Computational Materials Science 95 (2014) 651–662

Contents lists available at ScienceDirect

Computational Materials Science

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

Numerical modeling of dual phase microstructure behavior under deformation conditions on the basis of digital material representation

L. Madej [a,*], J. Wang [b], K. Perzynski [a], P.D. Hodgson [b]

[a] AGH University of Science and Technology, Mickiewicza 30 av., 30-059 Krakow, Poland
[b] Institute for Frontier Materials, Deakin University, Geelong, Victoria 3217, Australia

ARTICLE INFO

Article history:
Received 5 March 2014
Received in revised form 5 July 2014
Accepted 22 August 2014
Available online 16 September 2014

Keywords:
Numerical modeling
Dual phase steels
Digital material representation
Micro-compression

ABSTRACT

Development of a digital material representation (DMR) model of dual phase steel is presented within the paper. Subsequent stages involving generation of a reliable representation of microstructure morphology, assignment of material properties to component phases and incorporation of the model into the commercial finite element software are described within the paper. Different approaches used to recreate dual phase morphology in a digital manner are critically assessed. However, particular attention is placed on innovative identification of phase properties at the micro scale by using micro-pillar compression tests. The developed DMR model is finally applied to model influence of micro scale features on failure initiation and propagation under loading conditions.

1. Introduction

There is high demand in the automotive industry to develop new metallic materials that have superior mechanical properties but low weight. As a result, the number of new steel grades has increased exponentially for the last decade [1], and this trend continues. A series of innovative steels (e.g., DP – dual phase, BH – baking hardening, IF – interstitial free, CP – complex phases, TRIP – Transformation Induced Plasticity, TPN – three-phase nano, nano-bainitic) as well as other metallic materials (e.g., aluminum, magnesium, titanium or copper alloys) are being developed in various research laboratories around the world [2–6]. These modern steels are characterized by elevated material properties, resulting from sophisticated microstructures with a combination of features such as large grains, small grains, inclusions, precipitates, nanoparticles, different phases, Luders bands, Portevin-le-Chatelier bands, and shear bands. Interaction among these features at the micro scale and the surrounding material under loading conditions results in the required properties at the macro scale.

To obtain these highly sophisticated microstructures, complex thermo-mechanical operations are applied. Due to the above mentioned extraordinary properties, a significant increase in the use of modern steels to manufacture auto body components is observed [7–9]. The automotive industry is primarily focused on the application of the second generation of advanced high strength steels (AHSS). These steels make it possible to reduce automobile weight to improve fuel efficiency, while maintaining or even increasing safety (crash worthiness). Dual Phase (DP) thin steels, with the tensile strength of 400–1200 MPa (Fig. 1), is the most commonly used material for industrial use.

As seen in Fig. 1, DP steels have been successfully applied in automobile structural parts. This is because they have a combination of good formability, high bake hardenability and high crash worthiness. These elevated properties are the result of precisely designed microstructure morphologies, which consist mainly of ferrite matrix (around 70–90%) and hard martensitic phase (around 10–30%) as seen in Fig. 2a. The continuous annealing process is commonly used to obtain DP ferritic–martensitic steels in industrial practice. Thin strips of cold rolled steel of a ferritic–pearlitic structure are annealed in the ferrite (α) + austenite (WW) two-phase region— called intercritical annealing—and then control cooled, enabling the austenite to transform into martensite (Fig. 2b). Properties of DP steels are affected by many factors, including the volume fraction of martensite, average carbon content and carbon distribution in martensite, ductility of martensite, distribution of martensite, ferrite grain size, carbon and alloying elements content in ferrite, etc. [11,12].

The required combination of DP steel properties is usually obtained by a proper balance between chemical composition of DP steels and processing parameters. However, it seems that the higher the strength level of a DP grade, the more complicated the manufacturing process of those steels becomes due to high deformation forces and failure probability. In general, response of DP

* Corresponding author. Tel./fax: +48 12 617 5154/2921.
E-mail address: lmadej@agh.edu.pl (L. Madej).

http://dx.doi.org/10.1016/j.commatsci.2014.08.035
0927-0256/

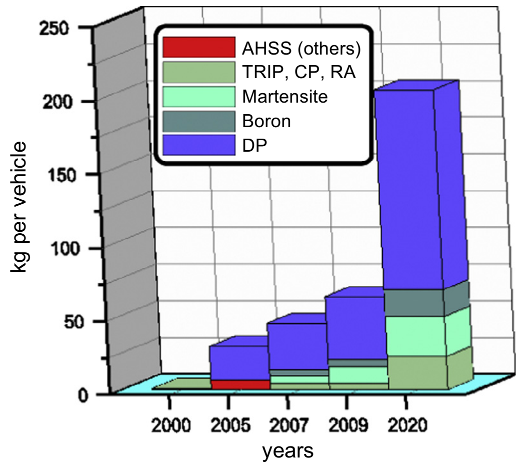

Fig. 1. Development of parts made of DP steels in a car body [10].

steels to deformation modes is very complex and depends on many factors.

The fact, that soft ferrite matrix and hard martensite constituent have significantly different strength properties, leads to inhomogeneous material deformation and the possibility of failure during manufacturing should not be underestimated. Technical literature describing the effect of microstructural parameters on the properties of DP steels provides adequate knowledge [11–13], however, the problem of failure has not yet been solved. And this issue plays a crucial role in practical applications. For investigation purposes the state-of-the-art experimental equipment must be used (e.g., in-situ deformation, electron microscopy, SEM/EBSD/FIB). Initial results obtained on the basis of such equipment has been recently realized in several research institutes and has proven its efficiency in micro scale analysis of cracks [14].

To support this fundamental experimental research and lower the costs of such investigations, numerical modeling techniques can be applied. The finite element (FE) method is the main tool usually used in many research facilities to simulate various deformation processes, and it gives satisfactory results [15]. This method is used to describe material behavior as a continuum and is based on general relationships between strains and stresses despite the presence of various phases in a DP steel. To obtain accurate flow stress data that are necessary for FE analysis, a series of plastometric tests in various deformation conditions (temperatures and strain rates) is performed [16]. Furthermore, inverse analysis can be applied to take into account the heterogeneities related to experimental conditions (e.g., friction) [17]. Thus, a stress–strain relationship can be obtained that is insensitive to a sample's geometry, type of test, etc. Because large samples containing billions of grains are investigated, a major assumption of the approach is that behavior and interactions of subsequent grains are averaged in the form of a single flow stress model. This procedure is widely used in modeling metalforming operations [18].

However, recent experimental research has proven that the size, shape or position of the hard martensitic phase directly influences material behavior under loading conditions, especially when phenomena such as fracture are considered [19,20]. Therefore, it is crucial to create a robust model of DP steels based on modern numerical approaches that take into account the influence of microstructure on failure initiation and propagation during simulation. One of the solutions to create such a micro scale model is Digital Material Representation (DMR), which has been intensively developed in scientific literature [21–25].

2. Digital material representation (DMR) concept

The DMR is expected to create the possibility of analyzing material behavior in conditions that are difficult or even impossible to be monitored experimentally [26]. The general concept of the DMR approach is presented in Fig. 1.

As seen in Fig. 3, there are three main issues that have to be addressed when the numerical model on the basis of the DMR approach is created:

- The first, is generation of the material microstructure with specific grain shapes. The best way is to create digital microstructures as exact replicas of real microstructures. In this case an image of real microstructure is required, what always employs a series of experimental analysis. This procedure is becoming quite complex when 3D digital microstructures are necessary. The other solution is to use a statistically equivalent microstructures created using only numerical methods. That way a 2D and 3D digital microstructures can be obtained in a fast and efficient way.
- The second, is assignment of material properties to particular microstructure features. Usually nano-indentation tests [27] or monocrystal deformation [28] are used to investigate material behavior at the micro scale level.
- The third issue that influences accuracy of the results obtained from simulations with DMR is the mesh density and its topology. Limited amount of research is devoted to this subject (see for example [21]).

These DMR are further used in numerical simulations of processing or simulation of behavior under exploitation conditions based on e.g. finite element or cellular automata methods. The more accurate the digital microstructure morphology, assigned

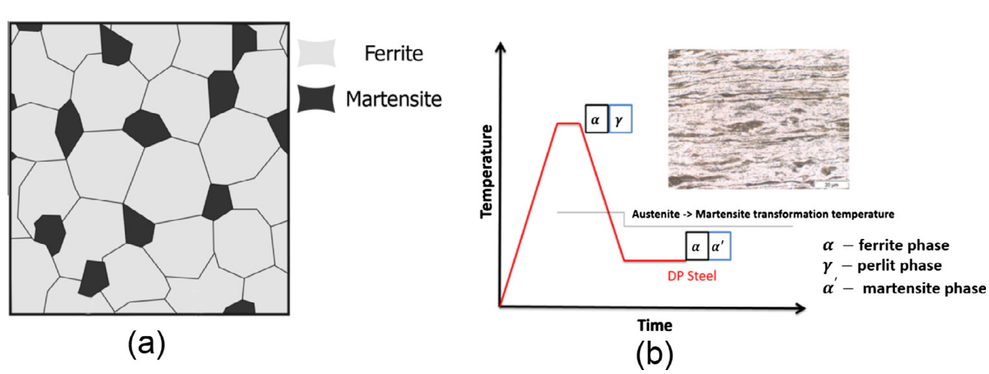

Fig. 2. Schematic illustration of the (a) two-phase microstructure and (b) controlled annealing thermal cycle [13].