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Assessment of crystal plasticity finite element simulations of the hot deformation of metals from local strain and orientation measurements

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Simulations of the deformation of microstructures at high homologous temperatures have been carried out using a Crystal Plasticity Finite Element (CPFE) model to predict texture and grain structure deformation in Face-Centred-Cubic (FCC) metals deformed under conditions representative of hot forming operations. Results show that the model can quantitatively predict the location and intensity of the main deformation texture components of a AA5052 aluminium alloy deformed at 300 °C under Plane Strain Compression (PSC). Simulations also reasonably predict the range of strain values measured using microgrids in the microstructure of a Fe-30wt%Ni alloy deformed at 1000 °C using a new experimental procedure. However, the model fails to reproduce accurately intra-granular strain distribution patterns. Results at room temperature, after a tensile test carried out inside a Scanning Electron Microscope (SEM) on the same model alloy, show a much closer match between simulation and experimental results. Despite discrepancies for some local deformation features, the model predicts the formation of intense deformation bands running at 45° with respect to the tensile axis and located along the same grain boundaries as in the experiment. Results, therefore, highlight the limitations of deterministic CPFE simulations for situations where the grain size to sample thickness ratio is small and for which the sub-surface grain geometry strongly affects surface strains. They also show that reliable predictions of the statistical response of a polycrystalline aggregate can be obtained for the hot deformation of metals which controls microstructure evolution during the processing of metals.

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1. Introduction

The mechanical properties of metals such as steels and aluminium alloys are dependent on their processing conditions and are a direct result of the microstructure evolution taking place during both hot and cold forming operations. For instance, recrystallisation occurring at high homologous temperature during a hot forming process such as industrial rolling followed by phase transformation upon subsequent cooling affect both the grain size and texture of metals. The numerical simulation of microstructure evolution during such process is, therefore, of paramount importance for the metal industry, with the aim of reducing production cost by predicting the properties of the final product. Microstructure-based simulations of recrystallisation and/or phase transformation using techniques such as Cellular Automata (Lan et al., 2005; Popova et al., 2015; Rollett and Raabe, 2001; Zheng and Raabe, 2013), Monte-Carlo (Radhakrishnan et al., 1998; Zhang et al., 2012) or Phase-Field (Lan and Pinna, 2012; Takaki and Tomita, 2010; Takaki et al., 2014) have been developed in recent years for microstructure and recrystallisation texture prediction at high temperature. Such physical phenomena are affected by the energy stored in the microstructure during deformation and, therefore, the accurate prediction of strain and stress distributions in these microstructures is key to the successful simulation of subsequent microstructure evolution. Crystal Plasticity Finite Element (CPFE) models of the deformation of polycrystalline metals are particularly well suited for the coupling with the numerical techniques mentioned above as they predict intra-granular state variable distributions which can then be used as input for recrystallisation/phase transformation simulations. Improved computing performance over the past decade has enabled the development of statistically meaningful simulations of the deformation of grain structures in metals using CPFE models. These models have been used extensively in published research studies for the prediction of deformation texture and mechanical response of metals at both room (Alharbi and Kalidindi, 2015; Bachu and Kalidindi, 1998; Erinosho et al., 2013; Gerard et al., 2013; Kalidindi et al., 2009; Khan et al., 2015; Sabnis et al., 2013; Sarma and Dawson, 1996; Tamini et al., 2014; Van Houtte et al., 2002; Zhang et al., 2015b) and elevated temperatures (Li et al., 2004; Quey et al., 2012) with good agreement with experimental measurements. They have also been used to simulate the deformation of grain structures at room temperature for polycrystals (Heripre, 2007; Kanjarla et al., 2010; Musienko et al., 2007; Pokharel et al., 2014; Raabe et al., 2001; Rossiter et al., 2010; Rotters et al., 2010; St-Pierre et al., 2008) but comparison with intra-granular strain measurements usually only shows qualitative agreement with clear local discrepancies between modelling and experimental results. Better agreement is usually obtained for the deformation of oligocrystals (Delaire et al., 2000; Kalidindi et al., 2004; Klusemann et al., 2012, 2013; Lim et al., 2011, 2014; Turner et al., 2013; Zhao et al., 2008) for which the geometry of the grain structure is better represented in three dimensions in the simulations.

Studies focussing on similar prediction of intra-granular deformation of metals at high homologous temperatures are scarce due to the difficulty of measuring strain distributions at that scale, especially under large deformation conditions typical of hot forming operations, in order to validate the models.

Several experimental techniques have been developed to measure strain distributions at the scale of microstructures. Methods based on Digital Image Correlation (DIC) (Sutton et al., 1991) are now commonly used but most studies have been carried out at room temperature, usually by combining DIC with in-situ testing conducted inside the chamber of a SEM (e.g. Ghadbeigi et al., 2012 for large deformation applications). One such study has been carried out at 950 °C recently (Torres et al., 2014). However, deformation conditions from the tensile test carried out in the latter study are not representative of the large compression experienced by metals in a hot rolling process. An alternative technique based on microgrids used in a PSC test carried out at 950 °C has enabled the measurement of strain distributions within the two-phase microstructure of a Duplex steel (Martin et al., 2013). However, the grids had to be engraved through chemical etching to ensure successful results, which affected strain resolution measurements and potentially subsequent microstructure evolution due to the grooves generated at the surface of the metal. Furthermore, the study did not include local orientation measurements at the microstructural scale.

The aim of this work is, therefore, to develop a CPFE model for the simulation of the hot deformation of single phase Face-Centred-Cubic (FCC) metals, such as aluminium alloys or steels rolled in their austenitic range during hot rolling, and assess the reliability of the results through comparison with experimental measurement of local strains and orientations. A new procedure has, therefore, been developed to measure both local intra-granular strain distributions and orientations in the microstructure of a single-phase steel deformed at 1000 °C under conditions representative of hot forming operations.

2. Experimental procedure

Experiments have been carried out at both high homologous and room temperatures in order to assess the reliability of CPFE predictions at various scales and temperatures. Statistical prediction from the model has been assessed through comparison with texture measurements, using Electron-Back-Scattering-Diffraction (EBSD), following a PSC test carried out at 300 °C on an aluminium alloy AA5052. A PSC sample 60 mm long along the rolling direction (RD), 50 mm wide along the transverse direction (TD) and 10 mm thick along the normal direction (ND) of the as-received hot rolled plate was heated from room temperature to 300 °C with a heating rate of 10 °C s^{-1} and soaked at this temperature for 10 s. The sample was then deformed in air to a thickness reduction of 60% with a strain rate of 9.0 s^{-1} using a state-of-the-art 500 kN Servotest thermo-mechanical-compression (TMC) machine capable of applying controlled strain rates up to 200 s^{-1}. A schematic drawing of the PSC test is shown in Fig. 1(a). The recommended aspect ratios to ensure plane strain conditions are: $b_0/w \geq 2$, $h_0/w \leq 0.67$ and $l/w \geq 3$, with b_0 and h_0 being the initial breadth and thickness of the specimen before deformation, w the width of the platen

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