Chapter 13
Numerical Simulation of High Temperature Deformation Behavior of Nickel-Based Superalloys Using Crystal Plasticity Models and Finite Element Method

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ABSTRACT

Development of reliable computational models to predict the high temperature deformation behavior of nickel based super-alloys is in the forefront of materials research. These alloys find wide applications in manufacturing of turbine blades and discs of aircraft engines. The micro-structure of these alloys consists of the primary gamma-prime phase and the secondary and tertiary precipitates (of Ni_3Al type) are dispersed as gamma-prime phases in the gamma-matrix. It is computationally expensive to incorporate the explicit finite element model of the micro-structure in a crystal plasticity based constitutive framework to simulate the response of the polycrystalline micro-structure. Existing models in literature do not account for these underlying micro-structural features which are important for simulation of polycrystalline response. The aim of this chapter is to present a physically-motivated multi-scale approach for simulation of high temperature response of Nickel-based super-alloys. At the lower length scale, a dislocation density based crystal plasticity model is developed which simulates the response of various types of micro-structures. The micro-structures are designed with various shapes and volume fractions of gamma-prime precipitates. A new model for simulation of the mechanism of anti-phase boundary shearing of the gamma-prime precipitates, by the matrix dislocations, is presented in this chapter. The lower scale model is homogenized as a function of various micro-structural parameters and the homogenized

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model is used in the next scale of multi-scale simulation. In addition, a new criterion for initiation of micro-twin and a constitutive model for twin strain accumulation are developed. This new micro-twin model along with the homogenized crystal plasticity model has been used to simulate the creep response of a single crystal nickel-based super-alloy and the results have been compared with those of experiment from literature. It was observed that the new model has been able to model the tension-compression asymmetry as observed in single crystal experiments.

INTRODUCTION

Nickel-based super-alloys are used for manufacturing of aircraft engine turbine blades, disk and other high temperature components such as combustion chambers, casings, liners, exhaust ducting and bearing housings etc (Furrer & Fecht, 1999). This is because of their superior mechanical properties such as excellent high temperature stability, oxidation resistance, creep resistance and mechanical strength. These properties are as a result of the two-phase structure (often called the $\gamma - \gamma'$ microstructure) (Sugui et al., 2011; Goff et al., 2004; Hopgood & Martin, 1986). The γ phase is mainly an alloy of Ni, Cr with the presence of small wt. % of other alloying elements. This phase is of face-centered cubic crystal structure and it remains stable up to its melting point. The γ' phase is a coherent ordered inter-metallic reinforcing phase of $L1_2$ crystal structure and of Ni_3A1 type. This phase often appears as a distribution of cuboidal precipitates embedded in a disordered Ni-Cr solid solution. However, the shape and size of these precipitates depends largely on the cooling rate (Babu et al., 2001; Epishin et al., 2001) as well as internal stress gradients (Ignat et al., 1993) encountered during casting and further heat treatment process of these alloys. Because of their shape and ordered structure, the γ' reinforcing precipitates act as effective obstacles to the motion of dislocations in the super-alloy.

When stresses are high, the dislocations will either bypass or shear the precipitates. The mechanism depends on the temperature and the stress level. The dependence of the super-alloy behavior on deformation conditions has been extensively analyzed in the last several years both for polycrystalline (Torster et al., 1997; Hong et al., 2009; Knobloch et al., 1997; Soula et al., 2009) and single crystal based super-alloys (Chatterjee et al., 2010; Cormier et al., 2007; Milhet et al., 2010). As is the case for other alloys reinforced with a dispersed hard second phase, the volume fraction of the γ' precipitates, their mean size and spacing have a major effect on the mechanical properties of these super-alloys. Another important micro-structural property controlling the behavior of super-alloys is related to high temperature changes in structure. When these super-alloys are deformed under creep conditions at temperatures above 850°C, their microstructure undergoes morphological changes. These changes have been described by models in literature (Manonukul et al., 2002; Ma et al., 2008) which take into account the intrinsic properties of a super-alloy (precipitate and matrix elastic moduli and volume fractions, misfit between the precipitate and matrix lattices, precipitate matrix interfacial energy), and also the experimental conditions (applied stress and temperature).

The creep deformation behavior of nickel-based single crystal super-alloys controls the service life of turbine blades used in modern aero-engines. Recently, there has been substantial effort to predict the life of the nickel based super-alloy components in literature (Brown et al., 1986; Koul & Castillo, 1991). Some of the modeling efforts for both single crystal and polycrystalline nickel based alloys are presented in literature (Coakley et al., 2011; Prasad et al., 2006; Kim et al., 2007; Zhan et al., 2008; Piard et al.,