grain size effects in Ti alloys, and no published studies of the effect of grain size on creep response. Mills at OSU is pursuing such studies on single phase Ti-6Al, which has the advantage of offering a relatively “clean” measurement of grain size effects, unlike studies of two-phase α - β alloys where the shape and dimension of the individual phases can obscure the grain size effects. These results will be used to calibrate the crystal plasticity model, thereby including scale effects directly. Due to the planar nature of slip in these short-range-ordered alloys, extended pile-ups, local stress concentrations and grain-to-grain “communication” of slip is observed experimentally using SEM and TEM.

Consistent with the discussion in section 4, this work will explore size dependent models in which strain gradient related production of GND's enable the prediction of size dependent behavior for intragranular and global strain gradients [81]. In this model the evolution of SSD's during crystallographic slip increases the number of short range interactions, which leads to isotropic hardening. The SSD density is affected by generation and annihilation of SSD's on each slip system and is expressed in the form:

$\dot{\rho}_{SSD}^\alpha = \frac{1}{b} \left(\frac{1}{d_e^{\alpha\zeta} L^\zeta} - 2y_c \rho_{SSD}^\alpha \right) d_e^{\alpha\zeta} |\dot{\gamma}^\zeta|$ due to a balance of accumulation and annihilation of dislocation

density rate. The geometrically necessary edge and screw dislocations can be obtained from relations to the gradients of plastic slip corresponding to the undeformed configuration as [76,102]:

$$\rho_{GND}^\alpha = \rho_{GND_0}^\alpha - \underbrace{\frac{1}{b} \sum_{\zeta} d_e^{\alpha\zeta} (\nabla_0 \gamma^\zeta \cdot \mathbf{m}_0^\zeta)}_{\text{edge}} + \underbrace{\frac{1}{b} \sum_{\zeta} d_s^{\alpha\zeta} (\nabla_0 \gamma^\zeta \cdot \mathbf{p}_0^\zeta)}_{\text{screw}}. \text{ Any gradient normal to the glide plane do}$$

not affect the lattice. A nonuniform GND distribution results in additional residual stresses and consequently a back stress term is entered in the crystal plasticity formulation. This counteracts the local resolved shear stress and obstructs crystallographic slip through long range kinematic hardening. Such models will be incorporated and will be tested with experimental results. Parameters in the size dependent hardening model will be calibrated from experiments on polycrystals of varying sizes.

5.3 Fatigue Crack Evolution with Cohesive Zone Models

Fatigue crack evolution in the microstructure takes place in multiple stages. In the first phase, plastic flow concentration due to crystallographic slip and interaction between grains lead to intense micro-shear band formation in the grains. The second is the crack nucleation phase, in which damage accumulates to form a crack, while the third stage is the small crack growth phase, where the crack size is on the order of the microstructure. The final stage is a long crack growth phase, where the crack size is large compared to the microstructure. Each stage is driven by different mechanisms and will be distinctly modeled.

The fatigue mechanisms will be explicitly modeled in this task for polycrystalline microstructures to examine the effects of local morphology. Fatigue crack growth is the result of the competition of material separation processes near the crack tip and the deformation processes in the surrounding material. An irreversible cohesive zone traction-separation law, which represents the physical processes of material deterioration, will be used to model crack initiations and growth in the material microstructure. A variety of cohesive zone models have been proposed in literature [103,104,105]. In this work, an irreversible CZM of the form developed in by [106] will be used to model fatigue crack growth.

$$T_n = \sigma_{\max,0} e \exp\left(-\frac{\Delta u_n}{\delta_0}\right) \left\{ \frac{\Delta u_n}{\delta_0} \exp\left(-\frac{\Delta u_t^2}{\delta_0^2}\right) + (1.0 - q) \frac{\Delta u_n}{\delta_0} \left[1.0 - \exp\left(-\frac{\Delta u_t^2}{\delta_0^2}\right) \right] \right\}$$

$$T_t = 2\sigma_{\max,0} e q \frac{\Delta u_t}{\delta_0} \exp\left(1 + \frac{\Delta u_n}{\delta_0}\right) \exp\left(-\frac{\Delta u_n}{\delta_0}\right) \exp\left(-\frac{\Delta u_t^2}{\delta_0^2}\right)$$

This model incorporates loading and unloading conditions, as well as effects of accumulation of damage during cyclic loading on cohesive zone model parameters. The traction-separation behavior is irreversible and history dependent, due to the fact that tractions depend on the current state of damage, and hence on the loading history. Parameters in the cohesive zone models will be calibrated using inverse methods using observations from fatigue experiments, consisting of mechanical testing and OIM scans of selected regions. The model applies to material systems where crack bridging dominates the crack growth behavior, and no energy dissipation takes place outside of this zone. The cohesive zone model will be tested extensively for effectiveness with intra-, inter- or grain boundary failure. Figure 11 shows the results of a preliminary polycrystalline model with the cohesive zone interface.

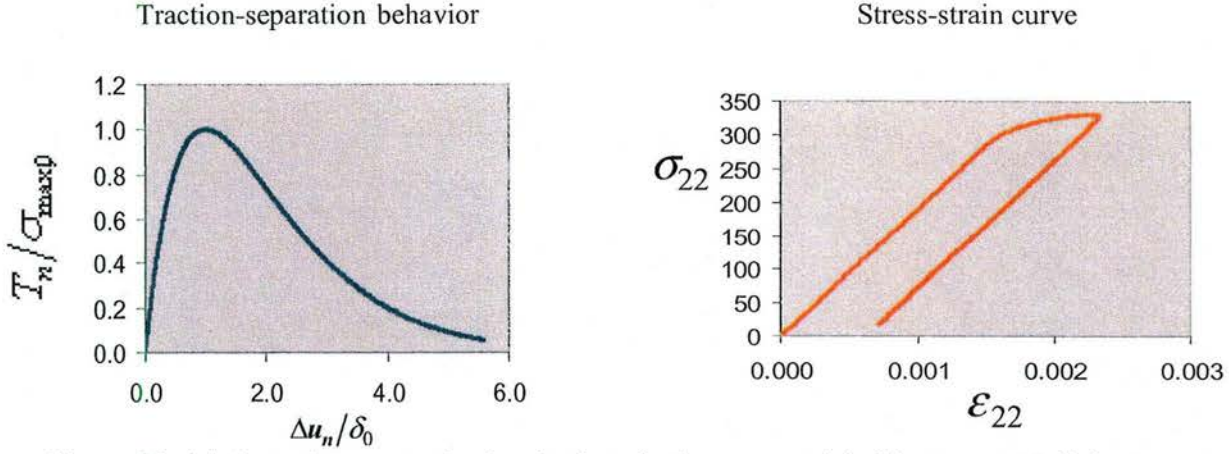


Figure 11: (a) A traction-separation law in the cohesive zone model, (b) stress-strain behavior in a single loading-unloading cycle.

5.4 A Novel Grain-Based Finite Element Model (GBFEM) for Finite Deformation

General purpose finite element codes like ABAQUS are severely limited in modeling large microstructural regions of polycrystalline aggregates due to prohibitively high computing requirements. The computing demands are even intensified when numerous time steps are required for modeling cyclic deformation. It is inevitable that specialized models of computational mechanics endowed with adaptive capabilities can bring considerable payoffs in this regard. In the proposed task, a special grain based adaptive finite element model (GBFEM) will be developed for accurate and efficient analyses and overcome limitations of conventional FE models in fatigue life prediction. The model will incorporate the real material morphology from task 5.1. Rate dependent crystal plasticity constitutive models and microstructural cohesive zone damage, as discussed in tasks 5.2 and 5.3, will be included in this large deformation GBFEM. This development will follow the highly successful *Voronoi Cell FEM (VCFEM)* [25-31] that has been proven to offer a tremendous advantage in accurate and efficient, *image-based* multi-scale modeling of nonuniform composite and porous materials. Early formulation and modeling of GBFEM have shown significant promise in modeling polycrystalline materials (see figure 12).

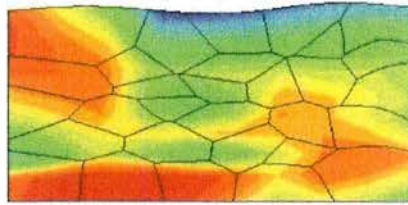


Figure 12: A preliminary attempt with GBFEM.

The GBFEM formulation will be based on the enhanced strain formulations that have been successful in modeling non-homogeneous and localized strain fields. Each element in GBFEM will manifest a single grain or crystal. Plastic flow concentration due to crystallographic slip and interaction between grains is a source of micro-shear band formation. GBFEM elements will be selectively enriched adaptively to differentiate between regions of high and low deformation gradients and impart preferential resolutions to sub-domains. *Adaptive methodologies* will be instrumental in identifying regions of evolving localized deformation and preferential resolutions will be imparted by local enrichment of sub-grain domains. In addition, intra-, inter- and grain boundary failure will be modeled by using the cohesive zone models in GBFEM as well. Incremental adaptivity will be necessary for modeling the evolution of fracture and bridging nascent surfaces.

A necessary ingredient for the success of this computationally intensive research is the incorporation of advanced high performance computing techniques. Effective use of high performance computing will be explored to reduce the overall execution time. Novel computational frameworks and programming environments will be developed to support efficient multi-scale simulations on different high performance computing platforms. Parallel programs will conform to the latest message-passing interface (MPI and OpenMP) standard for portability. Implementation focus will be on aspects of (a) *Parallel scalability*, (b) *Mapping and scheduling*, (c) *Run-time environment*: (d) *Parallel I/O*:

5.5 Multi-Time Scaling Algorithm for Modeling Long Range Cyclic Loading

Modeling cyclic deformation using conventional time increments can be an exorbitant task for crystal plasticity computations. Most simulations performed with 3D crystal plasticity are in the range of 100 cycles [82,83,84] and the results are subsequently extrapolated for fatigue predictions. In modeling fatigue, it is however desirable to conduct simulations for a significantly high number of cycles to reach local states of damage initiation and growth. Conventional methods of time integration using semi-discretization present numerous challenges due to the variation in time scales ranging from the scale of the entire process to the time resolution required by the damage evolution and crack propagation

For this purpose, a multiple time scaling methodology will be developed in this task, for compression and rarefaction of time scales. This will enable large time scale homogenization in relatively benign periods of deformation, to very fine time scale simulations in temporal regions of evolving localization or damage. The multi-time scaling will be based on homogenization with the asymptotic expansion method in the time domain for polycrystals. This basic idea of multi-time scaling has been developed in Asai and Ghosh [4], where a fast time scale τ , and a slow time scale t are related by the relation $t = \varepsilon \tau$, where ε is a small number. Variables in the crystal plasticity laws can be written using the double temporal scale asymptotic expansion is of the form $u^\varepsilon = u^0(x, t, \tau) + \varepsilon u^1(x, t, \tau) + o(\varepsilon^2)$. The various order terms can then be uncoupled and averaged to transcend time scales. Figure 13 shows a comparison of a cyclic deformation problem solved by (a) a detailed single time scale time integration scheme called reference solution, (b) a homogenized solution using a compressed slow scale and (c) a region of de-compression at a critical region to revert to the detailed time resolution. The comparison with the reference solution shows excellent accuracy while the efficiency gained through time compression can be enormous. This promising technique will be developed to complete fruition in this task.

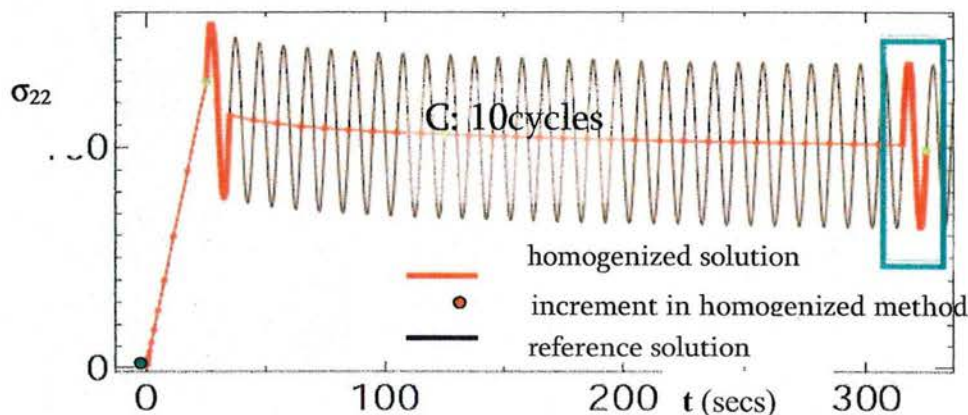


Figure 13: Stress-time plot in a cyclic deformation simulation showing different methods of time integration.

In summary, the tasks proposed for this complex set of problems are highly challenging. The PI believes that his prior and current accomplishments in related fields, and the collaboration with experts in complimentary fields will give him a strong impetus to satisfactorily execute this ambitious project.

6. IMPACT ON AIR FORCE SYSTEMS

Assessment and enhancement of life of structural materials in aerospace structural components, especially in aircraft engines is currently a priority at the US Air Force and other agencies. A number of multi-year major funding opportunities like the DARPA AIM and Prognosis initiatives have been announced in the recent years to address this very important but challenging problem. The scope of the proposed research project fits well into the grand scheme of objectives. Computational mechanics has traditionally played and will continue to play an important role in the development of novel materials and systems. The proposed project aims to advance the state of the art in computational mechanics for the specific objective of better prediction of material/structural life and reliability. It is expected that the approaches for reliable analysis and design will be established and technology will be transferred to the engine design community. The model and technology will benefit various applications of metallic materials with high structural integrity for aerospace systems.

7. DESCRIPTION OF ORGANIZATION

Information on the Department of Mechanical Engineering at the Ohio State University is available on the web [103]. OSU has had extensive contracting experience with the government.

8. OTHER AGENCIES RECEIVING THIS PROPOSAL

No other funding agency will receive this proposal

9. IMPACT ON ENVIRONMENT

The proposed effort will have no impact on water, atmosphere, natural resources and human resources.

10. PROPOSED PROJECT SCHEDULE

TASK	YEAR 1	YEAR 2	YEAR 3
5.1 A			
5.1 B			
5.2 A			
5.2 B			
5.2 C			
5.2 D			
5.3			
5.4			
5.5			

11 JUSTIFICATION OF BUDGET

- **S. Ghosh**

Support for 1 summer month is being requested. The PI will coordinate the entire collaborative effort and be involved in the development of computational models, in the planning and execution of experiments, and be the link between all participants in this research. He will be responsible for all deliverables resulting from this research, including papers, and project reports.

- **Graduate Students**

Support for 2 Ph.D. students has been requested. One student will be responsible for major developments of the computational models and algorithms and material characterization. The other student will be mainly responsible for the validation with experimental results and probabilistic modeling. The students will also help with the experiments at AFRL and OSU-MSE.

- **Travel**

Monthly meetings with the collaborators at AFRL are planned. In addition, students will also travel to AFRL to conduct experiments, and stay there for extended periods as required. Two national meeting will be attended every year to present the developments.

- **Services at No Cost to AFOSR**

Dr. Dennis Dimiduk and his research group will participate in this research at no additional cost to AFOSR. Specifically a student will be supported under the STW-21 initiative to provide experimental assistance to the program under their supervision. In addition, Professor M.J. Mills, who is supported by AFOSR will work with the PI for experimental validation and constitutive modeling.

12 DESCRIPTION OF AVAILABLE FACILITIES

Computer code developments will be performed on workstations in the PI's Computational Research Laboratory at the Ohio State University. A high-end computer workstation is being requested with this proposal for code development and debugging. Large-scale simulations will also be done on the SGI Origin, CRAY SV1 and Beowulf cluster at the Ohio supercomputer center.

Experimental component of the proposed research will be conducted in the Materials Testing Air Force Research Laboratory Materials and Manufacturing Directorate. Facilities at AFRL will be available for the program.

12 LETTERS OF INTENT

The letters of intent from collaborators are included near the end of this proposal.

1. **Dr. D. Dimiduk**, Materials and Manufacturing Directorate, AF Research Laboratory
2. **Professor M. J. Mills**, Materials Science & Engineering, The Ohio State University
3. **Professor Hamish Fraser**, Materials Science & Engineering, The Ohio State University

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