USING DIGITAL TWINS TO ACCELERATE QUALIFICATION OF FATIGUE CRITICAL COMPONENTS

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Abstract: Fatigue of engineering alloys is a major challenge in aerospace applications. Developing and qualifying fatigue critical components for use in aerospace requires manufacturing and testing of a significant number of test coupons. This process is highly time-consuming and expensive. QuesTek's ICMD® modeling software can provide reliable property predictions that can significantly lower the amount of testing required while still yielding a robust material property dataset. Utilizing integrated computational materials engineering methodologies, QuesTek has been developing microstructure sensitive fatigue models that can account for both intrinsic (e.g., grain size, grain morphology, phase fractions, crystallographic texture, etc.) and extrinsic (e.g., inclusions, surface roughness, porosity, etc.) features that drive fatigue life in engineering alloys. QuesTek uses a fatigue modeling framework combining crystal plasticity finite element method to predict fatigue indicator parameters at the mesoscale, with microstructurally small crack propagation and physically long crack propagation algorithms, to predict the full fatigue life from incubation to ultimate fatigue failure in both high and low cycle fatigue. This approach depends on both microstructure characterization used to generate the inputs for a microstructure digital twin, as well as a select few experiments to calibrate the physics-based models. By simulating the majority of loading scenarios of interest, testing can be targeted to just the most informative experiments during qualification. This approach offers three key benefits when compared with traditional design of experiment approaches; (1) decreased cost of qualification, (2) decreased time for qualification, and (3) improved mechanistic understanding of the key driving features for fatigue failure in a given alloy system, enabling optimization and improvements. QuesTek has recently made major strides in improving this modeling approach by decreasing the computational cost of simulations, making the approach feasible on QuesTek's cloud-based software, and by incorporating key microstructure features of interest for additively manufactured alloy such as anisotropic grain morphology/texture, porosity, and surface roughness. While this toolkit can be applied to traditionally manufactured alloys, it is particularly impactful for additively manufactured alloys due to their complex microstructures which result in difficult and expensive qualification processes when microstructure sensitive models are not utilized.

Keywords: Fatigue, Qualification, ICME, Additive Manufacturing, Digital Twin

INTRODUCTION

Qualification and certification are two important steps in the development and deployment of a new material and/or component in the aerospace industry [1]. These processes can be expensive and time consuming, but they are critical to ensure the safety and reliability of metals and components used in aerospace applications.

Qualification refers to the process of demonstrating that a material or component meets specific requirements and standards for a particular application. This involves performing various tests and evaluations to assess the material or component's performance under different conditions, such as temperature, pressure, and stress. The goal of qualification is to ensure that the material or component will perform reliably and safely in the intended application.

Certification, on the other hand, refers to the process of verifying that a material or component meets specific regulatory requirements and standards for use in aerospace applications. Certification is typically performed by regulatory agencies such as the Federal Aviation Administration (FAA) in the United States, the European Aviation Safety Agency (EASA) in Europe. Certification involves reviewing test data and documentation, performing inspections and audits, and ensuring compliance with regulatory requirements.

In the aerospace industry, both qualification and certification are critical to ensuring the safety and reliability of materials and components used in aircrafts. Qualification is typically performed by manufacturers and suppliers of materials and components, while certification is typically performed by regulatory agencies. The ultimate goal is to ensure that all materials and components used in aerospace applications are safe, reliable, and meet the necessary requirements and standards.

In the context of additive manufacturing (AM) of metallic aerospace components, the qualification and certification process is a major bottleneck that represents a large obstacle to adoption of this innovative manufacturing process. For traditional manufacturing routes, the qualification process can be scaled up and an economy of scale with large scale production reduces the burden of qualification cost per unit. However, many of the advantages enabled by AM (e.g., design flexibility, customization, supply chain independence, etc.) work in opposition to an economy scale. AM instead enables an economy of scope, achieving cost savings by having more versatile manufacturing capabilities with one machine being able to rapidly develop parts for several different products. The advantages of AM have been well documented, with applications in aerospace, space, automotive, energy, and biomedical. However, there is a need to reduce the cost and time required for qualification and certification of AM parts, especially for fatigue-critical applications [2].

Qualification is particularly challenging for fatigue-critical alloys because of the cost, time, and uncertainty associated with generating a reliable dataset for fatigue [3]. The challenges with fatigue are threefold. First, individual fatigue tests are costly and time consuming when compared with simpler testing required for static properties like tensile strength. Second, fatigue is an extreme value statistical (EVS) phenomenon, meaning that for minimum fatigue life, we are not concerned with the mean behavior of the bulk material, but rather the tails of the statistical distribution of local behavior, where fatigue cracks initiate and propagate – requiring extensive testing to achieve statistically rigorous characterization of minimum fatigue life. Lastly, Fatigue is not as well understood as many other mechanical properties, owing to the EVS nature of the problem, we don’t always know exactly what aspects of the microstructure are most important to the fatigue life and modeling of this inherently multi-scale problem is complex and computational expensive.

Integrated computational materials engineering (ICME) is an approach to materials design and development that integrates computational modeling, experimental measurements, and materials characterization to accelerate the discovery, optimization, and qualification of new materials and processes [4]. ICME involves using models and simulations to predict materials properties based on the microstructure, and in turn predict microstructure based on chemistry and processing. By establishing the process-structure-property (PSP)

linkages as a systems design chart for a material system in a given application, and filling in the linkages with well validated physics-based models, ICME enables goal-oriented design and optimization of materials for their applications, as well as enabling more rapid prediction of how properties vary as a function of the ranges of possible chemistry and processing inputs, to both enable robust design [5], and reduce the quantity of testing required to arrive at a statistical significant property dataset for qualification [6].

The accelerated insertion of materials (AIM) methodology, established through the DARPA AIM program [7-9] takes advantage of predictive PSP modeling along with selective data from experiments to predict minimum properties for qualification. This provides a massive advantage in the qualification process by enabling acceleration and parallelization of steps of the process while de-risking the expensive testing required to achieve A- or B-basis qualification of properties. By pre-determining 99th percentile minimum properties with only ~15 experiments combined with the AIM methodology, any necessary optimization can be carried out before investing in additional expensive testing, and further, the overall time to deployment can be accelerated by carrying out multiple steps of the process in series once a producer is confident in the high likelihood of successful qualification.

Previously, AIM has been successfully demonstrated for use in accelerating qualification in applications where static properties (e.g., yield strength, modulus of elasticity, etc.) are the critical properties of interest. However, ICME modeling of fatigue properties has not previously been introduced into this framework due to the inherent computational challenges associated with modeling minimum fatigue life. Unlike static properties which largely depend on bulk microstructure properties and mean behavior, fatigue depends on local features at the mesoscale ranging from sub-grain scale, to the scale of ~1000 grains. Additionally, both intrinsic and extrinsic microstructure features have significant impacts on fatigue performance. In fact, for high cycle fatigue (HCF) life, it is the extrinsic features like porosity and inclusions which typically play the most critical role. For that reason, modeling fatigue reliably at the microstructure scale requires the superposition of the worst case of each feature to determine the true minimum fatigue life [10-13].

The concept of a digital twin for the microstructure has enabled the explicit modeling of all the relevant intrinsic and extrinsic features at the mesoscale for fatigue life prediction in both low cycle fatigue (LCF) and HCF [14]. This paper will discuss the development of modeling tools to predict the fatigue crack initiation driving forces as a function of statistical distributions of each structural attribute, combined with microstructurally small crack (MSC) growth and in turn physically long crack growth models, along with the numerical methods and strategies used to make this modeling framework computational feasible. QuesTek has developed a fatigue simulation toolkit on the ICMD® software platform that makes this entire modeling framework commercially available to users in a cloud-based software environment to help accelerate qualification and certification of fatigue critical alloys for aerospace applications.

BACKGROUND

In this section the prerequisite background for the relevant concepts and methodology is provided. First, the qualification process for metal alloys in aerospace applications is discussed with particular focus on AM components. Next, ICME and its use to accelerate the qualification and certification of new alloys is reviewed. Lastly, computational modeling of fatigue and the concept of a fatigue digital twin is established.

Qualification and Certification Process

The gold standard for qualification of metallic alloys for aerospace applications in the US is set by the Metallic Materials Properties Development and Standardization (MMPDS) which acts as a primary source of statistically-based design allowables for metallic materials and fasteners used many different commercial and military aerospace applications around the world [1].

MMPDS defines three basis levels (A-basis, B-basis, and S-basis) that key static properties are required to achieve depending on the application of a given material. A-basis represents a statistically calculated 99th percentile with a 95 percent confidence interval exceeds the minimum for a given property. B-basis represents a statistically calculated 90th percentile with a 95 percent confidence interval for a given property. An S-basis represents the minimum property value specified by the relevant specification of the governing industry, federal, or military standard for the material. Typically, in aerospace applications, A-basis values are used for single load-path applications while B-basis values are used for redundant load-paths. The three basis levels are widely used to define the minimum required datasets to qualify and certify static properties such as yield strength for new materials and processes. However, when it comes to minimum fatigue life properties, there are no defined A-, B-, or S-basis allowables provided by MMPDS.

MMPDS provides guidance for defining the mean fatigue life, stating that normally the fatigue curves should be based on at least six data points for each of three or more stress or strain ratios, and the data should cover at least two orders of magnitude in life. Further, in discussion of the minimum bound life for fatigue, MMPDS states that methods used to define lower bounds of life must be accepted by the appropriate regulatory agency and may be negotiated by type certificate applicants and the regulators. This means that there is a not a one size fits all solution to fatigue qualification, but rather, the OEM and the certifying body must work together on a case-by-case basis to determine an acceptable dataset to achieve the necessary design allowables for safe and reliable certification of fatigue critical aerospace components.

In the present work, a methodology of improving the understanding of fatigue data to reduce risk associated with the qualification and certification as well as accelerating the testing process is discussed. This approach enables the safe and economically feasible adoption of new manufacturing processes such as metal AM. By using ICME with a fusion of experimental data and well validated physics-based models, the qualification process can be accelerated without reducing the reliability of fatigue critical components.

ICME and its Uses for Accelerated Qualification and Certification

ICME is a systems approach of computational materials engineering that integrates processing, structure, properties, and performance relations for the conceptual design, optimization, and insertion of materials for engineering applications [4]. Over the past 25 years ICME has grown in use and acceptance and has become a widely successful approach to accelerating development and adoption of new materials [15]. In addition to its application for the rapid design of novel alloys, ICME has proven effective in optimization of chemistry and processing of existing alloys and for insertion of materials highly regulated industries.

The AIM methodology relies on a combination of ICME, statistical approaches, experimental characterization, and mechanical testing, to generate minimum design allowables for new material with a significant reduction in testing. This is achieved by using well validated ICME models to predict the statistical distribution of mechanical properties that would occur due to associated statistical distribution in the chemistry and processing parameters due arising from the inherent uncertainty in the processing of materials. By propagating the uncertainty of chemistry and processing parameters using the allowable specification bounds, statistics of microstructure attributes associated with the specification can be predicted, and in turn, the statistics of mechanical properties can be predicted. Combining the predictions with a small test dataset, the predictions can be calibrated and a cumulative distribution function for the properties of interest can be established [7].

In practice, the AIM methodology was shown to be able to achieve 99th percentile yield strength predictions with just 15 experimental data points. In the case of static properties in the aerospace industry, typically the MMPDS A- or B-basis testing allowables are still required to be met before a component can meet certification requirements to fly. However, despite the need to ultimately complete the full testing dataset, the AIM methodology provides two major advantages for accelerated qualification for static properties; (1) If there is a potential to fail the qualification process, the AIM methodology will identify this with a fraction

of the tests, significantly reducing the cost and time required and allowing the producer to pivot and optimize earlier in the process, and (2) if AIM predictions indicate that there is no significant risk of failing the qualification processes when the full A- or B-basis datasets are generated, the steps toward qualification can be parallelized as the risk of failure is drastically reduced. The latter of these two scenarios was used to develop Ferrium M54® from clean sheet concept to in service as a hook shank component on a T-45 jet for the US Navy in just seven years, signifying a major acceleration of the insertion of a new material for a military aerospace application [8].

While the AIM methodology has not previously been formally applied to microstructure-sensitive fatigue modeling for accelerated qualification, these models have been used to improve understanding and reliability of fatigue testing and accelerate development and insertion of materials. McDowell et al. [16] first established the concept of using multi-scale ICME for multi-stage fatigue modeling and demonstrated its application to the development of cast A356-T6. This framework was expanded to additional materials [17] and applied to the development of fatigue critical automotive components [18]. Harlow et al. demonstrated the synthesis of modeling with limited experimental fatigue life data to predict S-N curves for SUJ2 steel [7, 9]. Further, McDowell and Dunne [14] reviewed the use of microstructure-sensitive computational modeling of fatigue crack formation and its application to high-strength martensitic gear steel, α/β titanium alloys, and nickel-based superalloys. Moore et al. [19] applied similar methodology to model and successfully accelerate the development of NiTi-based shape memory alloys for ultra-high-cycle fatigue applications. Hennessey et al. [20] extending this work to 7000 series aluminum alloys. Later, Prithivirajan and Sangid [21] demonstrated a similar microstructure sensitive fatigue modeling framework in application on AM nickel-based superalloys and the modeling of relevant microstructure attributes for AM alloys such as surface roughness [22] and porosity [23] have been demonstrated. Traditionally, the challenge for application of these microstructure-sensitive fatigue modeling tools is the large computational expense of such modeling which make it difficult to capture the full range of potential properties to truly identify a minimum fatigue life [24]. Recent advances in both machine learning [25] and numerical simulation methods and tools [26] have lowered the barrier to practical application of these models.

Fatigue Modeling and Digital Twin

The fatigue life of polycrystalline metal alloys can be broken into two regimes: crack initiation life (N_{init}) which is most critical for HCF, and crack propagation life (N_{prop}) which is most critical for LCF. The current state of the art in industry fatigue modeling, NASGRO [27], only deals with crack propagation by assuming the number of cycles to initiate a crack and an initial flaw size from empirical data. This means extensive materials testing data is necessary to predict the complete fatigue life of a component, limiting the utility of modeling to design and qualify components for service. Researchers in academia have been developing and using high-fidelity CPFEM simulations to predict the initiation and early growth of cracks more explicitly for a variety of engineering alloys. These efforts have enabled a better understanding of the origins of fatigue cracks, which can decrease reliance of fatigue life predictions on experimental data, as well as provide a deeper understanding of the underlaying mechanics involved in crack growth. It has been found that underlying mechanics for fatigue crack growth differ depending on the length scale of the crack. As such, the propagation life of a fatigue crack can be further split into three different regimes based on crack size, as shown in Eqn. 1, with models addressing the different driving forces at each stage.

$$N_{Total} = N_{init} + N_{prop} = N_{init} + N_{MSC} + N_{PSC} + N_{LC} \quad (1)$$

Crack initiation typically occurs over a sub-grain size volume referred to as the damage process zone over which slip accumulation can initiate a crack. Physically long crack (LC) growth is typically well described, for metals, using linear elastic fracture mechanics (LEFM) based on stress intensity factors [28]. However, for cracks that are small, the mechanics are no longer well-described by LEFM. This divides the crack propagation life into MSC growth, physically small crack (PSC) growth, and finally giving way to LC growth [29]. MSCs are generally considered to extend to up to 3-10 grains, and PSCs up to about one

millimeter, both depend on the applied stress amplitude and cyclic stress-strain behavior. Crack initiation and MSC growth through the first few grains is highly dependent on localized driving forces, linked directly to the cyclic crystallographic slip intensity within the microstructure [30]. These localized driving forces can be characterized using fatigue indicator parameters (FIPs). The physically small to physically long crack growth regime sees a transition from local driving forces to bulk driving forces as the number of grains in the plastic zone at the crack tip exceeds the threshold, thus averaging out the effects of individual grains. The transition to bulk driving forces can be characterized using the modified-NASGRO equation.

FIPs have been employed in both macro- and micro- scale fatigue studies to characterize driving forces for fatigue crack formation and early crack growth [31, 32]. FIPs intended to relate to transgranular fatigue crack formation are essentially local surrogate measures of driving force based on reversed slip intensity in a damage process zone at the microscale. Brown and Miller [33] first discovered that the crack propagation process is best descr3ibed by the plane on which the largest range of maximum plastic shear strain occurs. Building on this, Fatemi and Socie [14] developed a damage parameter that accounts for the cyclic maximum plastic shear strain averaged over the damage process volume at the mesoscale, with a mediating influence of the peak tensile stress normal to this plane, which is referred to as the Fatemi-Socie FIP, defined by Eqn. 2.

$$FIP_{FS} = \frac{\Delta\gamma^{p}_{\max}}{2}\left[1 + k\frac{\sigma^{p}_{\max}}{\sigma_{y}}\right] \quad \textbf{(2)}$$

Here, $\Delta\gamma^{p}_{\max}$ is the maximum cyclic plastic shear strain range, $\sigma^{p}_{\max}$ is the maximum normal stress acting on the plane of maximum cyclic plastic shear strain range, σ_y is the macroscopic yield strength of the material, and k is a fitting parameter having a value between 0.5 and 1 [14].

In recent years, correlations of various FIPs with high-fidelity experimental studies for transgranular small fatigue crack formation and early growth within polycrystals have been explored [34], including variants of the Fatemi-Socie FIP described here. Additional FIPs have been introduced for fatigue crack formation driven by slip impingement on grain or phase boundaries [35, 36].

Along with establishing appropriate models, it is important to digitally represent realistic microstructures having simulated volumes that are representative of those found in real material systems. In order to analyze the properties of interest for a range of microstructure variants and materials, ensembles of statistical volume elements (SVEs) can be generated, and crystal plasticity finite element method (CPFEM) can be applied using a variety of finite element modeling tools, either commercially available [37] or open-source [38]. Additionally, a tool called DREAM.3D [39] is used to digitally reconstructs or instantiate statistically realistic geometric representations of the grains comprising a polycrystal. This tool is widely used to generate SVEs for polycrystalline alloys.

Common macroscopic polycrystal quantities of interest may be determined based on deformed configuration stress, elastic strain, and inelastic strain, such as elastic stiffness or yield strength. A statistically homogeneous representative volume element (RVE) suitable for computing these stiffness or strength responses is relatively limited in size in terms of number of grains/phases required for convergence (on the order of several hundreds or thousands of grains). However, the concept of evaluating a RVE to compute FIPs is not practical when the property of interest is the minimum fatigue life (e.g., corresponding to maximum FIPs among a large population) [40], as it would require a RVE of excessive size and high computational cost of simulations. Consequently, ensembles of SVEs are typically used to compute the statistical distribution of FIPs [14]; both the SVE size (sufficiently large to incorporate important nearest

neighbor grain/phase spatial correlations) and number of SVEs in each ensemble of simulations needs to be determined to compute meaningful estimates of EVS FIP responses.

To summarize, FIPs serve as a surrogate measure for the driving forces for fatigue crack formation and subsequent growth. FIPs have been shown to correlate well with both LCF- and HCF-crack initiation and early crack growth in various engineering alloys including Ni-based superalloy Inconel 100 [41], martensitic gear steels [42], airframe aluminum alloys [43], and titanium alloy Ti64 [44].

Ultimately, the fatigue failure of engineering alloys is an EVS phenomenon that is initialized by local hot spots within the microstructure on the scale of the damage process zone. It is of vital importance to determine the statistical distributions of key microstructure attributes in a given materials system to examine the juxtaposition of the tail end of the statistical distributions of each microstructure attribute to capture the true minimum fatigue life performance. Liu [45] demonstrated that by adequately characterizing the size and number density of defects in shape memory alloys at two different length scales, the volume affect on fatigue could be accounted for to predict the limiting case for defect size at which the minimum fatigue life was simulated. The results were validated experimentally for various strain amplitudes. Extending this approach to other material systems requires similar characterization or predictive modeling of the relevant statistics of intrinsic and extrinsic microstructure attributes to simulate minimum fatigue life.

For MSC growth, Yeratapally et al. [46] demonstrated, that crack growth can be predicted using computed FIPs based on correlations with crack tip displacement using Eqn. (3) below. This approach provides MSC growth prediction from FIPs, which can be used to predict the minimum fatigue life for HCF. Additionally, this approach can be combined with NASGRO to predict minimum fatigue life for LCF.

$$n_{grain}^{i} = \frac{1}{\sqrt{c_1 c_2}} tanh^{-1}\left(D_{avg}\sqrt{\frac{c_1}{c_2}} \right) \tag{3}$$

Where,

$$c_1 = 2\theta\beta_i FIP_o^{\alpha} - \theta\Delta CTD_{th}$$
$$c_2 = \frac{4\theta\beta_i A(FIP^{\alpha})^b}{D_i^2}$$

Where, n_{grain}^{i} is the number of cycles required to crack the ith grain, D_{avg} is the average grain size while D_i is the size of the ith grain, θ is a material constant accounting for crack tip irreversibility (typically 0.33 to 0.5), β_i is the ratio between the size of the ith and the average grain size, FIP_o^{α} is the FIP on the α^{th} slip plane in the ith grain calculated prior to the crack while FIP^{α} is the value of the FIP with reduction of grain size factored in as the crack propagates. A and b are scaling constants that depend on the microstructure, ΔCTD_{th} represents a threshold below which no dislocations are emitted from a crack.

Lastly, the long crack growth regime is captured by the modified-NASGRO equation which takes over when the MSC grows to a point where the crack length equates to the initial flaw size for the long crack propagation model. Eqn. 4 below shows the modified-NASGRO model.

$$\frac{da}{dN} = C_{FM}\left[\left(\frac{1-\gamma}{1-R}\right).\Delta K_I\right]^n \frac{\left(1-\frac{\Delta K_{th}}{\Delta K_I}\right)^p}{\left(1-\frac{\Delta K_{max}}{\Delta K_{IC}}\right)^q} \tag{4}$$

Where a is the crack length, N is the number of cycles, C_{FM}, n, p, and q are material constants, γ is the Newman's crack opening function, R is the stress ratio, and ΔK_I, ΔK_{th}, ΔK_{max}, and ΔK_{IC} are the stress intensity factor, and the threshold, max, and critical stress intensity factors, respectively.

In the current work, the models for each regime of fatigue crack life are discussed and a framework combining these models to capture full fatigue life is presented as a path to accelerating qualification for fatigue critical components by reducing the number of experiments needed.

ACCELERATED QUALIFICATION FRAMEWORK

In this section, the step-by-step framework for prediction of minimum fatigue life and how it can be used to accelerate the qualification of fatigue critical components is discussed. First, a digital twin of the alloy is generated using experimental characterization of key features. Next, the mechanical properties are calibrated to experimental stress-strain data. Then the fatigue life is split into the relevant fatigue crack length scales and the initiation and MSC growth is captured with FIP-based models at the microstructure scale using CPFEM while the long crack regime is captured with a modified-NASGRO model. Finally, the results of these models are combined to capture the full fatigue life and they are experimentally calibrated and validated with HCF, LCF, and fatigue crack growth rate (FCGR) data.

To build a digital twin, one must first identify the relevant intrinsic (grain size, morphology, orientations, and phase fractions) and extrinsic (porosity, inclusions, and surface roughness) features for a given material, process, and application. Experimental characterization must be carried out to generate statistics on each of the key microstructure attributes identified. Characterization of 3D surface roughness can be achieved using coherence scanning interferometer-based 3D surface analysis. Both keyholing and lack of fusion porosity as well as inclusions can be characterized either with x-ray CT methods or by cross-sectioning samples and examining them with a scanning electron microscope. The latter approach lacks the ability to capture the exact 3D morphology of each feature but does provide a cheaper method to characterize the statistics of pore/inclusion volume fraction and sizes. Electron backscatter diffraction (EBSD) can be used for the rest of the intrinsic features like grain size and morphology, phase fractions, and crystallographic texture. More advanced techniques like serial-sectioning EBSD or diffraction CT can be used to characterize the 3D grain structures if necessary. Using DREAM.3D, statistical distributions of each of these microstructure attributes can be used to generate digital instantiations of the microstructure as shown in Figure 1.

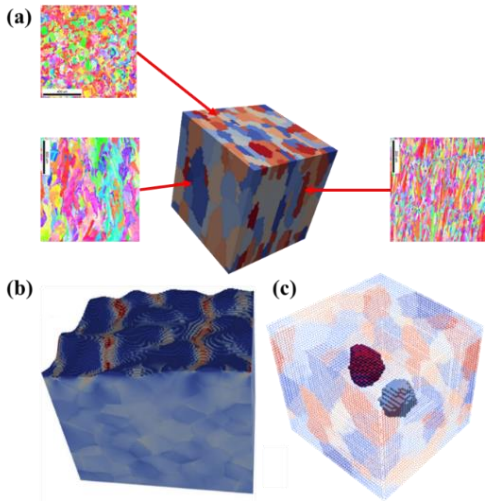

Figure 1. Digital twin of microstructure including key attributes such as (a) grain size, orientation, and morphology from EBSD data, (b) surface roughness adapted from [22], and (c) porosity and inclusions.

Once a digital twin of the microstructure has been generated, the next step is to calibrate the CPFEM model to the material system at hand. In this step, the bulk stress-strain response of a polycrystal is used to calibrate the model. Tensile testing can be used to generate calibration data. Figure 2 shows an example of a crystal plasticity model originally developed for Inconel 100 that was adapted and calibrated for additively manufactured Inconel 625 using monotonic stress-strain data to about 45% strain at room temperature. This is an illustrative example, but in practice one may want to calibrate to cyclic stress-strain data to capture the back stress during compression, as well as considering more than one strain ratio and loading direction, particularly for as-printed or otherwise anisotropic materials.

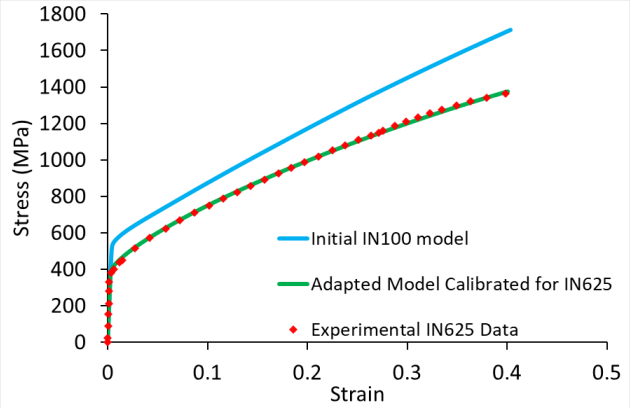

Figure 2. Calibration of CPFEM model to printed Inconel 625 experimental monotonic stress-strain.

Having calibrated a digital twin for the microstructure, the next step is to predict the minimum fatigue life for the relevant loading scenarios. Fatigue life can be described in multiple stages with different relevant lengths scales as previously discussed in the Background section. To summarize, fatigue initiates due to accumulation of slip at the sub-grain scale over a material dependent volume called the damage process zone. Once a crack nucleates, it grows along a meandering path of least resistance through grains, that slows as it reaches grain boundaries and accelerates through grains, making up the MSC/PSC portions of fatigue life, extending up to about one millimeter. Lastly, once the stress field at the crack tip grows large enough that the local microstructure effects are averaged out, and bulk effects takeover, long cracks tends to grow perpendicular to the loading direction in a relatively straight line as shown in Figure 3.

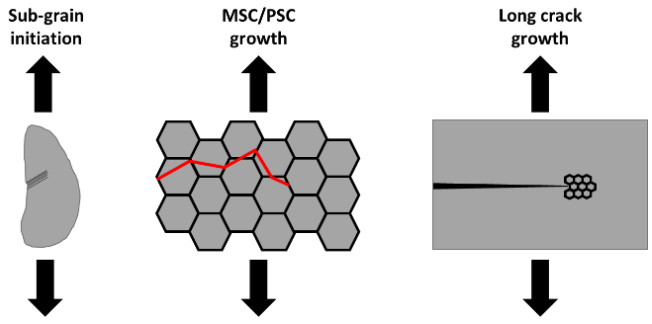

Figure 3. Regimes of fatigue crack initiation and growth for full fatigue life.

To predict crack initiation and MSC growth through the first few grains, a CPFEM model is used to simulate cyclic applied strain for several cycles until stress redistribution takes place and a stable stress-strain response from one cycle to the next is observed. The EVS distribution of FIPs across an ensemble of SVEs is characterized to determine the relative driving forces for fatigue crack initiation in different microstructures and under different applied strain scenarios. Figure 4 shows examples of ensembles of

SVEs and their associated distributions of the maximum computed FIPs from simulations. On the right side of the figure, a comparative analysis of the resulting distributions of FIPs in additively manufactured Ti64 with three different maximum pore sizes compared with Ti64 with zero porosity is shown. Qualitatively, plots like these can be used to determine the effects of microstructure attributes on the relative fatigue performance of a material. In this case it was shown that when maximum pore size is kept below a threshold of ~10μm, the pores do not initiate fatigue cracks in HCF. In general, the maximum FIP from an ensemble of SVEs can be calibrated to minimum life data and used to predict minimum fatigue lives for HCF, VHCF, and UHCF because the fatigue life in these applications is dominated by crack initiation.

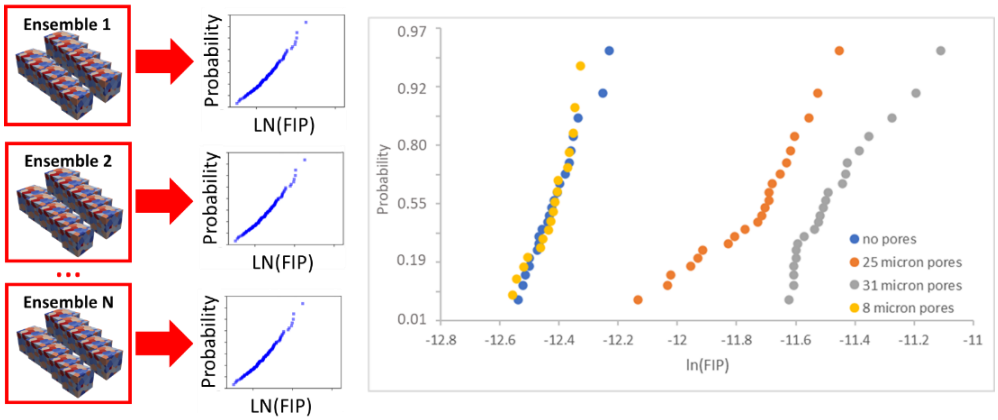

Figure 4. Example of several ensembles of SVEs and the resulting FIP distribution from each (left) and the comparison of FIP distributions for varied maximum pore size in additively manufactured Ti64 demonstrating that HCF life is not influenced by pores below a threshold size (right).

In higher strain LCF applications crack propagation becomes more important. Figure 5 shows an example for the same alloy of fatigue crack propagation through the first three grains, representing the MSC propagation regime. This is predicted with the non-deterministic crack growth model discussed previously in the Background section. This approach predicts the number of cycles required for a crack to grow through every possible grain in three dimensions outward from the crack initiation site. It determines a minimum fatigue life for crack propagation accordingly. This can be calibrated using LCF life and FCGR data.

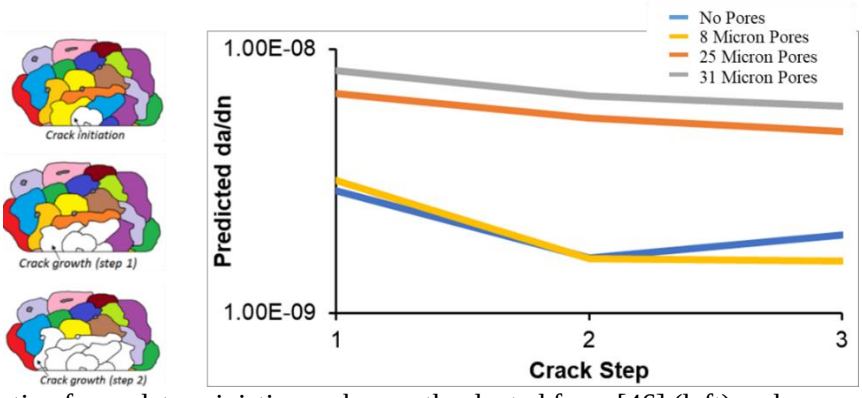

Figure 5. Schematic of non-deterministic crack growth adapted from [46] (left) and example of application of MSC model to additively manufactured Ti64 with varied maximum pore size (right).

As the crack grows beyond ~1mm in length, the crack tip stress field begins to encompass enough grains to average out the local effects and the crack begins to grow according to the bulk stress intensity factor. In this stage the modified-NASGRO model is applied and calibrated the FCGR data to predict the remaining

cycles before fatigue failure. As the number of cycles decreases this stage becomes more important, dominating minimum life for some LCF scenarios. Additionally, in scenarios where an initial flaw exists that is significantly larger than the grain size, such flaws can be considered a pre-initiated crack. Fatigue cracks will propagate from the flaw following the long crack propagation model. Figure 6 shows an example of the modified-NASGRO model calibrated using FCGR data for additively manufactured Ti64 in LCF.

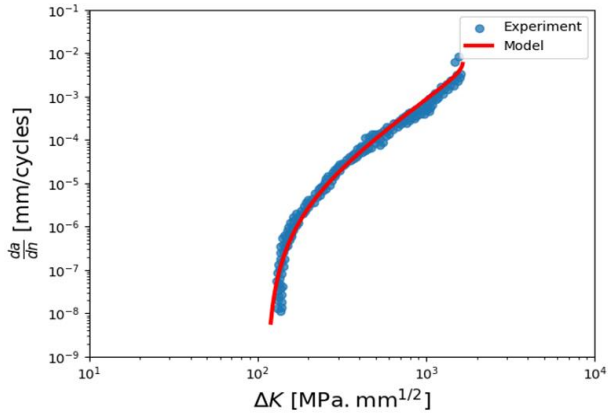

Figure 6. Example of long crack growth predicted using the modified-NASGRO model and calibrated to experimental FCGR data for additively manufactured Ti64.

Finally, the crack initiation life, MSC/PSC propagation life, and long crack propagation life can be combined to predict the full minimum fatigue life of a material under selected loading conditions. Figure 7 shows a schematic representation of what a combined fatigue crack growth curve would look like. Note that the crack growth in red is representative of MSC/PSC growth through the first several grains. Peaks and troughs in the crack growth rate are common in this regime as the crack tip slows at impediments like grain boundaries. Ultimately, once the grain grows long enough the long crack growth curve takes over and the full fatigue life can be captured by combining the two curves.

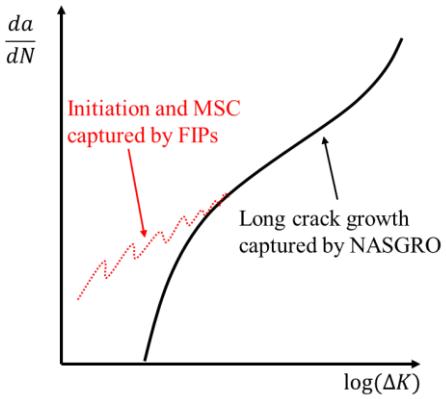

Figure 7. Schematic of how FIP-based microstructure sensitive model and NASGRO model can be combined to capture full minimum fatigue life.

The framework laid out here can be carried out for various microstructures resulting from changes in alloy composition or processing (e.g., as-printed or post processed material) as well as for various loading conditions (e.g., room temperature, elevated temperature, varied loading ratios/amplitudes, uniaxial, multiaxial, LCF, HCF, etc.). Calibrating each model and the overall framework to the minimum fatigue life in a limited number of strain scenarios can enable the prediction of minimum fatigue life for other strain scenarios and ultimately the generation of S-N curves with greatly reduced experimental time and cost.

REDUCING THE BARRIER TO TECHNOLOGY ADOPTION

AM offers several valuable advantages in the aerospace industry when compared with traditional manufacturing, including complex geometrical freedom in design, reduced reliance on supply chains, reduced complexity of mechanical systems by combining parts, and rapid prototyping and development of new components. However, the qualification process currently acts as a major barrier to the widespread adoption of this advanced technology. Qualification for aerospace typically requires extensive material testing to establish initial property datasets, followed by delta qualification for any new versions of machines, and witness coupon testing on each heat. This process is geared largely toward mass production manufacturing to reduce the cost and time burden of qualification. This approach is generally slow and costly and is especially so in the case of AM where economy of scale is less of a factor. Additionally, for minimum fatigue life, which is inherently an EVS phenomenon due to the local microstructure scale of the driving forces, even with extensive, time consuming, and costly experimentation, it is very difficult to truly characterize the minimum fatigue life of an alloy with any realistically feasible number of experiments. Using ICME in the qualification process for fatigue critical components provides three major advantages:

1. Cost: Pure factorial testing methods will require more raw material, sample printing, heat treatment, machining, and ultimately more experimental fatigue testing, significantly driving up the cost of qualification and certification. With an ICME approach, the number of tests, and in turn the number of fabricated test coupons needed to arrive at the same statistically rigorous dataset will be significantly lower, since a subset of the experiments can be used to calibrate and validate the models and the remaining loading scenarios can be simulated.
2. Speed: The use of ICME will decrease the time-consuming process of qualification by reducing the number of tests needed to arrive at the same statistically rigorous dataset, and the remaining scenarios can be rapidly simulated using parallel computing resources.
3. Reliability: There is always a tradeoff between cost and uncertainty in experimental approaches. To understand the true 99th percentile fatigue life for a given loading scenario requires 100 fatigue tests per loading scenario, which is typically not feasible. With well calibrated and validated physics-based models, and the relatively low cost/time required for simulations compared with experiments, it is more realistic to arrive at the true statistical minimum fatigue life as characterized by EVS. Additionally, by controlling the simulation inputs, a more fundamental understanding of how each microstructure attribute affects fatigue life can be attained, enabling future iterations and refinement on materials development to improve fatigue performances.

A typical fatigue qualification may consider 2-4 stress amplitudes in the LCF regime, another 1-2 in the HCF regime (including runouts) giving 3-6 different loading scenarios. Additionally, both as-printed and post processed samples are typically tested, doubling the number of tests. Next, for any material potentially used at elevated temperatures, tests are carried out at both room temperature and elevated temperatures, again doubling the number tests. In the case of AM materials which tend to be anisotropic, testing may be required in both parallel and perpendicular to the build direction to capture the range of fatigue properties as a function of loading direction. Already this adds up to 48 different scenarios. In some cases, strain-controlled fatigue testing is also required, and typically fatigue crack growth rate experiments are carried out to understand damage tolerance. To even captures the 90^{th} percentile minimum fatigue life for each of these scenarios, ten fatigue tests need to be carried for each, putting the total testing on the order 500+ fatigue tests to generate a reasonable dataset for qualification of fatigue critical components. This level of extensive fatigue testing from multiple batches of powder and from multiple AM machines can cost on the order of $1 million dollars for each new alloy or process parameter set developed. With the use of well validated and calibrated physics-based modeling in an ICME framework as discussed in this work, the costs can be drastically reduced while also providing better fundamental understanding of the physical metallurgy at play.

CONCLUSION

An ICME framework for modeling the full fatigue life of polycrystalline engineering alloys was discussed. An approach for the application of this framework to accelerate qualification of fatigue critical components was presented. By implementing this framework, the insertion of new materials for fatigue critical components can reliably and safely be carried out with reduced cost and time. The components of this modeling framework have been developed and validated over the past 20+ years in the academic and industrial R&D communities and in recent years several key advances in computational power, numerical methods to improve the efficiency and scalability of simulations, fundamental understanding of fatigue, and modeling of key microstructural attributes that drive fatigue crack initiation and propagation, have all combined to make this framework possible.

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