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Multiscale modeling of polycrystalline nickel-based superalloys accounting for subgrain microstructures



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ABSTRACT

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This paper focusses on the use of the parametrically homogenized crystal plasticity to simulate polycrystalline ensembles of Ni-based superalloys that are governed by the characteristics of the subgrain scale $\gamma - \gamma'$ precipitate morphology. Critical parameters representing the effect of subgrain-scale morphology are incorporated in the grain-scale crystal plasticity model, which then has the capability of representing mechanisms occurring at three scales, viz. the sub-grain scale of precipitates, the grain scale of single crystals and the scale of polycrystalline aggregates in a unified framework. A dislocation density crystal plasticity constitutive model with APB shearing of γ' precipitates is developed for modeling the subgrain scale representative volume element delineating explicit morphology of the $\gamma - \gamma'$ microstructure. A framework is developed for a parametrically homogenized activation energy-based crystal plasticity (AE-CP) model at the scale of single crystals by homogenizing the sub-grain model response and incorporating critical morphological parameters of the sub-grain morphology. Nucleation and evolution models for micro-twins are also incorporated for manifesting tension-compression asymmetry. The grain-scale AE-CP model is used to analyze polycrystalline microstructures.

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1. Introduction

Ni-based superalloys are widely used in propulsion components of the aerospace industry such as turbine engine blades, disks, casings and liners. These alloys possess a desirable combination of high temperature strength and toughness, oxidation and creep resistance, and high temperature stability [1,2], attributed to a subgrain scale two-phase $\gamma - \gamma'$ microstructure as shown in Fig. 1. The continuous γ -matrix phase has a face-centered cubic (fcc) lattice structure, and is an alloy of Ni and Cr with a small fraction of other alloying elements. The precipitate phase γ' is a coherent ordered inter-metallic reinforcing phase of L1₂ crystal structure of Ni₃Al type, which appears as a distribution of cuboidal precipitates in a solid solution as shown in Fig. 1. Fig. 1 shows the polycrystalline microstructure, the sub-grain $\gamma - \gamma'$ microstructure in a single grain, the discretized sub-grain $\gamma - \gamma'$ microstructural RVE, and the homogenized crystal plasticity FE model for a grain. The shape and size of the γ' -phase depend largely on the cooling rate and internal stress gradients during processing [3–5]. Slower cooling rates lead to the formation of bimodal populations of large (>500 nm) secondary and small (<50 nm) tertiary γ' precipitates, while higher

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cooling rates yield a predominantly unimodal distribution of secondary γ' precipitates (300–500 nm). The γ' precipitates act as effective obstacles to the motion of dislocations by virtue of their shape and ordered structure. The volume fraction of γ' precipitates, their mean size and spacing have a major effect on the mechanical properties of these superallovs [6,7]. Micro-mechanisms controlling creep in polycrystalline Ni-based superalloys are complex [6,8]. At intermediate temperatures $650 \circ C \le \theta \le 800 \circ C$ and moderate stress levels ~650 MPa, dominant deformation mechanisms include anti-phase boundary (APB) shearing and micro-twinning. The probability of occurrence of a given mechanism depends on the load, crystal orientation and microstructural morphology. At lower temperatures (θ < 650 °C) and higher stresses, creep is governed by different types of dislocation-based shearing processes, while at higher temperatures ($\theta > 800 \circ C$), the creep deformation is controlled by Orowan looping and cross-slip mechanisms [9].

Deformation behavior under various loading and temperature conditions has been analyzed both for single crystal [10,11] and polycrystalline [12,13] Ni-based superalloys. Meso-scale modeling of the $\gamma - \gamma'$ phases in single crystal Ni-base superalloys with unimodal precipitate sizes and periodic distributions has been conducted in [14-17] using phenomenological viscoplastic constitutive laws.

Crystal plasticity finite element models (CPFEM) have been implemented to model creep and deformation response of

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Fig. 1. Schematic representation of multiple scales in the development of a crystal plasticity finite element model for Ni-based superalloys: polycrystalline microstructure, subgrain microstructure in a single grain, discretized subgrain microstructural RVE (homogenized crystal plasticity FE model for a grain).

single crystal and polycrystalline Ni-based superalloys in [18–20]. In these models, the behavior of single-crystal superalloys with high volume fraction of cuboidal precipitates has been simulated using a gradient-dependent plasticity model. Phenomenological crystal plasticity models are based on the power law description [21], or the thermally activated theory of plasticity law [22]. The latter model has been shown to accurately model a large range of strain rates and temperatures. A limitation of these models is their lack of incorporation of the underlying microstructural characteristics at the sub-grain scale, which affect single crystal and polycrystalline behavior. Three scales are dominant when modeling polycrystalline behavior of Ni-based superalloys using CPFEM. They are:

- i. Sub-grain scale, characterized by size of γ' precipitates and their spacing or γ channel-width;
- ii. Grain-scale of single crystals characterized by grain-boundary distance;
- iii. Scale corresponding to representative volume elements of polycrystalline aggregates.

Crystal plasticity models should hierarchically incorporate information at each scale for generating constitutive models that can be implemented for microstructure-property relations. It is computationally intractable to simulate the behavior of polycrystalline microstructures with explicit representation of the $\gamma - \gamma'$ microstructure. In [17], hardening parameters are expressed as functions of the average size of precipitates. Crystal plasticity models with implicit dependencies on grain and precipitate sizes and volume fraction, have been proposed in [23] by assuming random distribution of precipitate phases. Computational models involving hierarchical approaches for Ni-based superalloys have been proposed in [24,25]. In [24,25], dislocation-density based crystal plasticity models for creep and fatigue have been developed using an artificial neural network algorithm, implicitly incorporating effects of grain size, volume fraction and size. It is evident that efficient, hierarchical crystal plasticity models with explicit relations to microstructural features are necessary for unraveling the dependence of properties on microstructure. The hierarchical framework may be accomplished for Ni-based superalloys through the homogenization of lower (sub-grain) scale response to develop higher (grain) scale constitutive relations. This is achieved by incorporating parametric forms of subgrain-scale morphological characteristics in grain-level constitutive relations. Ghosh et al. have implemented computational homogenization approaches using asymptotic expansion methods to develop reduced order homogenized constitutive models for continuum plasticity of polycrystalline metals [26] and ductile fracture in heterogeneous metals [27,28]. In recent papers [29,30], the authors have developed a hierarchical model for Ni-based superalloys from subgrain-scale to grain-scale crystal plasticity constitutive model.

The present paper focusses on the use of the parametrically homogenized crystal plasticity developed in [29,30] to simulate polycrystalline ensembles of Ni-based superalloys that are governed by the characteristics of the subgrain scale $\gamma - \gamma'$ precipitate morphology. Critical parameters representing the effect of subgrain-scale morphology are directly incorporated in the grain-scale crystal plasticity model, which then has the capability of representing mechanisms occurring at three scales, viz. the sub-grain scale of precipitates, the grain scale of single crystals and the scale of polycrystalline aggregates in a unified framework. This is novel development for modeling Ni-based superalloys. The hierarchical framework for realizing the crystal plasticity model for polycrystalline superalloys is shown in Fig. 1. The time-scales of both the sub-grain and the grain-scale slip activity are similar. Hence, the strain-rates do not have to be homogenized in the temporal scale. The strain-rates involved in this model are in the range small to moderate range ($\leq 10^3$), for which plasticity occurs primarily due to dislocation glide on slip planes.

The paper briefly discusses the sequence of steps pursued to create the framework. Section 2 introduces a dislocation density crystal plasticity constitutive model with APB shearing of γ' precipitates for modeling the sub-grain scale representative volume element delineating explicit morphologies of the $\gamma-\gamma'$ microstructure. Section 3 provides a framework for the development of an activation energy-based crystal plasticity (AE-CP) model at the scale of single crystals by homogenizing the sub-grain model response and incorporating critical morphological parameters of the sub-grain morphology [29,30]. This section also introduces nucleation and evolution models for micro-twins. Section 4 incorporates the grain-scale AE-CP model in a framework for analyzing polycrystalline microstructures.

2. Sub-grain scale RVE model

The two-phase binary Ni-based superalloy consists of a primary matrix γ phase (pure Ni) and a secondary intermetallic γ' (Ni₃Al) phase as shown in Fig. 1. The primary phase is a solid solution with a face-centered cubic or *fcc* crystal structure, with four planes of inelastic slip corresponding to the {111} family, i.e. γ in Miller indices. The secondary γ' phase has an ordered crystalline lattice of type $L1_2$. In contrast to the γ phase, cube slip systems of the {100} family accompany the octahedral slip systems of the {111} family for this phase for some temperature ranges. Atoms of aluminum are placed at the vertices of the cubic cell, while atoms of Ni are located at centers of the faces as shown in Fig. 1.

The intermetallic γ' phase has been known to exhibit an anomalous dependence of the flow stress on temperature [31,32]. The flow stress increases with increasing temperature to a peak value at a critical temperature of around 1000 K. Beyond this critical temperature, the flow stress drops rapidly with increasing temperature. At its peak, the flow stress is almost four times larger than its value at room temperature. This anomalous mechanical behavior of γ' phase is governed by a complex combination of underlying dislocation mechanisms. In the anomalous range (~below 1000 K) slip occurring on octahedral slip systems dominates the deformation process. Most of the dislocations in this temperature range are immobile screw dislocations that lock in a Kear-Wilsdorf (or KW) configuration [31]. A secondary mechanism that is responsible for this behavior is the activation of cube slip systems. Cube planes are not closely packed planes in fcc materials and activation of cube slip systems has been observed, especially at temperatures above the critical temperature of peak flow stress. Above this critical temperature, dislocations on cube planes are of both screw and edge dislocation type without any cross-slip. The major reason for the anomalous yielding behavior of Ni₃Al intermetallics is arguably the hardening caused by pinned segments of screw dislocations when they cross-slip from octahedral planes to the cube planes. While the anomalous behavior of the γ' phase has been developed in a recent paper [33], this paper will primarily focus on the temperature range $650 \degree C \le \theta \le 800 \degree C$ for which, dislocation glide on the primary octahedral plane is responsible for plastic deformation.

A signed dislocation density-based crystal plasticity model proposed in [34,35] is implemented to model rate-dependent plastic behavior. These models incorporate evolution of statistically stored (SSD) and geometrically necessary dislocations (GND) due to the plastic deformation. Plastic strain gradient at the $\gamma-\gamma'$ phase interface and grain boundaries lead to generation of GNDs. The micromechanical crystal plasticity model accommodates multiplication and annihilation of SSDs in the γ -channel and also accounts for APB shearing of γ' precipitates by matrix dislocations.

2.1. Dislocation density-based crystal plasticity model

Crystal deformation results from a combination of the elastic stretching and rotation of the crystal lattice and plastic slip on different slip systems. Large-strain kinematics is accommodated through a multiplicative decomposition of the total deformation gradient into an incompressible, inelastic component associated with pure slip, and an elastic component that accounts for elastic stretching and rigid-body rotations, expressed as:

$$\mathbf{F} = \mathbf{F}^{e} \mathbf{F}^{p}, \quad \text{s.t. det } \mathbf{F}^{e} > 1 \quad \text{and} \quad \text{det } \mathbf{F}^{p} = 1$$
 (1)

Evolution of plastic deformation is expressed in terms of the plastic velocity gradient, the plastic shear rate $\dot{\gamma}^{\alpha}$ on the slip system

 α , Schmid tensor $\mathbf{s}_0^{\alpha} \equiv \mathbf{m}_0^{\alpha} \otimes \mathbf{n}_0^{\alpha}$ (in terms of the slip direction \mathbf{m}_0^{α} and slip plane normal \mathbf{n}_0^{α} in the reference configuration) as:

$$\boldsymbol{L}^{p} = \dot{\boldsymbol{F}}^{p} \boldsymbol{F}^{-p} = \sum_{\alpha=1}^{N} \dot{\gamma}^{\alpha} \boldsymbol{m}_{0}^{\alpha} \otimes \boldsymbol{n}_{0}^{\alpha} = \sum_{\alpha=1}^{N} \dot{\gamma}^{\alpha} \boldsymbol{s}_{0}^{\alpha}$$
(2)

The stress-strain relation invokes the second Piola-Kirchhoff stress and its work-conjugate Lagrange-Green strain tensor in the intermediate configuration as:

$$\mathbf{S} = \det(\mathbf{F}^e)\mathbf{F}^{e-1}\boldsymbol{\sigma}\mathbf{F}^{e-T} = \mathbf{C}: \mathbf{E}^e, \quad \mathbf{E}^e \equiv \frac{1}{2}\{\mathbf{F}^{eT}\mathbf{F}^e - \mathbf{I}\}$$
(3)

I is the identity tensor, **C** is a fourth order anisotropic elasticity tensor and $\boldsymbol{\sigma}$ is the Cauchy stress tensor. The plastic shearing rate on a slip system α is expressed using the Orowan equation as $\dot{\gamma}^{\alpha} = \rho_{m}^{\alpha} b v^{\alpha}$, where ρ_{m}^{α} is the density of mobile dislocations, **b** is the Burgers vector and v^{α} is the velocity of dislocations that is a function of the applied shear stress τ^{α} , the passing stress τ_{pass}^{α} in the slip system and other slip system resistances, is written as:

$$v^{\alpha} = v_{\circ} \exp\left(-\frac{Q}{K_{\rm B}\theta}\right) \sinh\left(\frac{\left|\tau^{\alpha}\right| - \tau_{\rm pass}^{\alpha}}{\tau_{\rm cut}^{\alpha}}\right)^{p} \operatorname{sign}\left(\tau^{\alpha}\right) \tag{4}$$

The velocity of dislocations is a function of the applied shear stress, the passing stress in the slip system and other slip system resistances. Q is the activation energy barrier, $k_{\rm B}$ is the Boltzmann's constant and θ is the absolute temperature. Slip system resistances are represented in terms of the passing stress due to the interaction of mobile dislocations with other dislocations and their networks in the slip plane, and the cutting stress $\tau_{\rm cut}^{\alpha}$ due to the mobile dislocations cutting the forest dislocations with density $\rho_{\rm F}^{\alpha}$ perpendicular to the slip plane. The stresses are expressed in [29,30] as:

$$\tau_{\text{pass}}^{\alpha} = c_3 G b \sqrt{\rho_{\text{P}}^{\alpha} + \rho_{\text{m}}^{\alpha}}, \quad \tau_{\text{cut}}^{\alpha} = \frac{c_4 K_{\text{B}} \theta}{b^2} \sqrt{\rho_{\text{F}}^{\alpha}}$$
(5)

where c_3 and c_4 are material constants and *G* is the shear modulus. Contributions to the overall slip resistance are assumed to be due to both the density of immobile, statistically stored dislocations $\rho_{\text{SSD}}^{\alpha}$, and the vector field of geometrically necessary dislocation density $\rho_{\text{CND}}^{\alpha}$. The rate of evolution of statistically stored dislocation density $\dot{\rho}_{\text{SSD}}^{\alpha}$ has been identified in [35] as the net effect of components due to lock formation, dipole formation, athermal annihilation and thermal annihilation as:

$$\dot{\rho}_{\rm SSD}^{\alpha} = \dot{\rho}_{\rm SSD_{lf}}^{\alpha+} + \dot{\rho}_{\rm SSD_{df}}^{\alpha+} + \dot{\rho}_{\rm SSD_{aa}}^{\alpha-} + \dot{\rho}_{\rm SSD_{ta}}^{\alpha-} \tag{6}$$

Superscripts \pm correspond to multiplication and annihilation respectively. The rate increase due to lock formation, dipole formation, and decrease due to mechanisms of dislocation annihilation due to thermal and athermal annihilation are respectively given as [34]:

$$\dot{\rho}_{\text{SSD}_{\text{ff}}}^{\alpha} = \frac{c_5}{b} \sqrt{\rho_{\text{F}}^{\alpha}} \dot{\gamma}^{\alpha},$$

$$\dot{\rho}_{\text{SSD}_{\text{df}}}^{\alpha} = \frac{c_6}{b} \frac{\sqrt{3}Gb}{16\pi(1-\nu)} (|\tau^{\alpha}| - \tau_{\text{pass}}^{\alpha})^{-1} \rho_{\text{m}}^{\alpha} \dot{\gamma}^{\alpha},$$

$$\dot{\rho}_{\text{SSD}_{\text{aa}}}^{\alpha} = -c_7 \rho_{\text{SSD}}^{\alpha} \dot{\gamma}^{\alpha} \text{ and}$$

$$\dot{\rho}_{\text{SSD}_{\text{ta}}}^{\alpha} = -c_8 \frac{D_0 b^3}{k_B \theta} \exp\left(\frac{-Q_{\text{bulk}}}{k_B \theta}\right) (\rho_{\text{SSD}}^{\alpha})^2 |\tau^{\alpha}| \left(\frac{\dot{\gamma}^{\alpha}}{\dot{\gamma}_{\text{ref}}}\right)^{c_9}$$
(7)

where c_5 , c_6 , c_7 , c_8 and c_9 are material constants, D_0 is the diffusion co-efficient, Q_{bulk} is the activation energy for dislocation climb and $\dot{\gamma}_{\text{ref}}$ is a reference shear rate. Each of the contributing components in Eq. (7) are functions of the slip rate, forest dislocation density, density of statistically stored dislocations, component of applied shear stress and the absolute temperature. Thus, a general form is proposed as $\dot{\rho}_{SSD}^{\alpha} = \dot{\rho}_{SSD}^{\alpha}(\dot{\gamma}^{\alpha}, \rho_{SSD}^{\alpha}, \rho_{F}, \tau^{\alpha}, \theta)$. The vector GND density rates depend on the gradient of plastic strain, written in terms of Nye's dislocation tensor **A**. The three scalar components, viz. screw, edge and normal components of the GND density have been derived in (Ma et al., 2006). The material time derivative of the Nye's dislocation tensor is decomposed for individual slip systems,

i.e.
$$\dot{\mathbf{\Lambda}} = \left(\sum_{\alpha=1}^{N} \dot{\mathbf{\Lambda}}^{\alpha}\right)$$
 to derive the GND density components as:
 $\dot{\rho}_{\text{GNDs}}^{\alpha} = \frac{1}{b} [\nabla_{X} \times (\dot{\gamma}^{\alpha} F_{\text{P}}^{T} n^{\alpha})] . m^{\alpha},$
 $\rho_{\text{GNDet}}^{\alpha} = \frac{1}{b} [\nabla_{X} \times (\dot{\gamma}^{\alpha} F_{\text{P}}^{T} n^{\alpha})] . t^{\alpha},$
(8)
 $\dot{\rho}_{\text{GNDen}}^{\alpha} = \frac{1}{b} [\nabla_{X} \times (\dot{\gamma}^{\alpha} F_{\text{P}}^{T} n^{\alpha})] . n^{\alpha}$

where \mathbf{m}^{α} , \mathbf{n}^{α} and $\mathbf{t}^{\alpha} = (\mathbf{n}^{\alpha} \times \mathbf{m}^{\alpha})$ are unit vectors in the slip direction of the Burgers vector, normal to the slip plane α , and tangent to the edge dislocation direction respectively. Correspondingly, $\dot{\rho}_{GNDs}^{\alpha}$, $\dot{\rho}_{GNDet}^{\alpha}$ and $\dot{\rho}_{GNDen}^{\alpha}$ are the screw component and two edge components parallel to \mathbf{n}^{α} and \mathbf{t}^{α} respectively. ∇_{X} is the gradient operator in the material coordinate system. The forest and parallel dislocation densities are now written as functions of the SSDs and GNDs [34] with an interaction strength coefficient $\chi^{\alpha\beta}$ between different slip systems [37] as:

$$\rho_{\rm F}^{\alpha} = \sum_{\beta=1}^{N} \chi^{\alpha\beta} \begin{bmatrix} \rho_{\rm SSD}^{\beta} |\cos(\boldsymbol{n}^{\alpha}, \boldsymbol{t}^{\beta})| + \rho_{\rm GNDs}^{\beta} |\cos(\boldsymbol{n}^{\alpha}, \boldsymbol{m}^{\beta})| + \\ \rho_{\rm GNDet}^{\beta} |\cos(\boldsymbol{n}^{\alpha}, \boldsymbol{t}^{\beta})| + \rho_{\rm GNDe1}^{\beta} |\cos(\boldsymbol{n}^{\alpha}, \boldsymbol{n}^{\beta})| \end{bmatrix} c \qquad (9)$$

$$\rho_{\rm P}^{\alpha} = \sum_{\beta=1}^{N} \chi^{\alpha\beta} \begin{bmatrix} \rho_{\rm SSD}^{\beta} |\sin(\boldsymbol{n}^{\alpha}, \boldsymbol{t}^{\beta})| + \rho_{\rm GNDs}^{\beta} |\sin(\boldsymbol{n}^{\alpha}, \boldsymbol{m}^{\beta})| + \\ \rho_{\rm GNDet}^{\beta} |\sin(\boldsymbol{n}^{\alpha}, \boldsymbol{t}^{\beta})| + \rho_{\rm GNDe1}^{\beta} |\sin(\boldsymbol{n}^{\alpha}, \boldsymbol{n}^{\beta})| \end{bmatrix}$$

which evolve with the SSDs and GNDs due to plastic deformation and hardening mechanisms. The density of mobile dislocations is computed as a function of forest and parallel dislocation density and the temperature as [34]:

$$\rho_{\rm m}^{\alpha} = \frac{c_{10}k_{\rm B}\theta\sqrt{\rho_{\rm F}^{\alpha}\rho_{\rm P}^{\alpha}}}{{\rm Gb}^3} \tag{10}$$

2.2. Criteria for γ' phase anti-phase boundary shearing

Matrix dislocations in the disordered *fcc* matrix γ phase cannot enter the ordered γ' phase, characterized by crystalline lattice structure L_{1_2} , initially. However, the matrix dislocations can form super-dislocations at the $\gamma - \gamma'$ interface and enter the γ' phase through the mechanism of anti-phase boundary or APB shearing upon reaching a critical condition [6]. The γ' phase APB shearing is assumed to take place when the following conditions are met at the interface:

(i)
$$\tau^{\alpha} > \tau_{\rm c}$$
 and (ii) $\rho_{\rm m}^{\alpha} > \rho_{\rm c}$ (11)

The corresponding flow rule for the γ' phase is expressed as:

$$\dot{\gamma}^{\alpha} = \mathbf{H}(\rho_{\rm m}^{\alpha} - \rho_{\rm c})\rho_{\rm m}^{\alpha}bv^{\alpha} \text{ where}$$

$$v^{\alpha} = \lambda \upsilon \exp\left\{-\frac{Q}{K_{\rm B}T}\left(1 - \frac{\langle\tau^{\alpha} - \tau_{\rm pass}^{\alpha}\rangle\mathbf{H}(\tau^{\alpha} - \tau_{\rm c})}{\tau_{\rm cut}^{\alpha}}\right)\right\} \operatorname{sgn}(\tau^{\alpha})$$
(12)

where $\mathbf{H}(\rho_m^{\alpha} - \rho_c)$ and $\mathbf{H}(\tau^{\alpha} - \tau_c)$ are Heaviside functions, τ_c is the critical resolved shear stress and ρ_c is the critical density at the interface.

Table 1

Stiffness for the sub-grain model.

Phase	$C_{11} = C_{22} = C_{33}$	$C_{44} = C_{55} = C_{66}$	$C_{12} = C_{13} = C_{23}$
$\gamma \\ \gamma'$	201.7 GPa	104.5 GPa	134.4 GPa
	229.7 GPa	110.1 GPa	153.2 GPa



Fig. 2. Comparing CPFEM results with those for tension experiments under a constant strain rate 0.0001 s^{-1} with FEM model for cubic precipitates with the volume fraction of 70% and edge length 0.5 μ m.: volume-averaged Cauchy stress-true (log-arithmic) strain response.

2.3. Calibration and validation of constitutive model

Selected constitutive parameters in the crystal plasticity model with APB shearing have been calibrated with experimental data for the alloy CMSX-4 in [29,30]. Constants c_1 and c_2 in Eq. (5) and constants c_3 , c_4 , c_5 , c_6 and c_7 in Eq. (7) are calibrated using experimental data from tensile constant strain-rate tests in [37]. The critical shear stress τ_c and the threshold dislocation density ρ_c in Eq. (11) are calibrated from the tension creep experimental data in [38]. These are:

$$c_1 = 1.7 \times 10^{10}, \quad c_2 = 3.77, \quad c_3 = 4, \, c_4 = 100$$

 $c_5 = 1.0 \times 10^{-3}, \quad c_6 = 1.0 \times 10^{-4}, \quad c_7 = c_8 = 100$
 $c_9 = 100, \, c_{10} = 25, \quad p = 0.5.$

The elastic stiffness tensor $C_{\alpha\beta} = C_{\beta\alpha}(\alpha = 1, ..., 6, \beta = 1, ..., 6)$ is considered to be isotropic for both phases, for which the non-zero components at 800 °C are obtained from [39] as shown in Table 1.

In addition, b = 2.49 nm and $Q = 6.5 \times 10^{-19}$ J are handbook values.

To validate the crystal plasticity constitutive relations with APB shearing, the CPFEM analyses results have been compared in [29,30] with experimental data from [37,38]. The RVE is for a regular array of cubic precipitates with a 70% volume fraction, as shown in Fig. 2(a). Its dimensions are $0.5 \,\mu\text{m} \times 0.5 \,\mu\text{m} \times 0.5 \,\mu\text{m}$. The edge length of cubic γ' particles, allocated symmetrically at the eight corners, is 0.45 µm. The CPFE model of the microstructural RVE is discretized into 2200, 8-noded brick elements using selective reduced integration. CPFEM simulations are conducted with an applied strain-rate of $0.001 \, \text{s}^{-1}$ in the y-direction at $800 \,^{\circ}\text{C}$. A tensile constant strain-rate is applied to the top y-surface in Fig. 2 (inset), while rigid body modes are suppressed by applying boundary conditions on the bottom y-surface as: $u_y = 0$ on all nodes $u_x = 0$ on nodes on the line $x = 0.25 \,\mu\text{m}$ and $u_z = 0$ on nodes on the line z = 0.25 μ m. The volume-averaged Cauchy stresses $\bar{\sigma}$ = $\frac{1}{\Omega_{\rm RVE}} \int_{\Omega_{\rm RVE}} \sigma(x, t) dV$ over the RVE $\Omega_{\rm RVE}$ and the averaged true (logarithmic) strain expressed as: $\bar{\boldsymbol{\varepsilon}} = \ln(\boldsymbol{l}_y/\boldsymbol{l}_{0y}) = \ln(\boldsymbol{l}_{0y} + \bar{\boldsymbol{u}}_y/\boldsymbol{l}_{0y})$ are



Fig. 3. Effect of APB shearing for RVE with cubic γ' precipitates: mobile dislocation density evolution within γ channels and through γ' precipitates.

computed for the RVE where l_{0y} and \bar{u}_y are respectively the initial dimension and the *y*-direction displacement of the top surface of the RVE. The volume-averaged stress–strain response is compared with experimental data from [38] in Fig. 2. There is a good agreement between the experimental and model predictions.

A host of other simulations have been conducted in [29,34] to validate the sub-grain CP model as well as to explore the effect of variations in the microstructural morphology.

2.4. Effect of APB shearing and precipitate shape on overall response

The volume-averaged stress-strain response by dislocation density-based CPFEM simulations for the RVE in the previous section, with and without the activation of APB shearing of γ' precipitates is studied [30]. In the absence of the γ' phase, the overall yield strength, as well the hardening is considerably low. The stress-strain response is rather stiff if the APB shearing mechanism is not activated in the high volume fraction (~70%) γ' phase that has zero initial dislocation density. Accumulation of dislocation density at the $\gamma-\gamma'$ phase interface with high stresses leads to APB shearing, with super-dislocations entering the γ' -phase and softening the overall response. Accurate representation of the stress-strain response requires incorporation of APB shearing criteria and associated relations for γ' -phase plastic flow.

Three different stages of deformation are identified in the stress-strain response [30]. During initial deformation (state 1), both phases behave elastically and there is no plastic deformation in the domain. From the end of state 1 to the onset of volumetric yielding (state 2), the γ -phase experiences plastic deformation and SSDs start to evolve, with a plastic strain gradient building especially near the $\gamma - \gamma'$ interfaces. To preserve lattice continuity, the GNDs must evolve causing an increase in mobile dislocation density. The distribution of ρ_m along the *x*-axis at state 2 reveals little difference in $\rho_{\rm m}$ for states 1 and 2 in the γ' phase. However, this difference is significant in the γ – channel due to the evolution of GNDs. In the post APB shearing stage, the γ' -phase experiences plastic deformation with considerable rise in $\rho_{\rm m}$. At state 2, corresponding to the activation of APB shearing, the initial value of ρ_m does not change in the γ' phase. Beyond this state, $ho_{\rm m}$ starts to evolve and reaches the distribution in Fig. 3 at 5% strain.

3. Grain-scale crystal plasticity model

3.1. Homogenized activation energy-based crystal Plasticity (AE-CP) model

Results of simulation of the sub-grain RVE model, discussed in Section 2, are homogenized to generate constitutive parameters for a grain-scale activation energy-based crystal plasticity (AE-CP) model. Determination of parameters is assumed to be governed by the Hill-Mandel principle of macro-homogeneity [39] expressed as:

$$\langle \sigma \rangle : \langle \boldsymbol{D} \rangle = \frac{1}{\Omega_{\text{RVE}}} \int_{\Omega_{\text{RVE}}} \sigma dV : \frac{1}{\Omega_{\text{RVE}}} \int_{\Omega_{\text{RVE}}}$$
$$\boldsymbol{D} dV = \frac{1}{\Omega_{\text{RVE}}} \int_{\Omega_{\text{RVE}}} \sigma : \boldsymbol{D} dV = \langle \sigma : \boldsymbol{D} \rangle$$
(13)

Here σ and **D** correspond to the Cauchy stress and the rate of deformation tensors respectively and the symbol $\langle \cdot \rangle$ corresponds to volume averaging over the RVE domain. The constitutive parameters are formulated in terms of morphological variables and are calibrated by computational homogenization. The proposed grain-scale, homogenized crystal plasticity model for Ni-based superalloys follows the framework of activation energy-based crystal plasticity (AE-CP) models [22,40,41]. The homogenized constitutive model incorporates an evolving thermal shear resistance as well as an athermal shear resistance due to plastic deformation. For a slip system α , the plastic shearing rate follows from the Orowan equation as:

$$\dot{\gamma}^{\alpha} = \begin{cases} 0 & \text{if } \tau^{\alpha}_{\text{eff}} \leq 0 \\ \dot{\gamma}^{\alpha}_{*} \exp\left\{-\frac{Q}{k_{\text{B}}\theta}\left(1 - \left[\frac{|\tau^{\alpha}_{\text{eff}}|}{s^{\alpha}_{*}}\right]^{p}\right)^{q}\right\} \text{sgn}(\tau^{\alpha}) & \text{if } 0 \leq \tau^{\alpha}_{\text{eff}} \leq s^{\alpha}_{*} \end{cases}$$

$$(14)$$

Q is the activation energy Here barrier. $k_{\rm B}$ (= 1.3807 × 10⁻²³ JK⁻¹) is the Boltzmann's constant, θ is the temperature and exponents p, q are material constants. For the slip system α , $\dot{\gamma}_*^{\alpha}$ is a reference strain-rate, $\tau_{\text{eff}}^{\alpha}(=|\tau^{\alpha}|-s_a^{\alpha})$ is the effective resolved shear stress. The temperature-dependent critical slip resistance $s^{\alpha}(>0)$ is assumed to be comprised of a thermally activated obstacle to slip s_*^{α} and a part due to the athermal obstacles s_a^{α} . The athermal and thermal shear resistances s_a^{α} and s_*^{α} correspond to the passing and cutting stress barriers respectively. The difference between the athermal shear resistance and the resolved shear stress is the driving force for dislocation motion on the slip system α . $\dot{\gamma}^{\alpha}_{*}$ can evolve with the activation of APB shearing, when the γ -phase experiences plastic deformation with increasing dislocation density, especially near the $\gamma - \gamma'$ interfaces. This deformation effect can be significant for some γ' precipitate shapes, e.g. spherical, but not as strong for cuboidal. A yield point phenomenon is applied to introduce a morphology dependent functional form for $\dot{\gamma}^{\alpha}_{*}$ [29,30] as:

$$\dot{\gamma}_{*} = H(\bar{\varepsilon}_{\rm p} - l_{\rm p}) \dot{\gamma}_{0} \left\{ \frac{\tanh(k) + \tanh(kl_{\rm p})}{10 \{\tanh[k_{*}(\bar{\varepsilon}_{\rm p} - l_{\rm p})] + \tanh(kl_{\rm p})\}} - 1 \right\} + \dot{\gamma}_{0}$$
(15)

where *H* is the Heaviside step function, $\dot{\gamma}_0$ corresponds to the initial strain rate and $l_{\rm p}$, *k*, *k*_{*} are material constants. In this work $l_{\rm p} = 10^{-4}$ and *k* and *k*_{*} are derived in terms of morphological parameters. The equivalent plastic strain $\bar{\varepsilon}_{\rm p} \left(=\sqrt{\frac{2}{3}}\varepsilon_{ij}^p\varepsilon_{ij}^p\right)$ is defined in terms of the Lagrangian plastic strain $\varepsilon_{ij}^p = \frac{1}{2}(F_{ij}^{pT}F_{ij}^p - \delta_{ij})$. Consequently, evolution laws for thermal and athermal shear resistances, contributing

to the overall slip resistance s^{α} , are proposed in terms of the plastic strain rate. The thermal shear resistance, accounting for forest dislocations normal to the slip plane and the athermal shear resistance reflecting the effect of parallel dislocations in the slip direction m^{α} , are expressed as:

$$\dot{s}_{a}^{\alpha} = \sum_{\substack{\beta=1\\\beta=1}}^{n} h_{a}^{\alpha\beta} \left| \dot{\gamma}^{\beta} \sin(\mathbf{n}^{\alpha}, \mathbf{t}^{\beta}) \right|,$$

$$\dot{s}_{*}^{\alpha} = \sum_{\substack{\beta=1\\\beta=1}}^{n} h_{*}^{\alpha\beta} \left| \dot{\gamma}^{\beta} \cos(\mathbf{n}^{\alpha}, \mathbf{t}^{\beta}) \right|$$
(16)

where \mathbf{n}^{α} is slip-plane normal, $\mathbf{t}^{\alpha} = \mathbf{m}^{\alpha} \times \mathbf{n}^{\alpha}$, and the total shear resistance is $\dot{s}^{\alpha} = \sqrt{(\dot{s}^{\alpha}_{a})^{2} + (\dot{s}^{\alpha}_{*})^{2}}$. The initial values of the athermal and thermal shear resistances are respectively s^{α}_{a0} , s^{α}_{*0} . For convenience, coefficients accounting for the interactions between slip systems are taken to be the same i.e. $h^{\alpha\beta}_{a} = h^{\alpha\beta}_{*} = h^{\alpha\beta}$. Each component of $h^{\alpha\beta}$ is the deformation resistance on slip system α due to shearing on slip system β . It describes both self and latent hardening as:

$$h^{\alpha\beta} = q^{\alpha\beta}h^{\beta}, \quad \text{where}$$
$$h^{\beta} = \left[h_0 \left(1 - \frac{s^{\beta}}{s_{\text{sat}}^{\beta}}\right)^r\right] \text{sign} \left(1 - \frac{s^{\beta}}{s_{\text{sat}}^{\beta}}\right)$$
(17)

The parameter h^{β} denotes the resistance dependent selfhardening rate, s_{sat}^{β} is the saturation value of reference shear stress and r is a constant exponent. The coefficient is given as $q^{\alpha\beta} = q + (1-q)\delta^{\alpha\beta}$, where q is a latent-hardening parameter chosen as 1.4.

3.2. Sub-grain morphological parameters

Three characteristic parameters representing the sub-grain microstructural morphology in Fig. 1, are delineated as: (i) γ' volume fraction v_p , (ii) γ' shape factor n and, (iii) minimum limiting channel-width l_c between γ' precipitates. The volume fraction is expressed as the ratio of the γ' precipitate volume to the RVE volume, i.e. $v_p = \Omega_{\gamma'} / \Omega_{RVE}$. The shape factor is described in terms of the exponent of a generalized ellipsoid: $\left(\frac{x}{a}\right)^n + \left(\frac{y}{b}\right)^n + \left(\frac{z}{c}\right)^n = 1$, where a, b and c are the dimensions of the three principal axes and n is shape exponent. Here a = b = c is assumed to represent equiaxed precipitates. A value n = 2 corresponds to a sphere while $n \to \infty$ corresponds to a cube. To avoid a singular value of n a transformed shape factor $n_1 = \tan^{-1}(n)$ is used in the parameterization.

The effect of these morphological parameters on the volumeaveraged stress–strain response of the RVE using the sub-grain dislocation density CPFE simulations has been examined kin [29]. For each simulation conducted at $0.0001 \, \text{s}^{-1}$ and $800 \,^\circ\text{C}$, one of the parameters is varied, while the other two are held constant. Variables considered are (i) cubic precipitates of volume fractions 75.13% and 57.87%, (ii) shape factors n = 2.0 and ∞ , and (iii) channel-width $l_c = 0.29 \,\mu\text{m}$ and $l_c = 0.29 \,\mu\text{m}$ for cubic precipitates of 29.63% volume fraction. Results have shown that with increasing volume fraction, the post-yield plastic response does not change too much even though the yield strength increases. The yield strength changes and the plastic response diverges with increasing strain for different shapes. The plastic response changes with increasing channel-width, while the yield strength decreases only slightly.

Plastic slip and hardening parameters in the grain-scale AE-CP model are functions of the SSDs and GNDs. SSDs do not generally change much with morphological variables i.e. they are size independent, but GNDs can vary significantly with precipitate shape and size. Forest and parallel components of dislocation densities may be expressed as:

$$\rho_{\rm F}(\rho_{\rm SSD}, \rho_{\rm GND}) = \rho_{\rm F}(\gamma^{\alpha}, \nabla \gamma^{\alpha}), \quad \rho_{\rm P}(\rho_{\rm SSD}, \rho_{\rm GND}) = \rho_{\rm P}(\gamma^{\alpha}, \nabla \gamma^{\alpha})$$
(18)

Crystal plasticity hardening parameters are functions of the plastic slip γ^{α} due to SSD's. Morphological parameters should also be incorporated in these functions to account for the effect of GNDs or gradient of plastic shear strain. Sensitivity analyses indicate that the initial thermal shear resistance and its rate, the reference slip-rate $\dot{\gamma}_*$ and the saturation shear stress s_{aar}^{α} are functions of the morphology. In Eqs. (19)–(21) parameters are derived in terms of morphological parameters as well as ($\gamma^{\alpha}, \nabla \gamma^{\alpha}$) as:

$$\begin{split} \dot{s}_{*}^{\alpha}(n_{1},\nu_{p},l_{c}) &= \sum_{\beta=1}^{n} h^{\alpha\beta}(n_{1},\nu_{p},l_{c}) \left| \dot{\gamma}^{\beta} \cos(n^{\alpha},t^{\beta}) \right| \\ &= \sum_{\beta=1}^{n} \left[h_{0} \left(1 - \frac{s^{\beta}}{s_{sat}^{\beta}(n_{1},\nu_{p},l_{c})} \right)^{r} \right] sgn(1 - \frac{s^{\beta}}{s_{sat}^{\beta}}) \left| \dot{\gamma}^{\beta} \cos(n^{\alpha},t^{\beta}) \right| \quad (a) \\ \dot{\gamma}_{*}(n_{1},\nu_{p},l_{c}) &= H(\bar{\varepsilon}_{p} - l_{p}) \dot{\gamma}_{0} \\ &\times \left\{ \frac{\tanh[k(n_{1},\nu_{p},l_{c})] + \tanh[k(n_{1},\nu_{p},l_{c})l_{p}]}{10\{\tanh[k_{*}(n_{1},\nu_{p},l_{c})(\bar{\varepsilon}_{p} - l_{p})] + \tanh[k(n_{1},\nu_{p},l_{c})l_{p}]\}} - 1 \right\} \\ &+ \dot{\gamma}_{0} \quad (b) \end{split}$$

The initial strain rate $\dot{\gamma}_0$ and hardening parameter h_0 are insensitive to the morphology.

3.3. Calibrating the grain scale AE-CP model parameters

Eqs. (14)–(17) and (19) contain a number of material parameters, some of which vary with the morphology while others are independently constant. The constant material parameters that should be experimentally calibrated for the AE-CP model are the activation energy Q and exponents p, q in Eq. (14), $\dot{\gamma}_0$ in Eq. (15) and hardening parameter h_0 and exponent r in Eq. (16). These parameters have been calibrated in [29,30] for single crystal CMSX-4 using experimental data from tensile constant strain-rate and creep tests in [38,39]. The parameters are $Q(J) = 6.5 \times 10^{-1}$, p = 0.7, q = 1;15, $h_0 = 1300$, r = 1.115, $\dot{\gamma}_0(s^{-1}) = 5 \times 10^{-1}$ 10⁷. Subsequently, the morphology-dependent AE-CP parameters $s_{*0}^{\alpha}(n_1, \nu_p, l_c), \quad k_*(n_1, \nu_p, l_c), \quad k(n_1, \nu_p, l_c) \text{ and } s_{sat}^{\beta}(n_1, \nu_p, l_c) \text{ in Eq.}$ (19) are calibrated from the simulated volume-averaged response of the sub-grain RVE model. These simulations are conducted under a constant strain-rate of 0.0001 s⁻¹ in the [010] direction at 800 °C. The calibration process has involved 37 different RVE microstructures. The homogenized AE-CP model parameters are calibrated with the averaged stress-strain responses from the RVE model.

3.4. Functional forms of homogenized AE-CP constitutive parameters

Functional forms of the constitutive parameters $s_{*0}^{\alpha}(n_1, v_p, l_c)$, $k_*(n_1, v_p, l_c)$, $k(n_1, v_p, l_c)$ and $s_{sat}^{\beta}(n_1, v_p, l_c)$ in Eq. (19) are generated for representing the effect of morphology on the single crystal behavior. The functional forms have been derived by computational homogenization involving a large number of sub-grain RVE model simulations with varying volume fractions, channel-widths and shapes. In this process the homogenized material (e.g. stress–strain) behavior of the polycrystalline ensemble is first derived from the energy-equivalence in the

Hill-Mandel condition. The AE-CP model is then mapped on the homogenized constitutive behavior, for which specific constitutive variables and their evolutions are computed. Sensitivity analyses are conducted by varying each morphological parameter to assess functional dependencies. Following the establishment of the functional forms, coefficients are determined by solving a set of least square minimization problems [30,31]. They are expressed as:

$$s_{*0}^{\alpha}(n_{1}, v_{p}, l_{c}) = a_{1}(n_{1}, v_{p}) + \frac{b_{1}(n_{1}, v_{p})}{\sqrt{l_{c}}}$$

= 1039 + 559v_{p} - 99n_{1} - 136v_{p}n_{1}
+ \frac{-0.1 + 89v_{p} + 53n_{1} - 90v_{p}n_{1}}{\sqrt{l_{c}}} (20)

$$s_{\text{sat}}^{\alpha}(n_1, \nu_p, l_c) = a_2(n_1, \nu_p) + \frac{b_2(n_1, \nu_p)}{l_c}$$

= 3185 - 8905\nu_p - 1648n_1 + 6680\nu_p n_1
+ $\frac{-0.21 + 5008\nu_p + 363n_1 - 3599\nu_p n_1}{l_c}$ (21)

$$k_{*}(n_{1}, \nu_{p}, l_{c}) = 65 - 7500\nu_{p} + 33n_{1} - 2700l_{c} + 12768\nu_{p}n_{1} - 23120\nu_{p}l_{c} + 4080n_{1}l_{c} - 19847\nu_{p}n_{1}l_{c}$$
(22)

$$k(n_1, v_p, l_c) = a_3(n_1, v_p) + \frac{b_3(n_1, v_p)}{\sqrt{l_c}}$$

= 5.5 - 327.6v_p + 31.5n_1 + 221.4v_pn_1
+ $\frac{0.14 + 281.2v_p - 2.44n_1 - 176.5v_pn_1}{\sqrt{l_c}}$ (23)

The explicit dependence on channel-width l_c reflects the sizeeffect due to the presence of GNDs in the sub-grain dislocation density CP model. In Eqs. (20)–(23) the unit of l_c is μ m, while the units of initial thermal resistance and saturation shear resistance in Eqs. (20) and (21) are MPa.

3.5. Verification and validation of the homogenized AE-CP model

Two sets of verification and validation tests are conducted for the homogenized AE-CP constitutive model. In the first verification set, the results of a single grain, crystal plasticity FEM analysis with the calibrated homogenized AE-CP constitutive model are compared with the averaged response of a sub-grain RVE (SG-RVE) analysis. Three cases, corresponding to different microstructures, are considered for simulation. These are:

<u>Case 1</u> : $n = 10$,	$v_{\rm p} = 44\%$,	$l_{\rm c} = 0.135 \mu{\rm m};$
<u>Case 2</u> : $n = 1.5$,	$v_{\rm p} = 22\%,$	$l_{\rm c} = 0.260\mu{\rm m};$
<u>Case 3</u> : $n = \infty$,	$v_{\rm p} = 30\%$,	$l_{\rm c} = 0.576\mu{\rm m}$

Simulations for both the AE-CP and SG-RVE FE models were conducted for an applied strain-rate of $0.0001 \, \text{s}^{-1}$ in the *y*-direction at 800 °C. Excellent agreement is obtained has been seen between the homogenized grain-scale AE-CPFE model with morphological parameters and the explicit sub-grain RVE model. A notable advantage of the homogenized model is the significant efficiency gain over explicit RVE models. For this example, the gain in efficiency is of the order of 10^4 (few seconds for AE-CPFE model) with identical response.



Fig. 4. Reconstructing virtual microstructure of polycrystalline René-88 DT: (a) 3D EBSD data, (b) filtering fine scale features, (c and d) erosion, dilation, edge refinement (e and f) boundary smoothing process, and (g and h) transformation of the EBSD to a FE mesh.

The second example conducted in [30] involved validating the AE-CP constitutive model with results from creep experiments in [44] for single crystal CMSX-4 with 70% volume fraction of γ' precipitates for two tensile loads of 650 and 770 MPa in the [001] direction at 750 °C. CPFEM analyses with the homogenized parameters are conducted for a single grain under these conditions. The simulated logarithmic strain-time response by the simulations has been compared with the experimental results in [29] with good agreement.

Single crystal experiments on Ni-based superalloys also show considerable tension-compression asymmetry. Large difference in the creep response for single crystals loaded in the [001] and [011] directions under tension and compression conditions has been reported in [37,38]. APB shearing is responsible for the difference in tension and compression tests in the [001] direction. Transmission electron microscopy observations in [9] have reported micro-twinning mechanism for high temperature creep deformation. To account for this asymmetry, a micro-twinning model has been incorporated in the grain-scale crystal plasticity formulation, as described in [29,30]. The crystal plasticity FE model satisfactorily predicts single crystal experimental data, including micro-twin induced tension-compression asymmetry.

4. AE-CP model for polycrystalline microstructures

Polycrystalline microstructures of Ni-based superalloys are modeled using the homogenized AE-CP model with parametric representation of the $\gamma - \gamma'$ microstructure, together with micro-twin evolution models. For modeling polycrystalline microstructures however, the AE-CP model should be modified to account for grain boundary lattice incompatibility. Hardening laws, accounting for GNDs, have been proposed to address lattice incompatibility in [44] using the Nye tensor along the slip plane normal. In the present study, the dislocation density-based slip relations have been extended to take into account lattice incompatibility. The hardening parameters in Eq. (16) are augmented to account for lattice deformation incompatibility at grain boundaries due to plastic strain gradients leading to dislocation pileup. The athermal and thermal shear resistances in Eq. (16) are each divided into two parts, corresponding to SSDs and GNDs as:

$$s_a^{\alpha} = s_{a,\text{SSD}}^{\alpha} + s_{a,\text{GND}}^{\alpha}, s_*^{\alpha} = s_{*,\text{SSD}}^{\alpha} + s_{*,\text{GND}}^{\alpha}$$
(25)

where

$$s_{a,\text{GND}}^{\alpha} = \bar{c}_1 G b \sqrt{\rho_{\text{GP}}^{\alpha}}, s_{*,\text{GND}}^{\alpha} = \frac{Q}{\bar{c}_2 b^2} \sqrt{\rho_{\text{GF}}^{\alpha}}$$
(26)



Fig. 5. Virtual polycrystalline microstructural FE models of René-88 DT including twins: (a) generated by direct implementation, (b) generated by equivalence of statistical data and (c) stress-strain response from simulations of the DI and SEM generated microstructures with and without twins.

These relations are consistent with those in the sub-grain scale model in Eq. (5), where the cutting and passing shear resistances are expressed as functions of parallel and forest dislocation densities. In Eq. (26) \bar{c}_1 and \bar{c}_2 are material constants, and ρ_{GP}^{α} , ρ_{GF}^{α} are parallel and forest dislocation densities resulting from GNDs corresponding to Eq. (9). They may be written as:

$$\rho_{\rm GP}^{\alpha} = \sum_{\beta=1}^{N} \chi^{\alpha\beta} \left\{ \begin{array}{l} \rho_{\rm GNDs}^{\beta} |\sin(\boldsymbol{n}^{\alpha}, \boldsymbol{m}^{\beta})| + \rho_{\rm GNDet}^{\beta} |\sin(\boldsymbol{n}^{\alpha}, \boldsymbol{t}^{\beta})| + \\ \rho_{\rm GNDen}^{\beta} |\sin(\boldsymbol{n}^{\alpha}, \boldsymbol{n}^{\beta})| \end{array} \right\}$$

$$\rho_{\rm GF}^{\alpha} = \sum_{\beta=1}^{N} \chi^{\alpha\beta} \left\{ \begin{array}{l} \rho_{\rm GNDs}^{\beta} |\cos(\boldsymbol{n}^{\alpha}, \boldsymbol{m}^{\beta})| + \rho_{\rm GNDet}^{\beta} |\cos(\boldsymbol{n}^{\alpha}, \boldsymbol{t}^{\beta})| + \\ \rho_{\rm GNDen}^{\beta} |\cos(\boldsymbol{n}^{\alpha}, \boldsymbol{n}^{\beta})| \end{array} \right\}$$
(27)

where $\chi^{\alpha\beta}$ is the interaction strength coefficient and ρ_{GNDs} , ρ_{GNDet} , ρ_{GNDen} are the screw and two edge components of the GND densities respectively. Implementation of GND based hardness in the polycrystalline AE-CP model is discussed in [31].

4.1. 3D virtual polycrystalline microstructure simulation and mesh generation

Virtual polycrystalline microstructures are generated using methods and codes described in [45–47], by matching morphological and crystallographic statistics obtained from electron backscattered diffraction (or EBSD) data of microstructural sections provided by Pollock [48]. The virtual microstructures are subsequently used in the image-based CPFE models of the superalloy



Fig. 6. Stress states during various stages of uniaxial loading: (a) volumetric stress–strain response, (b) stress field in the deformed microstructure at 10% total strain, and (c) spatial distributions of the stress field at four different strain levels.

René-88 DT, dominated by annealing Σ 3 twin boundaries with a specific 60° misorientation angle about <111> directions [49]. The annealing twins that develop during material processing have large aspect ratios as shown in Fig. 4(a). The geometric disparity of these twins requires mesh localization at these areas relative to the remainder of the polycrystalline structure. In resolving the twin bands and maintaining a large sample size, the voxelized 3D reconstruction often contains flaws like disconnected defects or hooked features near grain boundaries, due to experimental resolution. The flaws are eliminated through filtration and smoothing techniques illustrated in Fig. 4.

Two methods are pursued for developing virtual images and finite element models of the actual microstructures. They are termed as (i) direct implementation (DI) method and (ii) statistically equivalent microstructure (SEM) generation method. The DI method uses the commercial code Simmetrix [50] to directly implement the actual microstructure derived from EBSD and serial sectioning-based reconstruction in the FE model. The structural data is filtered with minimal data treatment and a significant percentage of annealing twins is preserved in this method. The primary steps in transforming a voxel dataset into a finite element mesh include volume thresholding, erosion, dilation, edge refinement, boundary smoothing, vertex repositioning, and curvature refined meshing. The steps and the final polycrystalline FE model are shown sequentially in Fig. 4. The SEM method uses the code DREAM.3D [51] to generate statistically equivalent "synthetic representation" of the microstructure, based on statistical features of the 3D microstructure. The primary structural and crystallographic



Fig. 7. Analysis of a cross section normal to the loading direction at 4% total strain: (a) identification of twin boundaries, (b) variation of von Mises stress and (c) equivalent plastic strain over several grain boundaries.

characteristics such as grain size, number of neighboring grains, orientation, and misorientation are matched to the corresponding statistical distributions of the data. Fig. 5(a and b) shows the polycrystalline microstructure containing annealing twin generated by the two methods. Fig. 5(a) by the DI method contains 206 grains that are discretized into 180,203 linear tetrahedral elements with 99,975 degrees of freedom. Fig. 5(b) by the SEM method on the other hand, has 197 grains discretized into 138,290 tetrahedral elements having 75,468 degrees of freedom.

4.2. Polycrystalline microstructure simulation

The virtual polycrystalline microstructures developed by the DI method (Simmetrix/Actual) and SEM method (DREAM.3D/Synthetic) are prepared for crystal plasticity finite element simulations using the grain-scale AE-CP constitutive models. Results of a constant strain-rate tension test simulation for different microstructures, for various sub-grain morphological conditions are shown in the figures next. The competing activation of microstructural mechanisms controls the overall elastic-plastic response of the polycrystalline material. Local variations in stress and plastic strain are observed to be highly dependent on the grain structure and concentrate near twin bands, where favorably oriented grains reside.

The stress-strain response of the virtual polycrystalline microstructures generated by the DI and SEM methods (Fig. 6(a) and (b)) are compared in Fig. 5(c). The results for both microstructures show good agreement, which reveals that the



(a)



Fig. 8. Comparison of the stress response in virtual microstructures; (a) spatial distribution of stress and (b) contour plots in microstructures with and without annealing twins.

effects of morphology and crystallography can be captured by the statistics of EBSD scans. Implementation of statistically equivalent microstructures can reduce the effort required for material characterization and mechanical experiments. Fig. 5(c) also shows the response without considering annealing twins. Removal of twins reduces the elastic modulus of the superalloy as well as softens the material in the plastic region. This reduction of strength is solely due to the variation of microstructural features. The complex twinned structure creates a large degree of heterogeneity in the response fields of the material that cannot be captured by a volume-averaged measure.

Local stress variations are quantified by observing the spatial distribution over the entire polycrystalline domain. Fig. 6 shows the stress states in a DI method-based microstructure containing twins, with increasing strain. Fig. 6(c) shows the probability distribution of the stresses with increasing strain, illustrating the probability of observing a given stress state at any location in the volume. During elastic deformation, the stress distribution remains relatively uniform, while the spatial average quickly escalates to the yield strength. As strain increases further, the onset of plastic flow causes

a stagnation in the mean stress evolution while inducing a drastic redistribution of the remaining field. This redistribution of stresses indicates an increased likelihood of a localized events and large extremums, both in tension and compression.

Twin boundaries plays an important role in the mechanical response of the superalloy. Each grain boundary for a particular cross section of the microstructure is categorized, as shown in Fig. 7(a), to observe correlations between orientation and variations of local fields. Σ 3 twin boundaries are detected by measuring the misorientation angle and rotation axis between neighboring grains. The stress state oscillates significantly across the microstructure with a period corresponding to the geometry of the twins. Due to high aspect ratios, the twinned regions create large changes in stress, on the order of 500 MPa, over relatively small length scales (1-10 µm). This creates steep gradients at each shift in orientation. The local plastic strain also undergoes an oscillatory behavior throughout the twin structure. In this case, the peaks occur at the boundaries and vary within each individual grain. Furthermore, the triple junction composed of various grain boundary characters (a combination of boundaries 1, 2, and 3 in Fig. 7(a) promotes the



Fig. 9. Comparison for microstructures having varying sub-grain morphology: (a) depiction of the graded γ' volume fraction field, (b) increasing volume fraction path on a cross section normal to loading, (c) equivalent plastic strain along cross section, and (d) relative difference in plastic strain between graded and constant volume fraction microstructures.

largest accumulation of plasticity and is an active site for dislocation aggregation.

4.2.1. Effect of annealing twins on stress fields

The overall effect of annealing twins is assessed by comparing results of the DI method based polycrystalline microstructure (actual) to that with twins removed. A 15 degree tolerance is applied to the misorientation angle and rotation axis between grains to determine whether a twin boundary is present. Once identified, the twins are removed from the parent grains. The resultant microstructure is loaded in uniaxial tension. This removal of complex twins produces a significant reduction in the variance of the stress field. The spatial distributions, shown in Fig. 8(a), demonstrate a notable increase in the upper and lower bounds in the stress for the twinned microstructure indicating many regions of localization caused by the existence of twins. At 10% total strain, $\sigma_{zz} = 1550 \pm 3000$ MPa and $\sigma_{zz} = 1420 \pm 1850$ MPa with annealing twins and without twins, respectively. The bounds contain 99% of the stress field.

4.2.2. Effect of varying sub-grain morphology

In this example, the effect of varying constitutive response at the scale of the polycrystalline microstructures due to local variation in sub-grain morphology, is studied. A microstructure with sub-grain morphology is shown in Fig. 9(a). The volume fraction of the γ' phase is graded through the material in one direction, ranging from 25% to 70%. The equivalent plastic strain is computed along a line through a cross section of the microstructure and compared to the same polycrystalline structure with a uniform γ' volume fraction of 42%. At the locations where the graded material has lower volume

fraction, plastic strain becomes 10–15% higher due to a reduction in hardening from the depletion of the precipitate phase. On the other end of the microstructure where the volume fraction of the graded material is larger than 42%, the opposite effect is observed. The γ' phase strengthens the grains and resists plastic yielding. The capability of the model to account for the influence of the lower scale precipitate structure allows for great freedom in the design process of superalloys. A structural component can be functionally graded to optimize performance and design objectives, and the model can guide the manufacturing targets while minimizing needs for costly mechanical experiments.

5. Summary and conclusions

This paper uses a homogenized grain-scale crystal plasticity model for modeling polycrystalline microstructures of Ni-based superalloys. An activation energy-based crystal plasticity (AE-CP) FEM model is developed incorporating characteristic parameters of the sub-grain scale $\gamma - \gamma'$ morphology. Hardening evolution laws are developed to reflect the effect of dislocation density distributions from the sub-grain RVE model, which represents deformation mechanisms. The homogenized model incorporates the effect of important characteristics of the sub-grain $\gamma - \gamma'$ morphology, viz. the volume fraction and shape of the γ' precipitates and the γ channel-width. Parametric representations of these sub-grain morphology variables are incorporated in evolution laws of the homogenized AE-CP model that include both thermal and athermal shear resistance. Three homogenized parameters, viz. the thermal shear resistance, the saturation shear resistance and the reference slip-rate are expressed as functions of the sub-grain morphology

variables. Size dependence that is explicitly represented in the sub-grain dislocation density crystal plasticity model through the presence of geometrically necessary dislocations is reflected in the homogenized AE-CP model through the explicit dependence on the channel-width. The AE-CP model is found to accurately reproduce the stress-strain response of the RVE for a range of microstructural variations. It is also found to agree quite well with results of experimental studies on single crystal superalloys in the literature. A significant advantage of this homogenized AE-CP model is that its high efficiency enables it to be effectively incorporated in polycrystalline crystal plasticity FE simulations, while retaining the accuracy of detailed RVE models. It would be impossible to simulate polycrystalline microstructures with direct numerical simulation of the subgrain morphology otherwise. Grain-scale micro-twinning is taken into account through a micro-twin nucleation and evolution model that is incorporated alongside the homogenized AE-CP model. Tension-compression asymmetry, observed in creep experiments, is well represented by this model. The grain-scale model is also augmented with the effect of GNDs in the hardness formulations to compensate for lattice incompatibility. The parametrically homogenized AE-CP constitutive model implicitly retains the effect of microstructure morphology while reducing computational cost by several orders of magnitude without significant loss of accuracy. This is necessary for meaningful simulations that can be corroborated by experiments.

Virtual polycrystalline microstructural models of the superalloy René-88 DT are created by two methods, viz. the direct implementation (DI) method and the statistically equivalent microstructure (SEM) generation method. Constant strain-rate simulations of tension tests show similar behavior of both the instantiations. However, the simulations conclude that annealing twins have a significant influence on the overall polycrystalline behavior as well as on the local behavior. Finally, the effect of gradients in the subgrain scale morphological parameters on the overall polycrystalline behavior is demonstrated. In summary, the hierarchical model demonstrates the capability of representing mechanisms occurring at three scales, viz. the sub-grain scale of $\gamma - \gamma'$ precipitates, the grain scale of single crystals and the scale of polycrystalline aggregates in a unified framework for predicting deformation behavior under different loading conditions, This is a novel development in the literature of Ni-based superalloys, for which behavior at the macro-scales is strongly governed by behavior at the lower-scales. Most models in the literature do not explicitly incorporate parametric forms of the lower scales. In this regard, the present model is expected to provide a strong pathway to lower-scale material design.

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