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Microscale modelling of the deformation of a martensitic steel using the Voronoi tessellation method

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ABSTRACT

The deformation of a martensitic steel (P91) at the microscale is investigated using the finite element method. The approach takes into account the hierarchical grain–packet–block microstructure of the steel as determined experimentally by electron backscatter diffraction (EBSD). The orientation relationship for P91 between the prior austenite grain (PAG) and the martensitic packet/block is determined and found to be consistent with the Kurdjumow–Sachs (K–S) relationship. This relationship is incorporated within a finite-element model to represent the material microstructure, using a representative volume element (RVE) generated by a modified centroidal Voronoi tesselation (VT) approach. A non-linear, rate dependent, finite strain crystal plasticity model is used to simulate the mechanical response of the material at the micro- and macro-level and the sensitivity of the results to the model assumptions is investigated. It is found that the global (macro) mechanical response predicted by the RVE generated using the modified VT model is in good agreement with that predicted by an RVE taken directly from the measured EBSD microstructure. The influence of block/packet/grain boundaries on the local (micro) deformation is examined and it is found that the microscale prediction obtained using the RVE based on the modified VT microstructure, with an appropriate choice of microstructural parameters, is consistent with that obtained using the measured EBSD map.

1. Introduction

High-strength steels, containing between 9% and 12% chromium by weight, are widely used in current power generation plant due to their characteristics of high creep strength and excellent corrosion and oxidation resistance (Abe, 2016). In this work, the micro-mechanical response of a modified 9Cr steel (P91) with a tempered martensite microstructure is examined (Fournier et al., 2010; Hald, 2004; 2008; Shankar et al., 2006; Shibli and Starr, 2007). 9Cr steels after rapid quenching from austenite typically form a lath martensite microstructure (Abe, 2016). During the transformation from austensite (γ phase) to martensite (α' phase), each austenite grain, with a face-centred cubic (FCC) structure, is transformed into a number of packets with body centred cubic (BCC) structure, separated by high angle boundaries. Each packet is further subdivided into blocks, also separated by high angle boundaries. A block can be viewed as a single crystal containing dislocations, with martensite laths within these blocks distinguished by low angle misorientations (Krauss, 2005). The mechanical properties of martensitic materials depend strongly on the microstructure, for example the yield strength and toughness of as-quenched

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martensite, depend strongly on packet size (Swarr and Krauss, 1976). Therefore, the study of the deformation at relevant microstructural length scales is crucial for the understanding and optimization of the mechanical properties of these materials and it is expected that the deformation and failure at the microscopic length scale (micro-scale) will be strongly influenced by the packet–block morphology.

Martensitic transformation is a diffussionless and shear transformation on habit planes, the preferred crystallographic planes of the austenite where the martensite crystals form (Krauss, 2005). The morphology of martensite and the orientation relationship between the prior austenite grain and the transformed martensite blocks both depend on alloy composition. Generally, lath martensite forms in low carbon steel with carbon content less than 0.6% (Morito et al., 2003), with habit planes close to $\{111\}_\gamma$. As carbon content increases to 0.92%, the habit planes approach $\{225\}_\gamma$. In high carbon steels, carbon content up to 1.78%, plate martensite forms and the habit planes approach $\{229\}_\gamma$ (Greninger and Troiano, 1940). It has also been found that other chemical elements, such as Ni, affects the martensite morphology and habit plane orientation. As the Ni content increases, the morphology changes from lath to 'butterfly' or lenticular (plate) (Sato and Zaefferer, 2009). The habit plane of butterfly martensite, observed for alloys with Ni content between 17% and 19% and carbon content less than 0.5% approaches $\{252\}_\gamma$ (Zhang et al., 1989). For high Ni content alloys, the martensite morphology may be lenticular rather than lath, even at low carbon content (Klostermann and Burgers, 1964). A number of lath martensite steels have been reported to satisfy the Kurdjumow–Sachs (K–S) orientation relationship (Kurdjumow and Sachs, 1930), e.g. Fe–Si–Mn steel with carbon content less than 0.2%wt (Kitahara et al., 2006; Morito et al., 2003; 2006). Fe-28.5%Ni steel (Kitahara et al., 2005) forms plate martensite and has been reported to satisfy the Nishiyama–Wassermann (N–W) orientation relationship (Nishiyama, 1934; Wassermann, 1935). A combination of K–S, N–W and Pitsch has been used to describe the orientation of the BCC structure in TRIP Steels, based on electron backscatter diffraction (EBSD) studies (Verbeken et al., 2009). Sonderegger et al. (2007) found that a combination of the K–S and N–W relation could be used to represent the microstructure of a martensite steel similar to the material of interest here but with 11%Cr content. To our knowledge no similar studies have been carried out on P91 steel, which is widely used, particularly in high temperature power plant (Ennis and Czyrska-Filemonowicz, 2003).

Finite-element (FE) models, incorporating a crystal plasticity constitutive model, have been widely used to investigate the deformation of crystalline materials at the microscale, with the microstructure modelled by a representative volume element (RVE). This approach can capture the experimentally observed active slip directions in polycrystalline materials (Dunne et al., 2007) and can predict lattice rotations that agree well with experimental measurements (Dunne et al., 2012; Zhang et al., 2014) . In simulating deformation at the microscale, the microstructural morphology may be determined directly from experimental measurements (e.g. through electron microscopy and/or electron backscatter diffraction (EBSD)) or may be generated numerically (e.g. the Voronoi tessellation (VT) approach, Li et al., 2013; Okabe et al., 2009). The VT approach is to partition a volume/area into different regions with polygonal shapes representing equiaxed grains with random crystal orientation distribution. In our previous work, a combination of the VT approach and FE simulation was utilized to investigate deformation in austenitic steel in Li et al. (2011b) and the evolution of lattice strain for different crystallographic grain families, measured under uniaxial tension using in-situ neutron diffraction, was found to be consistent with the model predictions. Shanthraj and Zikry (2013) developed an integrated framework to examine dislocation interactions at block and packet boundaries to investigate failure of martensitic steel accounting for the morphology and orientation for a small number of packets/blocks. A dislocation-density based crystalline model proposed by Hatem and Zikry (2009) was applied to investigate the deformation and shear strain localization (Hatem and Zikry, 2010) in lath martensitic steel with a small number of prior austenite grains (PAG). A martensitic steel (M190) and two dual phase ferrite-martensite steels (DF140T and DP980) have also been analyzed using a VT-based approach (Chen et al., 2014; Ghassemi-Armaki et al., 2013) and predictions of deformation in micropillar compression tests were compared with experimental data. In Ghassemi-Armaki et al. (2013) it was found from the numerical analysis that deformation associated with block and packet boundaries contribute significantly to overall strain hardening of the material. The modelling approach taken here is similar to that in Ghassemi-Armaki et al. (2013), Chen et al. (2014). An equiaxed prior austenite grain microstructure is partitioned into packets and blocks using a VT approach, a periodic RVE is then constructed to represent the microstructure of martensite and the RVE analyzed within an FE model. The results obtained from the model constructed in this fashion are compared with measured tensile test data and with those of an RVE derived directly from measured block orientations. A systematic study of the influence of packet/block distribution within the PAGs is carried out to investigate how morphology influences microscale and macroscale deformation. The paper is laid out as follows: in Section 2, the K-S orientation relationship for martensite is reviewed. In Section 3, the experimental procedure to prepare and test the P91 sample is described and it is demonstrated that the K–S relationship is the most appropriate one to describe the morphology of the modified 9Cr steel P91. In Sections 4–6, the modelling results, including comparison with experimental data, are described. In Section 7, the summary and conclusions of the paper are presented.

2. Crystallographic analysis of orientation relationship between austentite and martensite

A number of relations have been developed to describe the relationship between the orientation of a PAG and the newly formed martensite (Verbeken et al., 2009). The difference between these relationships derives from the different assumptions for the habit plane and directions. Table 1 lists the orientation and habit planes for the most commonly used relationships. An early attempt to explain the mechanics of martensite transformation during rapid quenching is the relation