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Multiscale modelling of mechanical response in a martensitic steel: A micromechanical and length-scale-dependent framework for precipitate hardening

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Abstract

In this paper, a multiscale finite element (FE) modelling framework is developed with explicit representation of polycrystalline microstructure and sub-micron precipitate structure for a P91 tempered martensitic steel. A dislocation-mechanics-based and length-scale-dependent crystal plasticity model has been formulated to account for slip-based inelastic deformation in the material. The multiscale FE simulations have been validated through the use of uniaxial tensile test data at room temperature. Homogenization analysis is performed to connect the FE models at two length scales. The analysis indicates a strong dependence of dislocation mean free path on the morphology of the sub-micron structure. A linear relationship is found to represent the homogenized constitutive behaviour with respect to precipitate size. Softening effects with respect to precipitate and lath coarsening are identified and quantified at the macroscopic scale through the multiscale modelling framework.

Keywords: Multiscale modelling; Precipitate hardening; Strain gradient crystal plasticity; Dislocation mean free path; Tempered martensitic steels

1. Introduction

Tempered martensitic steels containing 9–12% Cr are widely used as structural materials in critical power plant components operating at elevated temperatures. To fulfil the current and future needs for safety, efficiency and flexibility of fossil fuel-fired power plants, there is a requirement for rigorous and accurate structural integrity assessment procedures, taking into account recent advances in multiscale computational and experimental techniques. The development of such approaches relies upon explicit incorporations of the underlying inelastic and microstructure-dependent deformation and failure mechanisms, operating at micron and sub-micron scales. Tempered martensitic steels have a complex microstructure exhibiting a hierarchical arrangement. The material has a body-centred cubic (bcc) lattice structure consisting of prior austenite grains, packets, blocks, laths and precipitates. A collection of packets forms within a prior austenite grain (with sizes between 10 and 500 μm) and a packet can be subdivided into blocks (of 2–10 μm) containing laths (0.2–1 μm thick) with precipitates (mean diameter in the order, 10–600 nm) dispersed mainly at lath boundaries [1–9]. In tempered martensitic steels, misorientated interfaces (the boundaries which separate packets, blocks and laths) and precipitates (such as carbides, carbonitrides, Laves phase and Z phase) represent two important classes of microstructural features contributing to the superior mechanical properties of these alloys by obstructing dislocation motion at micron and sub-micron scales.

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Quantifying the influence of microstructural features on the constitutive response of tempered martensitic steels is relevant to optimal design of such materials and structures, and to accurate structural integrity assessment. The effect of lath-boundary precipitates (carbides) on the creep strength has been experimentally investigated in Ref. [10] by comparing a tempered martensitic steel with a carbide-free material possessing a microstructure and composition closely similar to the tempered martensitic steel. It is pointed out in Ref. [10] that the presence of precipitates significantly enhances the creep strength of tempered martensitic steels by impeding dislocation motion and resisting the lath coarsening during high temperature creep. In a recent study [11], it has been shown that the addition of 3.0 wt.% cobalt into a martensitic steel can remarkably slow down the coarsening process of lath-boundary carbides during creep and consequently increase the creep life. However, the strengthening/hardening contributions associated with the hierarchical microstructure in tempered martensitic steels have not yet been fully quantified. Overall, the challenge of experimentally quantifying microstructural effects for materials with complex microstructure, such as martensitic steels, lies mainly in the difficulty of fabrication (varying just one type of microstructural feature, with the others remaining unchanged). Modern modelling techniques provide tools to directly quantify these effects and can assist in the understanding of issues relating to premature failure of martensitic steel components during creep [12,13], and in the application and design of high Cr martensitic steel components for the next generation of power plants [14,15].

The present paper addresses a multiscale modelling method to quantify precipitate hardening in a P91 martensitic steel by means of crystal plasticity finite element (FE) analysis. To date, crystal plasticity-based simulations for metals have provided extensive insights [16] into the understanding of inelastic deformation mechanisms, particularly when the models are combined with experiments at multiple length scales [17–23]. Crystal plasticity FE models in conjunction with a micropillar test [23] have been used to investigate block boundary-induced strain hardening in martensitic steels. Dislocation density-based crystal plasticity FE models have also been used to predict shot peening-induced residual stress at the block level [24], the effects of irradiation damage on tensile and creep properties [25], and microstructure-associated dynamic failure [26]. In recent years, crystal plasticity FE models with length-scale dependence incorporated have been developed and applied to investigate microstructural response in metals [20,27–31]. A key feature in these models is the consideration of strain gradient effects on the constitutive response to include length-scale dependence. Discrete dislocation dynamics simulation is another modelling technique which can be used to investigate effects of precipitates on deformation at very small length scales [32–34]. However, there are computational barriers to simulating bulk materials dealing explicitly with a large amount of dislocations. A multiscale method combining a discrete dislocation dynamics model with a crystal plasticity model [35] may be appropriate for a large volume of material.

Limited work has been reported on multiscale modelling for tempered martensitic steels and the importance of strain gradient (length scale) effects in these materials has not been fully studied. Thus, it is of practical interest to quantify the role of microstructure, in particular precipitates, in tempered martensitic steels by means of crystal plasticity modelling. The objectives of the present paper are as follows: (i) to develop a finite element model to explicitly represent the geometry of laths and precipitates in tempered martensitic steels and incorporating the influence of precipitate and lath size into the model; and (ii) to use a multiscale method to examine how precipitates at lath boundaries affect the evolution of dislocation density and influence strain hardening at different length scales.

The paper is laid out as follows: Section 2 describes the multiscale FE modelling strategy. Section 3 outlines the computational results which are discussed in Section 4, followed by concluding remarks in Section 5.

2. Multiscale finite element modelling framework

In the present work, the mechanical behaviour of a P91 martensitic steel at multiple length scales is examined. The FE method is employed to account explicitly for the microstructure, with strain gradient crystal plasticity theory used to represent the material's inelastic and length-scale-dependent constitutive behaviour. The constitutive model incorporates the evolution of statistically stored dislocations (SSDs), based on generation and recovery mechanisms, and geometrically necessary dislocations (GNDs), governed by the gradients of plastic strain.

2.1. Strain gradient crystal plasticity constitutive model

The gradient crystal plasticity model developed in Ref. [29] for faced-centred cubic crystals is adopted and modified for bcc martensitic steels. For simplicity, it is assumed that inelastic slip is activated on twelve {1 1 0}[1 1 1] slip systems.

As proposed in Ref. [36], a multiplicative decomposition can be applied for deformation gradient, $\mathbf{F}$, as follows:

$$\mathbf{F} = \mathbf{F}^e\mathbf{F}^p \tag{1}$$

where $\mathbf{F}^e$ is the elastic part of deformation gradient representing elastic stretching and rigid rotation, and $\mathbf{F}^p$ is the plastic part accounting for pure plastic deformation. Following Ref. [37] for slip-based plastic deformation in crystalline materials, the plastic velocity gradient is introduced, which depends linearly on crystallographic slip rate as follows:

$$\mathbf{L}^p = \dot{\mathbf{F}}^p(\mathbf{F}^p)^{-1} = \sum_{\alpha=1}^{N}\dot{\gamma}^\alpha\mathbf{m}^\alpha \otimes \mathbf{n}^\alpha \tag{2}$$