**INTRODUCTION**

Nickel-based superalloys are employed as one of the primary structural components in high temperature jet engine applications. Their unique ability to maintain mechanical strength and corrosion resistance over a wide range of temperatures highlights them as critically important engineering materials. However, modelling Ni-based superalloys is inherently a multiscale problem. The remarkable properties of the material are attributed to precipitate strengthening and other dislocation micromechanisms, which occur at the subgrain level. At this scale, the morphology and spacing of NiAl γ precipitates play a significant role in the thermoviscoplastic behavior.

**DISLOCATION DENSITY-BASED CRYSTAL PLASTICITY CONSTITUTIVE MODEL**

Subgrain Crystal Plasticity Finite Element Model

A two phase dislocation density-based crystal plasticity model is developed to explicitly simulate the precipitate-matrix structures at the subgrain scale. (Keshavarz, Ghosh 2013)

Thermally Activated Flow Rule (Orowan equation)

\[ \dot{\gamma} = \rho_\gamma \rho_0 \exp \left( -\frac{Q_\gamma}{RT} \right) \cos \theta \cdot \frac{1}{1 + \frac{c}{H_0}} \gamma \cdot \frac{\gamma \dot{\gamma}}{\gamma^2 + 1} \]

\[ \gamma \] Phase Critical Resolved Shear Stress (Keshavarz, Ghosh 2013)

\[ \sigma_{\gamma} = \frac{c_1}{c_2} \tau_{\gamma} \]

A distance to edge computation is performed to validate the virtual microstructure generation procedure.

**DISESTABLISHMENT OF SERVES**

SERVE Analysis

For the subgrain micromechanical analysis, it is important to generate statistically equivalent representative volume elements (SERVEs) for finite element simulation. The size of this SERVE is determined by studying the convergence of microstructural statistics, material parameters, and mechanical properties as the simulation volume is increased.

**MICROSTRUCTURE SERVES**

Microstructure SERVE (M-SERVE)

Experimental 3D subgrain γ/γ' microstructure data is collected through FIB-SEM serial sectioning and is statistically quantified in terms of precipitate morphology and spacing distributions.

**PROPERTY SERVES**

Property SERVE (P-SERVE)

Defining the concept of a SERVE is ultimately linked to which mechanical property or microstructural feature is of interest. Yield and plastic strain behavior under monotonic loading is analyzed to determine the appropriate size of SERVE needed to represent these mechanical responses.

Convergence of macroscopic response occurs before M-SERVE

Distributions of mechanical fields converge near 100-200 precipitates.

**CALIBRATION AND GLOBAL SENSITIVITY**

Calibration of Constitutive Law Parameters

A generic optimization procedure is executed to determine the constitutive law material parameters.

Convergence of parameters is observed in the optimization function.

Global Sensitivity Analysis

Global sensitivity analysis is performed, in the form of Sobol' index computations, to understand which material parameters most influence the model and the calibration.

It is observed that the calibration to experimental data is not strongly influenced by different microstructure realizations even at a low number of precipitates.

**PARAMETRIC HOMOGENIZATION**

Morphological Distribution Parameters

The morphological distributions of γ precipitates critically influence the dislocation mechanics at the subgrain scale. The effects of these statistics are brought to the polycrystalline scale by parameterizing the distributions into lower order representations.

Homogenized Constitutive Model

A thermally activated crystal plasticity constitutive law is adopted for the single crystal behavior of the larger scale. Two critical parameters (cutting stress τc and hardening constant h) are selected to become functions of the γ morphological descriptors.

Parametric Homogenization

By simulating a number of microstructural realizations at the subgrain scale with various γ microstructures, functional forms for the initial cutting stress and hardening constant are derived. The connection between scales is enforced through Hill’s conditions.

Precipitate Strengthening at Polycrystalline Scale

The lower scale precipitate-matrix microstructure can be designed and optimized to strengthen weak grains in the polycrystalline aggregate.

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