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Microstructure based and temperature dependent model of flow behavior of a polycrystalline nickel based superalloy

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ABSTRACT

A physics-driven and microstructure-based model has been formulated for monotonic stress–strain behavior and applied to a polycrystalline nickel based superalloy, René 104. While the yield strength of this alloy is strongly dependent on size and distribution of the ordered γ' precipitate, the post-yield behavior is found to be fairly insensitive to the same. Additionally, post-yield hardening and softening rates are found to vary quite significantly within the narrow range of test temperatures examined. For a model to be able to consistently explain all these observations (a) it must explicitly account for microstructural effects and temperature dependence, and (b) it must be aware of the specific strengthening mechanisms unique to nickel-based superalloys. Accordingly, the present effort starts with Estrin's dislocation based framework (Estrin (1996) [4]), and then extends the same to incorporate post yield strengthening/softening mechanisms. This paper presents details of this mechanism guided semi-empirical monotonic stress–strain model and its ability to describe flow behavior for different microstructures over a range of temperatures.

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1. Introduction

René 104 is a polycrystalline nickel based superalloy used for turbine disc applications in aero-engines. Development of a model for flow behavior of this material is essential for predicting location specific properties in turbine disc components, and for development of a damage tolerant model.

For the last 45 years, there have been considerable efforts towards constitutive modeling of stress–strain response of metallic materials [1–6]. An excellent review article on constitutive theories can be found in [7]. Chaboche's own constitutive theories [8] are based on yield surface considerations. These involved choice of the viscosity function following von Mises elastic domain equation and choice of isotropic and kinematic hardening equations. These models are phenomenological in nature and are not motivated by microstructure considerations. As a result, these are not capable of predicting material response beyond the range of experimental conditions used in the estimation of parameters. Roters et al. [9] have given a more recent overview of available constitutive laws. They have clearly differentiated between phenomenological models, where the material state is only described in terms of critical resolved shear stress and not in terms of lattice defect populations, and physics based constitutive models, which treat evolution of dislocation densities taken as internal variables, and calculate flow stress from them. Prominent phenomenological models were formulated by Rice et al. [10], Hutchinson [11], and Peirce et al. [12,13]. Other notable phenomenological formulations include KHL model [14–18] and JC model [19]. Phenomenological models are limited by their applicability for a specific set of conditions only. The aim of the present work is to develop a more generic physics based model with enhanced predictive capability. Literature of physics based models includes the following: [20–27]; however, these models do not account for the unique behaviors shown by polycrystalline nickel based superalloys over a range of temperatures. More recently Crystal Plasticity Finite Element (CPFE) models have gained considerable amount of interest. CPFE models have been proposed by a few authors [28–34]; in this approach crystal geometry is introduced into the modeling, where plastic deformation is calculated by considering the shear contributions of the crystal geometry based slip systems. Many of these models have incorporated microstructure at grain level in terms of size, shape and orientation of the grains; however, most of these have not taken into account either the effect of intra-grain precipitates or the effect of temperature. Chaboche [7] in his review paper indicated about constitutive models that have physical concepts incorporated in [1,2,35]. Motivated by Kock's approach [2] to constitutive modeling, where

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internal variables representing the micromechanical state of the material were related to the dislocation density, Estrin included microstructure data through equations describing the evolution of dislocation density [4,35,36]. However, these microstructure driven models are developed for materials which do not show various unique behaviors as shown by polycrystalline γ' strengthened nickel based superalloys. These unique behaviors include retention of or even improvement in strength with temperature, higher initial hardening rates at higher temperatures etc. A more recent work by Huang et al. [37] describes discrete dislocation dynamics modeling of nickel based single crystal superalloy, where precipitate size and shape effects have been accounted for, however, temperature variation effect and grain size effect (as it is developed for single crystal) have not been explicitly considered. Using similar dislocation dynamics approach, Zhang et al. [25] have developed constitutive model for fcc metals, however this model is applicable only for pure FCC metals. The work by Shenoy et al. and Pryzybyla et al. [38,39] introduced microstructural features as inputs in modeling flow behavior of a nickel based superalloy, IN 100™. However, this model is applicable only at a specific temperature. A more generic model would incorporate various deformation mechanisms operative over a range of temperatures.

The goal of our present work is to introduce both microstructure and temperature as input variables to the model, so that the model can be applied at different temperatures for various microstructural conditions. In the present work, Estrin's modeling framework [36] has been adapted and applied to the polycrystalline nickel based superalloy René 104. While the general framework has been maintained, a few additional strengthening mechanism terms, specific to this alloy group have been added to capture the uniqueness shown by the flow behavior of this type of alloys. Plausible deformation mechanisms operating at different temperature regimes have been first identified and the corresponding terms have been incorporated in the constitutive model for post yield stress–strain behavior of René 104 under monotonic uniaxial loading. The model has been made modular in nature, meaning that the yield strength and post yield strengthening contributions have been made additive. Hence, even though the temperature dependence of yield strength (YS) has been modeled empirically at this stage making the present model semi-empirical, further reduction in empiricism is possible over the present state of the model by incorporating physics of temperature dependency of the yield strength. Primary focus of the present work has been to introduce deformation mechanism guided physics in post yield behavior of the alloy at different temperature, where deformation mechanisms have been incorporated specifically in the post-yield regime. Data of different microstructures having different distribution of size and volume fraction of γ', from temperature regimes of interest have been used for estimation of material parameters.

Table 1
Nominal composition of René 104.

René 104	Al	B	C	Co	Cr	Mo	Nb	Ta	Ti	W	Zr	Ni
In wt%	3.4	0.025	0.05	20.6	13	3.8	0.9	2.4	3.7	2.1	0.05	Rest

2. Material, heat treatment and testing

The nominal composition of the present material René 104 is given in Table 1. This polycrystalline nickel based superalloy has a matrix of FCC γ phase that contains ordered γ' precipitates of various sizes, categorized in different populations. A typical heat-treatment includes solutionizing above the γ' solvus temperature ($>$ 1427 K) of the alloy, followed by cooling at a specific rate, and a two-step aging treatment. Post forging and solutionizing treatment, grain size of the material in the present work was found to be around 30 μm (ASTM 7). Post solutionizing cooling rate determines the size and size distribution of γ' precipitates. Fig. 1 shows representative microstructures for the samples cooled at two different cooling rates, 41.7 K/min and 111.0 K/min from solutionizing temperature followed by double aging treatment. All the samples used in the present study came from the same forging, and underwent the same solutionizing treatment, resulting in similar grain size for all the samples. Faster cooling (FC) rate (111 K/min) generates finer distribution of γ' size compared to the slower cooling (SC) rate (41.7 K/min). Henceforth, in the text these two cooling rates would be denoted by FC and SC respectively.

Monotonic tensile tests have been carried out at different temperatures and strain rate conditions for the two different microstructures obtained by SC and FC. The test conditions are given in Table 2.

3. Experimental data analysis

The initial analysis of the experimental data revealed that the effect of strain rate on flow behavior of this alloy is minimal over the temperature range of interest. The focus of the present study

Table 2
Mechanical test conditions.

Post solutionizing cooling rates (K/min)	Strain rate (1/min)	Temperature (K)
111.0 (FC)	0.005	477
		672
and	and	700
		811
41.7 (SC)	0.05	977

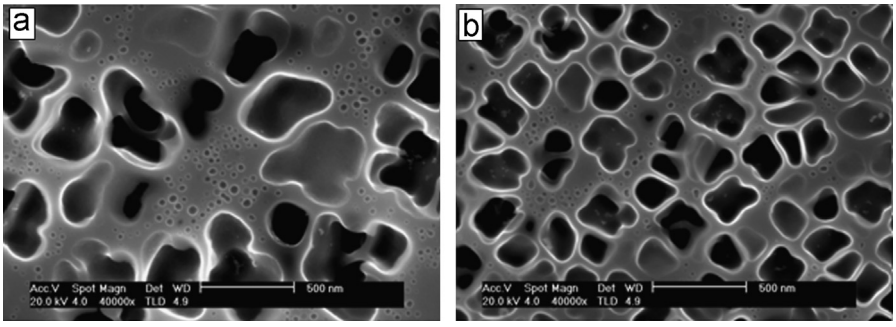

Fig. 1. SEM micrographs for two different cooling rates: (a) 41.7 K/min. (b) 111 K/min.

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