Development of a comprehensive fracture model, which takes into account crack initiation and propagation behavior at the microscale level in the Dual Phase (DP) steels is presented in the present paper.

At this stage of the research Authors proposed a numerical model, which takes into account ductile crack initiation and propagation through the ferrite phase. Developed model is based on digital material representation (DMR) of DP microstructure, which takes opportunity for modeling crack phenomena in an explicit manner. Proposed model of ductile crack behavior in the ferritic phase is based on the Johnson-Cook model. Particular attention is put on investigation of influence of martensite volume fraction in microstructure on failure behavior. Obtained results for two significantly different martensite volume fractions in the investigated microstructure are presented in this work.

Keywords: fracture, dual-phase steel, digital material representation

1. Introduction

Significant need presented by an automotive and aerospace industry for new metallic materials that can meet strict requirements regarding weight/property ratio has been recently observed. This need is a driving force for fast development of modern innovative steel grades. The number of new steel grades developed from the year 2000 has increased exponentially [1]. A series of innovative steels (TRIP, TWIP, DP, Bainitic, nano-Bainitic etc.) as well as other metallic materials e.g. aluminium, magnesium, titanium or copper alloys is being developed in various research laboratories around the world [2-6]. Complex thermomechanical operations are applied to obtain highly sophisticated microstructures with combination of e.g. large grains, small grains, inclusions, precipitates, multi-phase structures etc. It is commonly believed that these microstructure features and interaction between them at the micro-scale level during manufacturing or exploitation stages result in highly elevated material properties at the macro-scale. As a result significant increase in the application of these modern steels to auto body components production has been observed [7-9].

One of those new steel grades are advanced high strength steels (AHSS). They provide a possibility of reducing the automobile weight (increase of the fuel efficiency), while maintaining or even increasing their safety (crash worthiness). Example of those advances steels are Dual Phase (DP) thin steels, with the tensile strength of 400-1200 MPa. They have been successfully applied in the production of the automobile structural parts because they are characterized by combination of a good formability, high bake hardenability and crash worthiness. These elevated properties are the results of the properly designed microstructure morphologies, which consists mainly of ferrite matrix (around 70-90%) and a hard martensitic phase (around 10-30%) as seen in Fig. 1. The usual approach used to obtain a DP ferritic-martensitic steel is the annealing of a ferritic-pearlitic structure in the \(\alpha + \gamma\) two-phase region, called intercritical annealing, followed by controlled cooling, enabling the austenite to transform into martensite. Properties of DP steels are affected by many factors, includ-
ing: 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 [10-12].

Required combination of DP steel properties is usually obtained by 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 becomes the manufacturing of those steels, because of high deformation forces and failure probability. In general, response of the DP steels to deformation modes is very complex, and depends on many factors. Mentioned increase of the difference in strength between soft matrix and martensite constituent leads to inhomogeneous material deformation. Due to combination of two phases with significantly different properties, the problem of failure during manufacturing stages is of importance. Technical literature describing the effect of microstructural parameters on the properties of DP steels provides adequate knowledge, however, the problem of failure is still not solved. And this issue has a crucial character for practical applications. The majority of works dealing with failure is based on fundamental experimental research [13-15]. To investigate this complex issue a state-of-the-art experimental equipment have to be used e.g. in-situ deformation, electron microscopy, SEM/EBSD/FIB. Initial work realized on the basis of such equipment has been recently used in several research institutes and proved its efficiency in micro scale analysis of crack.

To support this fundamental experimental research and lower the costs of such investigation, a numerical modelling techniques can be applied. The finite element method is the main tool usually used in many research facilities to simulate various deformation processes and it gives satisfactory results. This method is used to describe material behaviour as a continuum and it 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 the FE analysis, a series of plastometric tests in various deformation conditions (temperatures and strain rates) is performed. To take into account the heterogeneities related, for example to friction, an inverse analysis is applied. That way stress-strain relationship that is insensitive to a sample geometry type of the test etc., is obtained. Due to the fact that large scale problems containing billions of grains are considered, the major assumption of the mentioned approach is that behaviour and interaction of particular grains is averaged in form of one single flow stress model. This procedure is well established and is widely used to solve problems occurring during material deformation at the macroscale. To extend numerical modelling capabilities the FE codes are usually combined with different crack models based on Johnson-Cook criterion or more sophisticated methods like eXtended Finite Element Methods [16]. It can be stated that the fracture modelling in these approaches is again mainly simulated at the macroscopic scale level because the morphology of the microstructure e.g. of dual phase steels is neglected. At the same time experimental research has proved that the size, shape or position of the hard martensitic phase directly influences failure initiation and propagation.

That why the main aim of the proposed approach by the Authors is to create a robust model of failure for DP steels based on modern numerical approaches that take microstructure explicitly during deformation. One of the solution to create such a micro scale model is a Digital Material Representation (DMR) idea intensively developed by the Authors [17-18].

2. Digital representation of the dual-phase steel microstructure

The concept of the DMR has been proposed recently and it is dynamically evolving. The main objective of the DMR is creation of the digital representation of microstructure with its features represented explicitly as seen in Fig. 2. The DMR basic concept creates possibility to describe material at various scales. Such approach offers gathering and processing of metallurgical data, which is related to each other at the different levels of description. Thus, the complex DMR system consists of several software modules. Some of these modules are dedicated to selected single scales, e.g. characterization of material microstructure (micro-scale). On the other hand, the rest of the modules span some of the scales together to perform multi-scale calculations, e.g. micro shear and shear bands or dynamic recrystallization.

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Fig. 2. a) Initial optical microstructure, b) digital microstructure obtained after image processing, and c) digital microstructure with the finite element mesh generated in mesh generator [19-21]
The more precise DMR is applied, the more realistic results of calculations regarding material behaviour are obtained. Due to that conclusion, the detailed virtual analysis of simulation results can be performed, while errors of calculations are minimized. This allows the replacement of the conventional methods, dedicated to determination of material properties, by the computer automatic analysis, which connects DMR with modelling of manufacturing processes and with digital analysis of results. The DMR can be used during calculations as a Unit Cell or Representative Volume Element (RVE), depending on what kind of information are required: local or global, respectively. Usually several Unit Cells are considered as RVE. Literature review on various methods that are used during creation of microstructure morphology of both single and two phase microstructures are in earlier authors works [22-23].

Due to the complex shapes of phases in an investigated dual phase steels, the DMR model will be created on the basis of real microstructures images obtained from optical microscopy. Developed model will be the basis for the creation and identification of robust ductile failure model for DP steels.

3. Preparation of digital material representation approach

Due to the fact that only part of the sample is replicated during numerical simulation to ensure the space continuity the periodic boundary conditions are taken into account. However, digital microstructures created on the basis of microscopy image are not periodic, that is why before adopting periodic boundary conditions to the DMR Authors added a specific buffer zone to create an investigated Unit Cell. That way transferring of displacement field between left and right border in the model is possible [24]. Schematic representation of the buffer zone with applied periodic boundary conditions is shown in Fig. 3.

As mentioned ductile crack prediction in microstructures with different amount of martensite fraction is addressed within the present research. Two numerical models based on two different digital material representations were created simultaneously. Both DMR were prepared from images representing real microstructures of the DP steel received after quenching process. Two various quenching conditions were applied to differentiate amount of martensite. In the first case cooling rate equal to 1°C/s was applied, while in the second case it was equal to 475°C/s. As a results two microstructure morphologies were obtained with martensite volume fractions: 24.5% and 64.5%, respectively as seen in Fig. 4. In the case of Dual Phase steels obtained morphology of micro scale features is closely related to e.g. cooling conditions, state of the initial microstructure, level of alloying elements etc. Thus, the problem of representatives of investigated microstructures both from experimental and numerical point of view remains open [25]. That is why for the purpose of development of DMR Unit Cell representations, Authors selected microstructures located in the center of the plate where the most uniform processing conditions are expected.

Fig. 3. Periodic boundary conditions applied for the two edges of the DMR model

![Fig. 3. Periodic boundary conditions applied for the two edges of the DMR model](image)

Fig. 4. Real microstructures of dual phase steel made after quenching process with speed a) 1°C/s and b) 475°C/s (courtesy of prof. Roman Kuziak IMŻ Gliwice)

![Fig. 4. Real microstructures of dual phase steel made after quenching process with speed a) 1°C/s and b) 475°C/s (courtesy of prof. Roman Kuziak IMŻ Gliwice)](image)

For both simulations the same material properties for the martensite and ferrite phases were used. Based on simple rule of mixture different material definitions were adopted to surrounding buffer zone for the two investigated cases (Fig. 4). As a results material properties of the buffer zone are associated with percentage amount of ferrite and martensite structure and can be considered as properties of homogenous material.
Obtained digital material representation were discretized with high mesh density along phase boundaries were large solution gradients are expected. Number of finite elements used for discretization was set to about 100000. Three node linear plane strain triangle finite elements (CPE3) were chosen for the discretization purposes. The applied specific mesh was obtained with developed FE mesh generation software [23]. Models were created in commercial Abaqus application and calculated using explicit solver. Boundary conditions presented schematically in Fig. 5 were applied during calculations.

4. Ductile failure investigation

Ferrite phase during large plastic deformation fails by ductile failure mechanisms. For resolving problem of ductile crack initiation and propagation Authors decided to use ductile criterion approach. In ductile criterion it is assumed that the equivalent plastic strain at the onset of damage, $\bar{\varepsilon}_{pl}^D$, is a function of stress triaxiality and strain rate [26]:

$$
\bar{\varepsilon}_{pl}^D(\eta, \dot{\bar{\varepsilon}}_{pl}) = \frac{e_t^+ \sinh[k_0(\eta^+ + \eta)] + e_t^- \sinh[k_0(\eta^- - \eta^-)]}{\sinh[k_0(\eta^- - \eta^+)]} + \epsilon_{+T} - T \sinh[k_0(\eta^- - \eta^+)]
$$

where: $e_t^+$ and $e_t^-$ – equivalent plastic strain for equibiaxial tensile and equibiaxial compressive deformation respectively, $\eta^+$ and $\eta^-$ – stress triaxiality (a ratio of the equivalent mean stress $\sigma_m$ to the Mises equivalent stress $\sigma_{eq}$) for equibiaxial tensile and equibiaxial compressive deformation respectively, $k_0$ – parameter obtained experimentally. These parameters depend on the material, strain rate and temperature of the process. Failure in this model occurs when state variable defined by (2) reaches value of 1.

$$
w_D = \int \frac{d\bar{\varepsilon}_{pl}^D}{\bar{\varepsilon}_{pl}^D(\eta, \dot{\bar{\varepsilon}}_{pl})} = 1
$$

where: $d\bar{\varepsilon}_{pl}^D$ – plastic strain increment per simulation unit time.

The crack initiation parameters for ferrite failure were adopted in the present work based on [27] and its evolution is presented in Fig. 6.

![Fig. 6. Derived damage curve for ferrite in DP steel [27]](image)

Examples of obtained results based on described DMR approach combined with ductile failure criterion are presented in Fig. 7. Because real microstructure morphology is taken into account highly inhomogeneous strain distribution is obtained during deformation. Major part of accumulated plastic strain is within the softer ferrite phase. Zones where strain value is high e.g. due to morphological features can be the locations of ductile crack initiation according to (2). In models with different martensite volume fractions, level of the strain localization during deformation between martensite islands is significantly dissimilar. As a results in the model with lower martensitic volume fraction cracks start to initiate and propagate in the end of the deformation. While in the second model due to higher strain localization resulting from large area fraction of hard martensite, cracks start to initiate earlier during the deformation. Differences in the failure process between these two investigated microstructures is clearly visible in Fig. 7.

![Fig. 7. Numerical results of ductile cracks for microstructures with a) 24.5% and b) 64.5% of martensite volume fraction](image)

Discrepancies that can appear during numerical simulation if failure model is not taken into account are presented in Fig. 8. The same process conditions were applied during

![Fig. 8. Stress-Strain curves representing comparison between models with and without included ductile crack model](image)
deformation. The only difference was consideration of ductile failure model. Such comparison clearly highlights how it is important to consider failure models in simulations of such complex microstructures.

However, not only detailed information regarding inhomogeneous strain distribution, and fracture propagation during deformation can be obtained. Using this approach a response in the form of flow stress model can be obtained as seen in Fig. 8. Then it can be used during macro scale calculation of behavior of a complete automotive components during the procedure of manufacturing chain modeling [28]. A relations between microstructure morphology and its properties can be directly established using the presented approach.

5. Conclusions and future work

Inhomogeneous strain distribution and crack propagation in the microstructure of dual-phases steel simulated on the basis of digital material representation was presented in the paper. The major conclusion from the research is that it is important to include representation of geometry of the phases structure during numerical simulations. Precise consideration of shape of the phases received after quenching process allow to predict inhomogeneous strain distribution across microstructure during further processing operation. The strain localization zones seems to be the locations for ductile cracks initiation. It can also be concluded that by application of the DMR with the ductile criterion it is possible not only to simulate crack initiation and subsequent propagation but also make relations between micro scale behavior and macroscopic response.

The next part of the work will be based on modeling brittle and ductile cracks at the same time, as based on experimental research ductile failure initiation in ferrite is also related to brittle cracks propagation in martensite phase.

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