Mechanics of Materials 101 (2016) 27–39

Contents lists available at ScienceDirect

Mechanics of Materials

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

Research paper

3D micromechanical modeling of dual phase steels using the representative volume element method

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ARTICLE INFO

Article history:
Received 25 February 2016
Revised 28 June 2016
Available online 18 July 2016

Keywords:
3D modeling
Dual phase steels
Micromechanical modeling
Microstructural design
Quantitative metallography
Representative volume element

ABSTRACT

There is a steady increase in the implementation of dual phase steels in stamped automotive components. Therefore, steel suppliers who develop dual phase steels are interested in predicting the microstructure-properties relationship for optimization of microstructural design. This goal is achievable by micromechanical modeling. The representative volume element (RVE) method has been a popular technique for micromechanical modeling of dual phase steels. It is generally considered that 2D modeling underestimates the flow curves and that 3D modeling predicts the experimental stress-strain curves more accurately. However, much of the research has focused on 2D modeling. This paper develops 3D micromechanical modeling of DP500 and bainite-aided DP600 steels by including statistical quantitative metallography data in the models. More than 3000 grains were analyzed in each steel. Hence, both volume fraction and morphology of martensite were statistically determined. This model predicted the ultimate tensile strength of these two dual phase steels with less than 0.5% error.

1. Introduction

1.1. Microstructure of dual phase steels

Dual phase steels have been used in the automotive manufacturing industry since the 1970s. Their combination of greater strength and ductility compared to conventional steels led to significant research on processing and microstructure-properties relationship of dual phase steels. Nowadays, dual phase steels are increasingly used for automotive inner panels and body-in-white components. Hence, steel suppliers are developing new grades of dual phase steels to meet the industrial requirements. Tasan et al. (2015) summarized recent microstructure-oriented advances for dual phase steels. They reviewed microstructure evolution of dual phase steels during processing, experimental characterization of micromechanical behavior, and the simulation of mechanical behavior, in order to understand the critical unresolved issues and to guide future research efforts.

The microstructure of dual phase steels consists of ferrite as the soft matrix and martensite as the hard phase, and small amounts of bainite may also be present. Ferrite is an interstitial solid solution of carbon in body centered cubic (bcc) iron. It is the predominant phase in low carbon steels including high strength low alloy steels (HSLA) and dual phase steels. The flow stress of the ferrite is generally controlled by chemical composition and grain size, and is also influenced by dislocations which are generated from the austenite to martensitic phase transformation during processing of steels (Liedl et al., 2002).

Martensite is a supersaturated solid solution of carbon in iron. Martensite is a secondary phase in dual phase steels which increases the strength of dual phase steels. The mechanical strength of martensite primarily depends on its carbon content. The mechanical properties of dual phase steels significantly depend on the volume fraction and morphology of martensite (Gündüz, 2009; Hwang et al., 2005). Martensite is the major cause of microstructural damage in dual phase steels at quasi-static and high strain rate deformation and at different strain paths (Samei et al., 2016, 2014a).

Bainite forms by decomposition of austenite at a temperature above the martensite start temperature (M_s) and below the pearlite formation temperature. Bainite is a combination of plate-shaped ferrite and carbides. Bainite is presented in two forms: lower-bainite and upper-bainite. Lower-bainite forms at temperatures closer to the M_s, while upper-bainite forms at higher temperatures. During heat treatment of dual phase steels, lower-bainite may form in the microstructure of dual phase steels. Bainite

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http://dx.doi.org/10.1016/j.mechmat.2016.07.011
0167-6636/

grains in dual phase steels commonly consist of cementite and dislocation-rich ferrite. Therefore, bainite is stronger than ferrite.

1.2. Plastic deformation of dual phase steels

Yielding and plastic deformation in dual phase steels starts in the ferrite grains. Hence, the yielding behavior of dual phase steels is controlled by the ferrite properties. During plastic deformation of dual phase steels, martensite generally exhibits elastic deformation unless the strain reaches high levels; however, martensite has a significant influence on work hardening of dual phase steels (Samei et al., 2014b, 2013)

Low carbon steels generally exhibit yield point elongation. The yield point phenomenon includes upper and lower yield points in the tensile stress-strain curve followed with oscillations of the flow stress. In low carbon steels, dislocations are locked by the interstitial carbon atoms. The shear stress required to cause dislocation movement inside the grain is less than the shear stress necessary to unlock them, and this causes a sharp drop in stress at the yield point (Cottrell and Bilby, 1949).

The yield point phenomenon is not usually observed in dual phase steels and the flow curves of dual phase steels normally exhibit continuous yielding due to the processing of dual phase steels. Austenite and martensite have face centered cubic (fcc) and body centered cubic or body centered tetragonal (bcc or bct) crystal structures, respectively. Hence, a volume expansion occurs during the austenite to martensite phase transformation during processing of dual phase steels. This volume expansion introduces plastic deformation and therefore, geometrically necessary dislocations (GNDs) are generated at the ferrite/martensite interface. By increasing the volume fraction of martensite the number of GNDs increases. There are mobile dislocations among the GNDs which can move immediately at the onset of yielding, and thus produce a smooth flow curve. However, in dual phase steels with low martensite content, the number of GDNs is not sufficiently high to cause continuous yielding. Hence, yield point phenomenon is observed in low-martensite dual phase steels. Calcagnotto et al. (2010) investigated the GNDs in two ultrafine grained dual-phase steels with different martensite particle size and volume fraction. They reported that steel with higher martensite fraction has a lower elastic limit. A detailed study of the influence of GNDs on the plastic deformation of dual phase steels is reported by Kadkhodapour et al. (2011).

1.3. Background and methodology

Dual phase steel sheets are used increasingly in automotive inner panels and body-in-white components because they provide a good combination of strength and formability which are required for design flexibility and weight reduction. Nevertheless, steel suppliers strive to further enhance the mechanical properties of dual phase steels by optimizing their microstructure. The representative volume element (RVE) method is a micromechanical modeling technique which predicts microstructure-properties relationship in multi-phase materials such as dual phase steels. It is a modeling method that helps to understand the influence of microstructure on mechanical properties and is therefore well suited for optimization of microstructural design. The fundamentals of the RVE technique are presented in Section 2.

Either 2D or 3D RVEs can be used for micromechanical modeling of flow behavior of dual phase steels. Al-Abbasi and Nemes (2003), Uthaisangsuk et al. (2011), and Ramazani et al. (2013a) have modeled flow curves of dual phase steels using 2D and 3D RVEs. They reported that 2D RVEs underestimate the flow curves of dual phase steels whereas 3D RVEs predict more accurate stress-strain curves. However, the use of 3D RVEs requires more advanced computational resources and significantly increases the time of calculations, therefore most of the research has focused on 2D modeling.

Most of the previous reports on 3D micromechanical modeling of dual phase steels have only included phase volume fraction of martensite in the 3D RVEs (Al-Abbasi and Nemes, 2003; Ramazani et al., 2013a; Thomser et al., 2009; Uthaisangsuk et al., 2011). However, electron back scattered diffraction (EBSD) was recently used for quantitative microstructural analysis of dual phase steels (Brands et al., 2011)(Tasan et al., 2014)(Yan et al., 2015). In their work, Brands et al. (2016) constructed statistical 3D RVEs using a 3D EBSD system equipped with a focused ion beam (FIB). Extensive EBSD scans were carried out on a 16×2 mm area to obtain volume fraction and morphology of ferrite and martensite. As expected, the models accurately predicted the flow curves of the dual phase steels.

The objective of this paper is to develop a 3D micromechanical model that is able to accurately predict the flow behavior of two commercial dual phase steels in uniaxial tension: a DP500 steel and a bainite-aided DP600 steel. Both volume fraction and morphology of martensite are taken into account. Hence, the influence of martensite morphology on the mechanical properties of dual phase steels can also be investigated using the present model. The purpose of this work is to present a simple methodology to facilitate the application of the 3D RVE model in the steel industry using the commercial software Digimat and ABAQUS.

2. The representative volume element method

Microstructural parameters have a significant influence on the flow behavior of materials; however, microstructural features are not considered in phenomenological finite element modeling of materials. In all mechanical modeling, elastic and plastic parameters such as Young's modulus, Poisson's ratio, yield stress, hardening modulus and hardening exponent are considered. In micromechanical models, chemical composition and volume fraction and morphology of phases and grain size are also taken into account. Different modeling scales and methods for micromechanical modeling of dual phase steels are summarized by Tasan et al. (2015). The representative volume element (RVE) is a popular technique for micromechanical modeling of materials. As presented in Fig. 1, micromechanical modeling of flow behavior of a material using the RVE method consists of four steps. These steps are described in Sections 2.1–2.4.

2.1. Definition of the RVE

An RVE is a small volume of microstructure that has the general characteristics of the whole microstructure such as volume fraction, morphology and randomness of the phases and over which modeling of specific characteristics is carried out. The results of the RVE modeling investigations should properly describe the characteristics of the whole microstructure. An RVE should be sufficiently large to include the essential microstructural characteristics. On the other hand, the RVE size should be as small as possible so that the states of stress and strain can be approximately considered as homogeneous in the whole RVE. Also, a smaller RVE requires less computational resources such as memory and calculation time to simulate the deformation. An advantage of micromechanical modeling using the RVE method is that the RVE provides a detailed description of the stress and strain distributions and their evolution in the microstructure during a metal forming process (Ramazani et al., 2014; Thomser et al., 2009; Uthaisangsuk et al., 2011).