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Development and validation of multi scale failure model for dual phase steels

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ABSTRACT

Development of finite element (FEM)/eXtended finite element (XFEM) numerical solution combined with the digital material representation (DMR) approach to simulate brittle/ductile fracture is the subject of the present work. The paper is divided into three main parts. In the first, proposed procedures for development of DMR model of investigated two phase steel are described. Then, details on the FE/XFE model to simulate interrelations between ductile and brittle fractures occurring within particular phases are presented. Finally, model validation stage based on comparison between experimental and numerical results is discussed. The typical industrial hole expansion test was used as a case study for validation purposes. To numerically describe material behavior at various length scales from microstructure to macro sample a multi scale concept was used in the part as well.

1. Introduction

In recent years significant amount of modern steel grades and light weight metals have been developed throughout the scientific laboratories to provide required materials for practical applications in various industries including automotive one [1–4]. To provide sufficient macroscopic in-use properties these modern materials have usually composite type microstructures, where micro scale feature interact locally between each other and surrounding matrix. These local interactions are directly related to specific elevated macroscopic properties. Thus, several thermomechanical operations are applied to obtain mentioned, highly sophisticated microstructures with combination of e.g. inclusions, nano-particles, multi–phase structures etc. With increasing understanding of behaviour of these microstructures under processing conditions comes also significant increase in their application to vehicle chassis as well as body components production [5,6]. An example of such a group of materials are advanced high strength steels (AHSS) in particular dual phase (DP) steels [7]. These steels due to multi-phase microstructure can provide reduction in the weight of the chassis and at the same time increase crash worthiness, which is of importance from safety point of view. However, composite microstructure with features characterized by significantly different properties are also susceptible to failure during manufacturing operations. Thus, to minimise this disadvantage a series of investigations should be performed to understand underlying physical mechanisms and redesign manufacturing cycle. Experimental investigation in laboratory or semi-industrial scales is usually used as it provides required information on mechanisms occurring at the microstructure scale. However, this investigation can also be supported by a modern numerical analysis with multiscale character, that can deliver high quality results faster and cheaper. The key aspect in this case is to take into account microstructure in an explicit manner during simulation as shape, position or dispersion of different microstructural features directly influence initiation and propagation of failure [8,9].

That is why authors developed a multi scale numerical model of failure based on the digital material representation (DMR) concept [10,11], that considers behaviour of particular microstructure features during simulation. Mentioned dual phase steels have been selected as a case study for model application and validation. These steels are composed of ferritic matrix and hard martensitic islands occupying approx. 20% of material volume. To simulate behaviour of each phase and their interactions proposed model has a hybrid character, where both ductile and brittle fracture that occur in ferrite and martensite, respectively, can be predicted. The ductile fracture is modelled by the Ductile Fracture criterion implemented within conventional FE model, while brittle fracture is predicted by more sophisticated eXtended Finite Element Method (XFEM). Proper data transfer protocols between these two methods were proposed within the paper to create a complex numerical model. Finally, the developed micro scale solution became the basis for the multiscale model, where micro model provides

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information about failure initiation to the macro scale level. The model was validated with the experimental hole expansion test and proved its good predictive capabilities.

2. DP fracture models based on the FEM approach

Modelling fracture in DP steels is a complex task because of the composite character of the investigated microstructure. There are two phases with significantly different mechanical properties: soft ferrite as a matrix and hard constituent phase as inclusions. Review of classical approaches to deal with this issue can be found in [12]. However, recently modelling of fracture initiation and propagation based on the DMR approach is becoming more popular and development of different models, which take into account fracture with various fracture criteria in DP steels can be found in scientific literature.

The first group of models resolves fracture in dual phase steel as a result of the maximum strain that is localized in the small area. Identification of maximum strain localization zones in material is the main subject of e.g. [13]. Authors compared experimental and numerical results obtained on DP800 steel grade. Real macroscopic tension experiment showed that crack initiates in zones where the sample starts necking and where strain reaches maximum value. Microscopic experiments showed small cracks existing in close proximity between hard constituent phase islands. Numerical investigation based on the representative digital microstructure obtained from metallographic analysis and combined with elasto–plastic material model revealed large stress localization, which generates accumulative shear strain. Similar experimental and numerical investigation was made on different DP grades in [14,15]. In these works authors prepared series of the DMR structures where martensite volume fraction varied from 7% to 90%. Numerical experiment based on the elasto–plastic material model without fracture criteria revealed sites with maximum localized strain values. These sites can be treated as future crack initiation locations. Similar works have been realized based on artificially generated digital microstructures, which statistically reflect real morphology [13,16].

The second group of fracture models consider damage initiation on voids. These models take into account nucleation, growth and coalescence of voids during material deformation. For this reason Gurson–Tvergaard–Needleman (GTN) model is often used.

Soyarslan et al. [17] developed numerical bending test for simulation of macrocrack formation in DP1000 steel grade. Calculations were supported by experimental investigation, which was used to determine GTN model parameters. Dalloz et al. [18] presented similar work on effect of shear cutting in DP steel, where GTN model was used to determine crack propagation directly during cutting process. Authors performed two plastometric tests for tension and crack opening processes to predict size and shape of micro voids observed through fractography. Experimental procedures were used to determine coefficients of the GTN damage model. Similar work was done by Ramazani et al. [19]. Authors prepared simulation of cross–die test with GTN model. The model was verified through forming limit diagram (FLD) curves recorded during experimental and numerical tests. In [20–22] authors took statistical representative volume element of the material into account. First, authors made simulations at the macro scale (the hole expansion or stretching tests), where deformation state was used as input parameter to create simulations at the micro scale. Maximum force leading to crack initiation was compared to the force received during experimental investigation.

Another widely used, fracture criterion that is calibrated through real experimental procedure for DP steels, is called Johnson–Cook (JC) criterion. There are a lot of works where authors prepared experiments and determined material state parameters for DP steel grades based on the criterion. The JC criterion is implemented in almost all of the commercial numerical applications and gives opportunity for qualitative explanation of the observed fracture phenomena. In [23] authors used JC criterion for modelling cracks in different DP steel grades during electro–hydraulic forming conditions. Another work [24] resolves problem consisting of multiscale fracture modelling in the sample during impact test. Deformation state from macro model was set as boundary condition to a micro model. DMR used during simulations was built with three different ferrite volume fractions. Materials constants for the JC criterion were determined during two plastometric tests: tension and impact, respectively. Behrens et al. [25] considered failure of two cold–rolled hot–dip galvanised dual phase steel grades for cold forming namely: HCT600XD and HCT780XD. In [26] authors prepared simulation of the microstructure deformation where ductile fracture was calculated by the JC model. This work emphasizes the large influence of the mesh sensitivity required for the successful execution of fracture calculations.

Fracture modelling techniques in commercial numerical applications are mostly based on the FE method. The above review presented a great number of models for fracture prediction in dual phase steel grades as a result of microvoids coalescence, ductility or brittleness. However, developed models do not take into account interactions between ductile and brittle fracture modes. Usually only one mechanism is considered during simulation, which is a great simplification.

That is why, the main goal of the present paper is development of reliable fracture model of Dual Phase steels based on digital material representation concept that can simulate not only ductile and brittle failure but also can take into account interactions between them. Thus, one of the key aspects in the approach is development of numerical procedure capable to provide digital microstructure models both in 2D and 3D spaces.

3. Monte Carlo grain growth algorithm for DMR of DP steel

The proposed algorithm is based on the Monte Carlo grain growth model [27] properly adapted to recreate not only morphology of DP microstructure but also required volume fractions of ferrite and martensite. The model is composed of several subsequent steps. The first, is responsible for preparation of initial states of MC cells in the computational domain. Generation of input data that describe an initial state of material in the form of a three–dimensional matrix of cells is realized. A random state Q_i that belongs to $Q = \{Q_0, \ldots, Q_{n-1}\}$ is assigned to each cell in the investigated space. Second step is combined with random sampling of the entire space and is performed in order to calculate the energy change of each cell. Random change in cell states from the Q_n available states is another step. After the change of state, the energy of the system is again calculated and the probability of change in the cell state is calculated as well. If the calculated difference of energy takes a negative value, a new value of cell state is accepted otherwise the state is accepted with a probability p. With successive MC steps, the energy value of the entire system is reduced. Using the MC approach for modelling DP steel grade where hard constituent volume fraction is e.g. approx. 30% the amount of cell states Q is limited in the solution space Ω only to three ($Q = \{Q_0, Q_1, Q_2\}$). Proposed solution provided a possibility to generate three similar phases as seen in Fig. 1.

Then to obtain proper phase fractions, developed algorithm assigns one phase as a hard constituent and two others as ferrite providing representative microstructure of the DP steel as seen in Fig. 2.

As seen in Fig. 2, the final DMR consists of two separate phases. Such digital representation is usually satisfactory for fracture modelling in DP steels. However, the approach neglects information on ferrite grains within the ferritic matrix, and this information is important when failure is investigated. Adding a ferrite grains was realized with the cellular automata (CA) grain growth algorithm in two distinctive steps.

First the CA algorithm was used to generate nuclei of ferrite grains within the continuous ferrite phase from MC simulation, and then to model their growth. Number of new nuclei is equal to the number of required ferrite grains. For the growth purposes the Moore neighbourhood and a single transition rule were implemented, see for details