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Microstructure-sensitive notch root analysis for dwell fatigue in Ni-base superalloys

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ABSTRACT

Macroscopic viscoplastic constitutive models for γ–γ' Ni-base superalloys typically do not contain an explicit dependence on the underlying microstructure. Microstructure-sensitive models are of interest in many applications since microstructure can vary in components, whether intentional or not. In such cases, the use of experiments from one microstructure condition to fit macroscopic models may be too limiting. The principal microstructure attributes that can significantly affect the cyclic stress–strain response of γ–γ' Ni-base superalloys are the grain size and γ' precipitate volume fraction and size distributions. An artificial neural network (ANN) is used to correlate the material parameters of a macroscale internal state variable cyclic viscoplasticity model with these microstructure attributes using a combination of limited experiments augmented by polycrystal plasticity calculations performed on other (virtual) microstructures within the range characterized experimentally. The trained model is applied to an example of a component fatigue notch root analysis with dwell periods at peak load to demonstrate the methodology and explore the potential impact of microstructure-sensitive constitutive models on life prediction for notched structures subjected to realistic load histories.

1. Introduction

Conventional macroscopic (referred to as 'macro') models for cyclic viscoplastic deformation do not typically contain explicit dependence on the underlying microstructure. Microstructure-sensitive models are of interest in view of variations of microstructure within heat-treated components. Moreover, components with functionally graded microstructures may exploit microstructure-property relations to achieve enhanced fatigue resistance. A macroscopic internal state variable model [16] that is sensitive to microstructure is potentially useful since it is capable of being used in notch root cyclic stress–strain behavior analysis of components, whereas polycrystal plasticity is formulated at too fine a length scale for practical component level analyses. Another important issue is the dependence of the notch root response, such as creep and stress relaxation, on microstructure under conditions of cycling with sustained peak dwell periods. These issues are difficult to resolve with high fidelity, component level simulations that employ polycrystal plasticity models with resolution at the scale of individual grains.

One means of informing macroscopic models is to employ a homogenization approach based on micromechanics of heterogeneous materials. Various forms of self-consistent models have been proposed for homogenization of polycrystalline response, for example. However, the microstructure considered here has attributes at multiple scales even below the grain level of strengthening precipitates that affect grain level response. Moreover, finite element polycrystal simulations of large numbers of grains offer adequate approximation of intergranular interaction effects. Accordingly, this paper employs a hierarchical approach shown in Fig. 1 to embed dependence on microstructure in the 'macro' model. In this work, constitutive models are formulated at two length scales: at the scale of individual grains with a microstructure-dependent model that employs a crystal plasticity framework [27,29], and a macroscale internal state variable (ISV) model. A combination of experimental stress–strain histories from actual microstructures and stress–strain responses computed using virtual (digital) microstructure simulations from the microscale model are used to inform the microstructure-dependent parameters in the macroscale model. There are three primary steps in the algorithm to embed microstructure dependence into the 'macro' model [26,27]:

- Step 1 – A stress–strain database is generated for different strain histories using the polycrystal plasticity (referred to as 'micro') model for a range of microstructures that are intermediate to 7–8 selected actual microstructures used for 'micro' model calibration.

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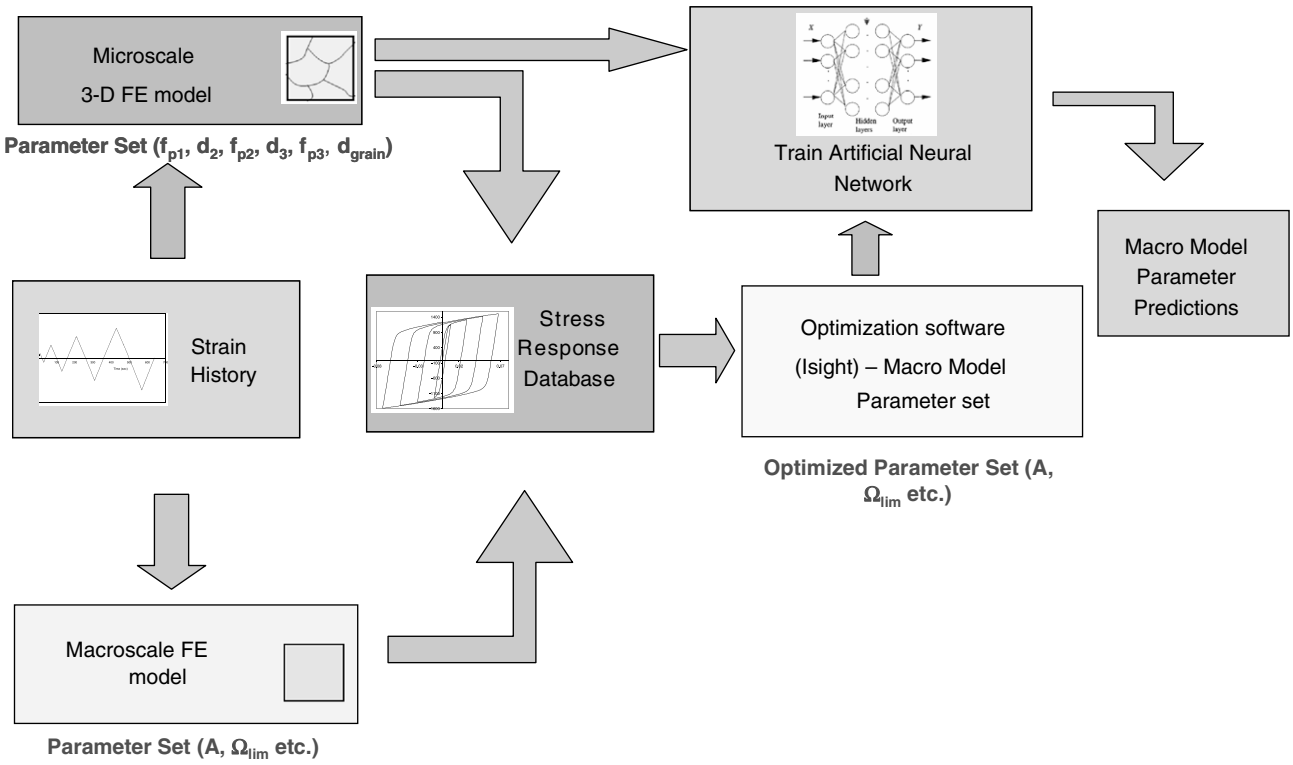

Fig. 1. Framework for linking the 'micro' model to the 'macro' model.

- Step 2 – The macroscopic ('macro') ISV model parameters are determined for the stress–strain data for each microstructure in the database, including virtual microstructures intermediate to those characterized experimentally, using an optimization scheme.
- Step 3 – An artificial neural network (ANN) is trained to relate the parameters in the 'macro' model to the corresponding microstructure attributes. The microstructure attributes for Ni-base superalloy IN 100 are varied randomly within the range shown in Table 1, subject to a constraint on an allowable total γ' volume fraction to lie between 0.5 and 0.6. A total of 150 microstructures are generated to train the ANN.

The primary microstructure attributes that can significantly affect the cyclic stress–strain response of Ni-base superalloys include the mean grain size and the sizes and volume fractions of the Ni_3Al γ' precipitates, with ranges based on experimentally characterized microstructures [27] in the present Ni-base superalloy listed in Table 1. The size of primary γ' is not listed in this table, as it is on the order of grain size and these particles are not sheared; primary γ' effectively enhances shear localization in surrounding matrix regions [27]. Both subsolvus and supersolvus heat treatments are considered. The response of this particular alloy is similar to that of IN 100 [20], which was used in our prior study [26,27]. Fig. 2 illustrates the various microstructure attributes listed in Table 1.

Table 1
Ranges of microstructure attributes used to generate the database for 150 IN 100 microstructures

Microstructure attribute	Minimum	Maximum
Volume fraction of primary γ' precipitate, f_{p1}	0.0	0.25
Volume fraction of secondary γ' precipitate, f_{p2}	0.29	0.46
Secondary γ' Precipitate size, d_2 (nm)	110	340
Volume fraction of tertiary γ' precipitate, f_{p3}	0.024	0.14
Tertiary γ' precipitate size, d_3 (nm)	7.0	21.0
Average grain size, d_{gr} (μm)	4.0	34.0

2. 'Micro' polycrystal plasticity model

Local crystal plasticity theory is used at the grain scale for IN 100, with slip occurring on both octahedral and cube slip planes. The kinematical foundation for single crystal elastoplasticity has been built from a continuum perspective [3–6,9,13,19,25]. The deformation of a single crystal is composed of contributions from (i) an overall "elastic" distortion of the lattice, and (ii) plastic deformation associated with dislocation glide that does not disturb the lattice geometry. The deformation gradient, F, is multiplicatively decomposed, i.e., $F = F^e \cdot F^p$. The linear hyperelastic relation (small elastic strain) is assumed. The kinetics of shearing on each slip system is assigned as a function of resolved shear stress, with effects of initial yield and work hardening incorporated through micromechanical relations that reflect size-dependent precipitate shearing versus looping, and dislocation density evolution. The model equations are summarized in Table 2. The linear hyperelastic relation is given by $\sigma^{pk2} = C : \varepsilon^e$, where C is the 4th rank anisotropic elasticity tensor of the crystal and σ^{pk2} is the symmetric 2nd Piola–Kirchhoff stress with respect to the intermediate configuration defined by $(F^e)^{-1} \cdot F$.

The model is integrated over a large number of grains characterized by a random crystallite orientation distribution function that constitutes a representative volume element for purposes of fitting complex cyclic deformation behavior of actual microstructures. Details may be found elsewhere, including values of constants, and are beyond the scope of this paper [26,27].

3. 'Macro' cyclic viscoplasticity model

Statistical variability of cyclic stress–strain behavior due to heterogeneous, polycrystalline microstructure either at the scale of