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Bayesian uncertainty quantification and propagation for validation of a microstructure sensitive model for prediction of fatigue crack initiation

Saikumar R. Yeratapally[a], Michael G. Glavicic[b], Christos Argyrakis[c], Michael D. Sangid[a,*]

[a] School of Aeronautics and Astronautics, Purdue University, West Lafayette, IN 47907, USA
[b] Rolls-Royce Corporation, Indianapolis, IN 46225, USA
[c] Rolls-Royce plc, Derby DE24 8BJ, UK

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ABSTRACT

A microstructure and deformation mechanism based fatigue crack initiation and life prediction model, which links microstructure variability of a polycrystalline material to the scatter in fatigue life, is validated using an uncertainty quantification and propagation framework. First, global sensitivity analysis (GSA) is used to identify the set of most influential parameters in the fatigue life prediction model. Following GSA, the posterior distributions of all influential parameters are calculated using a Bayesian inference framework, which is built based on a Markov chain Monte Carlo (MCMC) algorithm. The quantified uncertainties thus obtained, are propagated through the model using Monte Carlo sampling technique to make robust predictions of fatigue life. The model is validated by comparing the predictions to experimental fatigue life data.

1. Introduction

The majority of mechanical failures can be attributed to fatigue, which is a complex problem involving many independent factors that evolve during cyclic loading. Fatigue crack initiation in polycrystalline materials can be attributed to the heterogeneous microstructure forming complex stress states resulting in strain heterogeneities and localization. Additionally, cyclic loading manifests in deformation mechanisms leading to cyclic slip irreversibilities, which ultimately increase stress concentration and thereby lead to the formation of cracks. Many empirical [1,2] and physics-based models [3–6] have been proposed to predict fatigue life in polycrystalline materials. Uncertainties exist in every model, and before such computational models are employed (to predict the life of components), careful attention must be given to understand the degree in which these uncertainties influence the predicted quantity of interest (QoI), in this case the fatigue life. Rigorous uncertainty quantification for validation purposes is a pre-requisite for such predictive models to be used in a production environment. The current work focuses on identifying, quantifying and propagating the uncertainties in a microstructure based life prediction model [6] for the purpose of validating the model. In this study, model validation is performed based on:

i) Global sensitivity analysis (GSA) to identify the set of non-influential parameters in a factor-fixing setting, which in turn helps in reducing the computational cost of the uncertainty quantification problem [7,8].
ii) Bayesian inference to quantify uncertainties in the set of influential parameters determined using GSA [8–10].
iii) Monte-Carlo sampling to propagate the quantified uncertainties to obtain distribution of predicted life, which will be used in validating the model's predictions [8,10].

Researchers in various sub-disciplines of computational materials science and engineering including computational solid (and particle) mechanics [10,11], computational fluid dynamics [12], molecular dynamics (MD) [13,14], etc., have integrated uncertainty analysis into their modeling framework. Over the past decade, uncertainty quantification has been successfully applied to fatigue crack growth models pertaining to both metals [15–19] and composites [20,21]. Zhang and Mahadevan [15] used Bayesian inference technique to quantify uncertainties via statistical distribution parameters in two competing crack growth models for metals. Cross et al. [16] used a hierarchical Bayesian inference framework to quantify uncertainties in equivalent initial flaw size and crack growth rate parameters, and hence improved the predictive capabilities of their fatigue crack growth model. Sankararaman et al. [19] used a Bayes network to propose a methodology for uncertainty quantification and model validation in fatigue crack growth analysis. Chiachio et al. [21] used a full Bayesian approach to quantify uncertainties of a set of five damage mechanics

* Corresponding author.
E-mail address: msangid@purdue.edu (M.D. Sangid).

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models for composites and the best of the models was chosen based on an information-theoretic approach by calculating the relative probability amongst all other candidate models. The metal fatigue crack growth models discussed above are empirical in nature and are independent of the microstructure of the material, which has a great influence in crack initiation [3–6] and microstructurally small fatigue crack growth [22]. The fatigue life prediction framework which is used in the current study [6], differs from the above mentioned crack growth models in the following four ways. First, it is a microstructure based framework, where the morphological and crystallographic heterogeneities in the microstructure are considered and an attempt is made to link the variability of the microstructure with the fatigue life calculated. Second, it is not fully empirical in nature, as the model takes into consideration the physics of underpinning deformation mechanisms, which lead to cyclic slip irreversibilities during fatigue, thereby addressing fatigue at the slip system length-scale. Third, it considers complex stress states from grain-to-grain interactions. Finally, the model predicts number of cycles for fatigue crack initiation rather than calculating crack growth with number of cycles. While dealing with models that predict fatigue crack initiation, a phenomenon, which is dependent on both the local microstructure and deformation mechanisms, the number of epistemic uncertainties increases due to the complexities involving length-scale dependent deformation mechanisms. These uncertainties need to be quantified, in order to validate the model and identify an appropriate applicability regime. There is a great amount of work that needs to be done in quantifying uncertainties in complex physics based models and hence improving the predictive capabilities of such models [23].

Several micro-mechanical fatigue crack initiation models have been developed which take into consideration the heterogeneities within the microstructure and various parameters that quantify length-scale dependent deformation mechanisms [3–6]. The energy based model of Tanaka and Mura [3] takes into consideration parameters like the frictional stress, cyclic slip irreversibility and the specific fracture energy of the material. The fatigue crack initiation framework developed by Sangid et al. [4,5] takes into consideration, width of a persistent slip band (PSB), dislocation density, γ' volume fraction, grain boundary (GB) energies, extrusion height at intersection of PSB-GB, stacking fault and anti-phase boundary energies. There are uncertainties associated with all the parameters mentioned above, some of which are difficult to measure using experiments. Although these models provide great insights into understanding how certain microstructural features and competing deformation mechanisms lead to initiation of fatigue cracks, systematic sensitivity and uncertainty analysis, in an attempt to validate such physics-based models, is still lacking [23]. The current work fills this gap by using a sensitivity and uncertainty analysis framework, in order to validate a microstructure and deformation mechanism based life prediction model [6]. Although validation of the model is a driving motivation, the main contribution of the current work is the application of sensitivity and uncertainty analysis to a microstructure and deformation dependent fatigue life prediction model.

The rest of the paper is organized as follows: In Section 2, we provide a brief overview of the microstructure dependent fatigue life prediction model and an overview regarding how the sensitivity and uncertainty analysis are performed on the model. Section 3 lists all the uncertainties that prevail in the model and categorize the uncertainties. It also provides an overview of the uncertainty analysis framework used in this study. In Section 4, we show the application of GSA to identify the most influential parameters in the model, which contribute most to the uncertainty in the output. Section 5 describes Bayesian framework and the quantified uncertainties for the set of influential parameters. In Section 6, we use Monte Carlo simulations to propagate the uncertainties through the model to obtain distributions of life predictions. Section 7 discusses the dependence of various parameters on applied strain amplitude, and conclusions are presented in Section 8.

2. Overview of the microstructure based life prediction model

As uncertainty quantification and propagation are the main focus of the current work, we only present a brief overview of the PSB energy based life prediction model (or PSB model) in this section. For a detailed description of the model, please refer to Yeratapally et al. [6]. It must be noted that the PSB model takes information on state dependent variables like the resolved shear stress (τ^{α}), normal stress (σ_N^{α}), back stress (χ^{α}), critical resolved shear stress (g^{α}) and accumulated strain in a slip system (γ^{α}), output from crystal plasticity finite element (CPFE) simulations (of one-cycle loading) done on a statistically equivalent microstructure (SEM), which is sufficiently large to capture the statistics of microstructural attributes (like mean and variance of grain size distribution and percentage of twins in the microstructure) and strength properties (elastic modulus, yield strength, hardening response and reverse plasticity upon unloading) pertinent to the material of interest, RR1000, a powder processed superalloy developed by Rolls-Royce plc, is used in this study. This stress-strain information along with the GB energetics is used as input to the PSB model, to predict the potential location and number of cycles for crack initiation. Although CPFE is an integral part of the fatigue framework, the focus of the current work is to quantify the uncertainties in the PSB model itself. Quantifying all the uncertainties in CPFE framework requires information about how the stress and strain evolve relative to the microstructure with applied loading, which is beyond the scope of the current work.

Fig. 1 displays a schematic of a PSB traversing a low angle GB (or LAGB) and impinges upon a high angle GB (for example an annealing twin boundary), where the dislocations pile-up, form extrusions at the boundary plane, and thereby increase the stress concentrations at the GB, which could potentially lead to crack initiation.

With this established view of a PSB (based on experimental observations), we define the energy of a PSB as follows:

$$E_{PSB} = \sum_i \partial X_i \left(f \int_0^L \gamma_{APB} dL + (1-f) \int_0^L \gamma_{SFE} dL \right) n_{eff}^{layers} + \sum_i \partial X_i (E_{slip-GB}^{\gamma-MD} n_{ext-GB}^{dis} bh) + \sum_i \partial X_i (\sigma_{pile-up} - \Delta\tau_{CPFEM}^{\alpha} - \sigma_{hardening}) bL n^{layers}, \quad (1)$$

where ∂X_i is the incremental slip within PSB, f is the volume fraction of the γ' precipitate phase in the nickel-base superalloy, γ_{SFE} is the stacking fault energy of the γ phase, γ_{APBE} is the anti-phase boundary energy of the γ' precipitate, n_{eff}^{layers} is the number of effective layers contributing to SFE or APBE, and it decreases with a decrease in the degree of crystallinity, DC, in the PSB (see Section 3.3 for further explanation on DC), L is the length of the PSB, $E_{slip-GB}^{\gamma-MD}$ is the energy required for a dislocation to transmit across a GB, n_{ext-GB}^{dis} represents the number of dislocations forming an extrusion at the PSB-GB intersection, b is the magnitude of the Burgers vector (which represents the amount of lattice distortion due to the glide motion of a single dislocation in a crystalline lattice), h is the width of the PSB, $\Delta\tau_{CPFEM}^{\alpha}$ is applied cyclic stress on the PSB, $\sigma_{hardening}$ accounts for the hardening within the PSB, $\sigma_{pile-up}$ is the pile-up stress at the intersection of the PSB and the GB, and n^{layers} is the number of slip planes within the PSB, which is related to the PSB width, h, as $n^{layers} = \frac{h}{b}$.

Within the energy expression of PSB, the terms n_{ext-GB}^{dis}, $\sigma_{pile-up}$, σ_{stroh}, $\sigma_{hardening}$ are calculated using the following expressions:

$$n_{ext-GB}^{dis} = k \left| \frac{\tau^{\alpha} - \chi^{\alpha}}{g^{\alpha}} \right|^m \frac{L}{L_{avg}} \left(\frac{\tau^{\alpha} + \sigma_{pile-up} - \sigma_{stroh}}{\sigma_{stroh}} \right) \sqrt{n - n_{offset}}. \quad (2)$$

$$\sigma_{pile-up} = \frac{1.8 \mu \gamma^{\alpha}}{\pi(1-\nu)}. \quad (3)$$