Journal of the Mechanics and Physics of Solids 86 (2016) 42–52

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

journal homepage: www.elsevier.com/locate/jmps

Microscale deformation of a tempered martensite ferritic steel: Modelling and experimental study of grain and sub-grain interactions

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ARTICLE INFO

Article history:
Received 3 February 2015
Received in revised form
29 September 2015
Accepted 29 September 2015
Available online 9 October 2015

Keywords:
Mesoscale modelling
Strain gradient crystal plasticity
Tempered martensitic steels

ABSTRACT

In this paper, a finite-element modelling framework is presented with explicit representation of polycrystalline microstructure for a tempered martensite ferritic steel. A miniature notched specimen was manufactured from P91 steel with a 20,000 h service history and tested at room temperature under three point bending. Deformation at the microscale is quantified by electron back scattered diffraction (EBSD) before and after mechanical loading. A representative volume element was developed, based on the initial EBSD scan, and a crystal plasticity model used to account for slip-based inelastic deformation in the material. The model showed excellent correlation with the experimental data when the relevant comparisons were made.

1. Introduction

Tempered martensite ferritic steels with a high chromium content are widely used for critical applications within modern power generation plants on account of their excellent fatigue and creep resistance. Due to the importance of these applications, a rigorous and robust analysis of the materials response under a variety of conditions must be undertaken. Material modelling is an essential part of this process, as it provides a predictive capability that can be incorporated into the design process. Quantifying the influence of microstructural features on the constitutive response of tempered ferrite martensite is also crucial to the understanding of the performance of these materials, and to the accuracy of structural integrity assessment. The current work focuses on a particular steel, P91 (containing 9% Cr, 1% Mo and the balance primarily Fe Fournier et al., 2009). Tempered martensite ferritic steels (termed TMFS by Dronhofer et al., 2003) have a body-center-cubic (BCC) structure with a complex microstructure, exhibiting a hierarchial arrangement of grains and sub-grains (Rahnama and Qin, 2015; Panait et al., 2010). The largest of these sub-structures is called a 'packet' which can range in size from 15 to 500 μm. Within these packets, 'blocks' (grains) can be identified, usually between 2 and 10 μm in size. In turn, 'blocks'

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http://dx.doi.org/10.1016/j.jmps.2015.09.015
0022-5096/

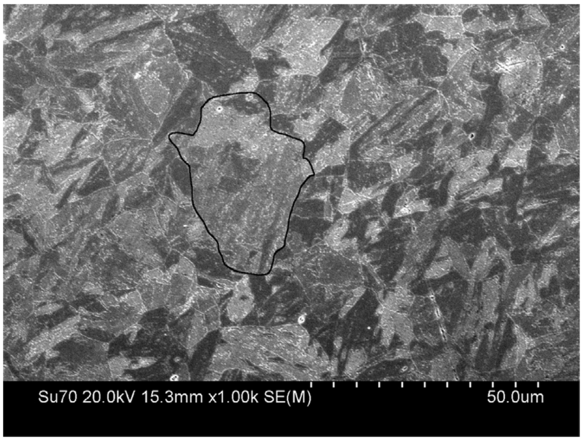

Fig. 1. SEM micrograph of the surface of P91, black outline represents a typical block.

are composed of subgrains called 'laths', which can range from 0.2 and 1 μm in width (Panait et al., 2010; Hald and Korcakova, 2003; Srinivas et al., 2011; Kipelova et al., 2011; Maruyama et al., 2001; Sawada et al., 2011; Aghajani et al., 2009; Rojas et al., 2011; Czyrska-Filemonowicz et al., 2006). Another important microstructural feature is the presence of precipitates, which form primarily at lath boundaries but also within laths (Rojas et al., 2011; Czyrska-Filemonowicz et al., 2006; Shibli and LeMatHamata, 2001; Shibli and Starr, 2007; Sawada et al., 2003). These precipitates contribute to the superior performance of P91 at high temperature by inhibiting dislocation movement during material deformation (Kitahara et al., 2006). The boundaries between lath, block, and packet can be identified by studying the misorientation of neighbouring grains. The misorientation between neighbouring blocks is typically 60°, while between laths the misorientation is typically 2°(Panait et al., 2010). Fig. 1 shows a typical P91 microstructure, from an SEM image, with the black outline showing an example of a block boundary.

In recent years significant progress has been made in the development and application of mechanistic, physically-based material models for engineering alloys, e.g. crystal plasticity has been used extensively (Dunne et al., 2007, 2012; Zhang et al., 2014; Erinosho et al., 2013) to model deformation mechanisms in polycrystalline materials (HCP Ti, FCC Ni and BCC steel). Crystal plasticity-based simulations for metals have provided deep insight into inelastic deformation mechanisms, particularly when these models are combined with experimental characterisation at multiple length scales (Cheong and Busso, 2004, 2006). There have been major advances in characterisation at the microscale, e.g. in Ghassemi-Armaki et al. (2013) micropillars, consisting of a single block of a martensitic steel, have been tested under compression and measured beam deflection compared to modelling predictions. Electron back scatter diffraction (EBSD) has been used to investigate microscale deformation in a wide range of materials, e.g. Endo et al. (2014), Mohseni et al. (2013), Beladi and Rohrer (2013), Spanos et al. (2008), Rowenhorst et al. (2005) and in Dunne et al. (2007, 2012) and Zhang et al. (2014) was used to validate computational predictions of deformation and rotation in a number of polycrystalline steels. In Kamaya et al. (2005), Kartel et al. (2012), Mayumi et al. (2011) and Hasebe et al. (2004) changes in grain orientation for a coarse grained (100 μm) stainless steel were examined, using the Wilkinson technique (Wilkinson et al., 2006), which involves measuring the changes in the Kikuchi pattern to determine the change in orientation in the material; the concept of crystal deformation was also introduced in Kamaya et al. (2005) to quantify average changes in grain orientation during deformation. In Kartel et al. (2012) EBSD (in conjunction with numerical modelling and the eigenstrain technique) has been used to determine the magnitude of the residual stress in large carbide particles (10 μm) in a nickel superalloy (MAR-M-200).

While significant progress has been made in computational and experimental characterisation of polycrystalline materials at the microscale, there have been few attempts to represent the hierarchical microstructure of martensitic steels in computational models. In Shanthraj and Zikry (2013a,b) a physically-based micro-mechanical model was used to analyse a martensitic steel, with grain boundary interactions and the evolution of dislocation density examined numerically using a 'constructed microstructure'. In Li et al. (2014b) a microstructurally based material model was used to predict the lattice (elastic) stress/strain response of a martensitic steel with the results validated by in-situ neutron diffraction measurements. The model was also used in Li et al. (2014a) to investigate lath size effects in a martensitic steel (P91). The current paper builds on our earlier work. As in previous work a finite-element (FE) approach is used, with an explicit representation of the material microstructure, focusing at the block level. In Li et al. (2011, 2013, 2014a,b), and Li et al. (2011), uniaxial loading of P91 was considered, with validation through neutron diffraction measurements in Li et al. (2013). In this work, we consider a complex multiaxial loading condition (notched three point bend) with validation carried out both at the macroscale, through overall specimen deformation and notch opening, and at the microscale through EBSD measurements. To our knowledge such an approach, using direct comparison of grain orientation change due to mechanical loading between experimental and modelling results has not previously been investigated for a martenstic steel. Significant work has been done using the change in orientation techniques presented in this paper (Dunne et al., 2007, 2012) but, to our knowledge,