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HYBRID FE/XFE FINITE ELEMENT MODEL FOR SIMULATION OF BRITTLE-DUCTILE FRACTURES IN DUAL-PHASE STEEL GRADES.

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Abstract. *Development of hybrid finite element/eXtended finite element numerical solution combined with the digital material representation (DMR) approach to simulate brittle/ductile fracture is the overall subject of the realized research. This particular work 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 procedure of creation of representative digital material representation model to simulate interrelations between ductile and brittle fractures occurring within particular phases are presented. Finally, based on evaluated model parameters examples of its application to numerical simulation of failure in DP steels are presented.*

The main outcome from this work is the hybrid FEM/XFEM model, which can be easily applied to various deformation processes. The approach fulfils industrial demand to create a computer aided design of processes were fracture is an issue. Presented model is designed for practical research and industrial applications.

1 INTRODUCTION

Modelling fracture in dual phase (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. Recently modelling of fracture initiation and propagation based on the digital material representation (DMR) approach is becoming popular and different models, which take into account mainly ductile fracture with various fracture criteria in DP steels are being developed [1, 2].

That is why, the main aim of the approach proposed by the Authors is to create a robust model of both brittle and ductile failure in DP steels based on modern numerical approaches that take microstructure explicitly into account during simulation of deformation.

Authors developed a combined model of ductile and brittle fracture that occur in ferrite and martensite, respectively. Ductile fracture is modelled by the Ductile Fracture criterion implemented within classical Finite Element (FE) model, while brittle one is predicted by more sophisticated eXtended Finite Element Method (XFEM). Proper data transfer protocols between these two methods were proposed to create a hybrid numerical model.

2 DIGITAL MATERIAL REPRESENTATION

The concept of digital material representation was suggested approx. a decade ago and is dynamically evolving [3, 4, 5, 6]. The main objective of the DMR is to create digital representation of microstructure with its morphological features (i.e. grains, grain orientations, inclusions, cracks, different phases etc.) represented explicitly. Generation of material microstructure with specific geometrical features and properties is one of the most important algorithmic parts of systems based on the DMR. Such DMR is further used in numerical simulations of material processing. Recently a lot of research is put on the development of methods responsible for creation of the 2D and 3D representations of analysed microstructures.

To obtain an accurate description of the 2D microstructure an image processing methods are usually applied. As an input data for this analysis SEM/EBSD results can be used. In this case not only information on microstructure geometry is obtained but also information on initial crystallographic orientation is provided. This approach was successfully used in [7, 8]. Unfortunately the approach is time consuming and expensive because each numerical simulation based on DMR requires a SEM/EBSD analysis. That is why image processing is also applied to the optical microscopy images that are more affordable. However, in this case only information regarding grain morphology is obtained see e.g. [9]. Details of such procedure applied to the DP steel can be found in [10]. The approach is generally composed of the three main stages responsible for image filtering (denoising), phases distinction and phases analysis. These subsequently applied methods aim to detect phases, phase boundaries, and, finally, to prepare the material microstructure in the DMR form for further numerical simulations (Figure 1).

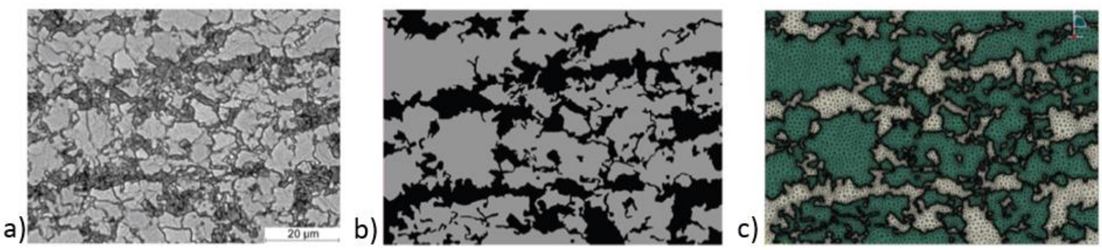

Figure 1: a) Real microstructure b) binary representation c) digital material representation with finite element discretization of dual phase steel [6].

However, the crucial aspect that has to be addressed, prior the numerical simulation, is evaluation of representativeness aspects of such digital models.

3 SELECTION OF THE REPRESENTATIVE VOLUME ELEMENT OF DUAL PHASE STEELS

In the literature [11, 12] there are two different approaches to the digital material representation. The DMR model can be considered as:

- the Representative Volume Element (RVE) – and in this sense it is a model of the material that can be used to determine the corresponding effective properties for the homogenized macroscopic model,
- the Unit Cell (UC) – in this sense it is a part of the RVE that enables obtaining results for particular part of the material. Thus, the Unit Cell is not representative for the whole numerical model

Consequently, before numerical investigation based on the RVE DMR approach a specific minimum size of the DMR model that can be considered as the RVE should be established. Research on this subject is presented within the chapter. However, aspects related with the mesh sensitivity have to be investigated first to eliminate numerical errors affecting final solution.

3.1 Mesh sensitivity analysis

The finite element method is mesh sensitive and obtained results depend to some extend on quality of the finite element mesh used for calculation. This is especially important for DMR models as local solutions are of particular interest. Thus, seven DMR models of the same microstructure ($100 \times 100 \mu m$) with different levels of the discretization were analysed to evaluate this issue. For all models the same sets of material properties for the martensite and ferrite phases, respectively, were used. Periodic boundary conditions were applied to maintain continuity of the computational domain. Number of finite elements used for discretization was set from 54 446 to 461 160. Four node bilinear plane strain quadrilateral reduced integration, hourglass control quad finite elements (CPE4R) were applied during discretization. DMR models were incorporated into the commercial ABAQUS application and calculated using the implicit solver. Selected microstructures used for mesh sensitivity analysis are presented in Figure 2.

a) b)

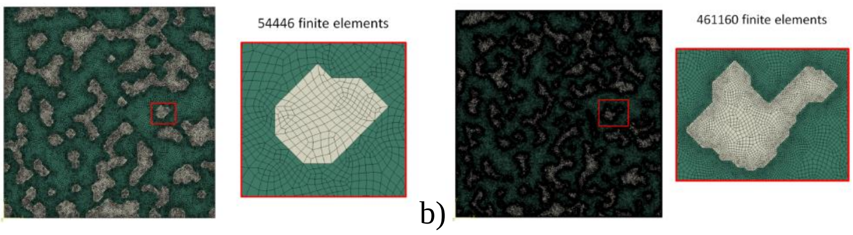

Figure 2: Microstructures discretized from a) 54 446 to b) 461 160 finite elements.

For low quality mesh, geometrical features of the martensitic phase are not replicated properly. All models were subjected to tensile test with displacement equal 20%. Examples of obtained results are presented in Figure 3. The figure confirms that mesh density has influence on obtained results. When mesh density is higher than 122 000 elements no visible differences in material behavior between models are visible. After the threshold value, obtained flow stress data converge to the same curve. So it can be stated that 224 000 finite elements per 100 μm^2 have to be used during the calculation to minimize the effect of mesh on quality of obtained results. Thus, this minimal value of FE *elements/*μm^2 is used in subsequent calculations related to evaluation of minimal size of the DMR model that can be considered as representative for the entire macro sample.

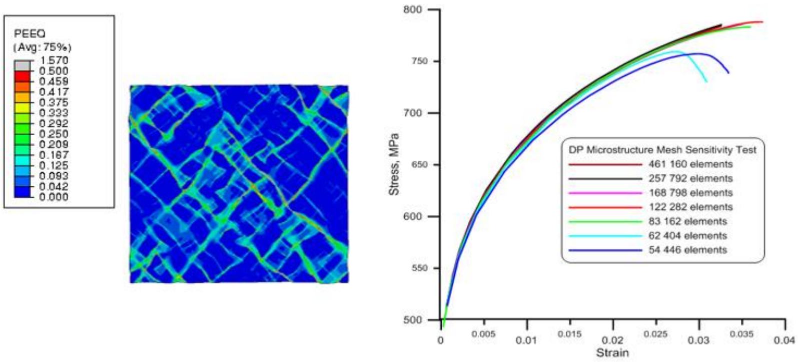

Figure 3: Homogenized strain–stress curves for 7 investigated microstructures.

3.2 Influence of DMR model size

To evaluate the minimal size of the DMR model that can be considered as RVE, four digital microstructure models were developed with the sizes: 50×50, 100×100, 200×200 and $300 \times 300 \mu m$. Authors decided to extract three smaller models from the largest microstructure in order to receive the same martensite volume fraction but different geometrical sizes as seen in Figure 4.

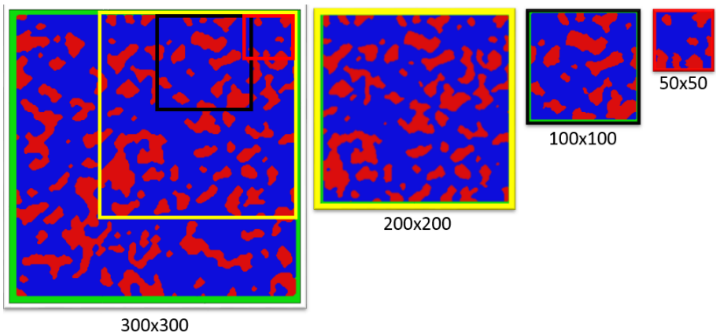

Figure 4: Digital material representation models with the same amount of martensite and different sizes: $50 \times 50, 100 \times 100, 200 \times 200$ and $300 \times 300\ \mu m$.

Digital models were incorporated into the finite element software. Periodic boundary conditions were applied and digital microstructures were deformed approx. $30 - 40\%$ of engineering strain. Number of finite elements used for discretization was set above the evaluated threshold value and varied between 190 000 to 335 000 nodes depending on microstructure complexity. Four node bilinear plane strain quadrilateral reduce integration, hourglass control quad finite elements (CPE4R) were used for the discretization purposes.

Because representative macroscopic response of the DMR models is under investigation, particular attention is put on homogenized flow curves obtained during deformation. Obtained homogenized stress–strain curves are shown in Figure 5.

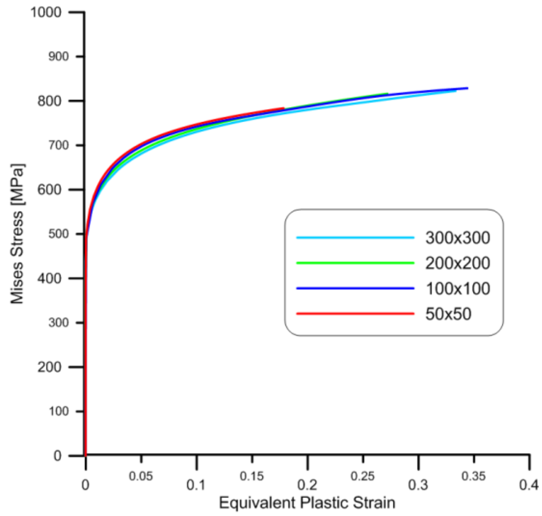

Figure 5: Homogenized stress–strain curves for investigated DMR models.

As seen in Figure 5 all microstructures provide quite similar material response to the applied deformation. Only the smallest microstructure $50 \times 50\ \mu m$ did not converge to the rest of the results due to the large local deformations in some regions – finite elements reached large degradation, which ended the simulation with solver error. Remaining models in a global sense behave consistently despite the investigated size. Additionally, to evaluate local material response strain distributions across the microstructure were analysed as seen in Figure 6.

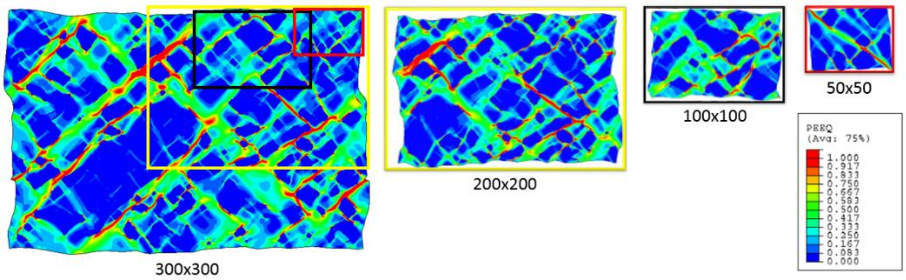

Figure 6: Equivalent strain distribution received in all DMR's after 30% of deformation.

As seen in Figure 6, maximum strain have similar values in all investigated microstructures. This information is crucial when the problem of cracks initiation in material is under consideration. Thus, it can be concluded that for the calculation accuracy microstructure larger than $100 \times 100\mu m$ should be used in further calculations.

These recommended DMR model parameters are then used during the numerical simulation realized with the developed model.

4 BRITTLE-DUCTILE FRACTURE MODEL

As mentioned, modelling of brittle-ductile fractures based on presented DMR approach requires combination of two numerical methods. In present work brittle martensite fracture was resolved with XFEM method implemented in the ABAQUS package. The most important model parameters are: martensite fracture initiation criterion based on the critical stress parameter σ_c and fracture propagation criterion based on critical energy condition (E_c). Model parameters were taken from literature investigation presented in [13] and were 1370 MPa, and 17.39 $\frac{J}{m^2}$, respectively.

Ferrite phase fracture during large plastic deformation fails by ductile failure mechanisms. Thus, a ductile failure criterion where the equivalent plastic strain at the onset of damage, ε_{iD}^{p} is a function of stress triaxiality and strain rate [14] was used:

$$\varepsilon_{iD}^{p}\left(\eta, \dot{\varepsilon}_{i}^{p}\right) = \frac{\varepsilon_{i}^{+} sinh[k_0(\eta^{-} + \eta)] + \varepsilon_{i}^{-} sinh[k_0(\eta - \eta^{+})]}{sinh[k_0(\eta^{-} + \eta^{+})]} \tag{1}$$

where: ε_{i}^{+} and ε_{i}^{-} – equivalent plastic strain for equibiaxial tensile and equibiaxial compressive deformation respectively, η – stress triaxiality (a ratio of the equivalent mean stress σ_m to the Misses equivalent stress σ_i), k_0 – parameter obtained experimentally. These parameters depend on the material, strain rate and temperature of the process. Finally, failure occurs when state variable w_D reaches 1:

$$w_D = \int \frac{d\varepsilon_{iD}^{p}}{\varepsilon_{iD}^{p}\left(\eta, \dot{\varepsilon}_{i}^{p}\right)} = 1 \tag{2}$$

The fracture initiation parameter for ferrite failure was adopted from literature [15].

Data transfer between the two models was realized with the developed python script. Example of results obtained from numerical simulation of deformation, under tensile stress state, based on developed model is shown in Figure 7.

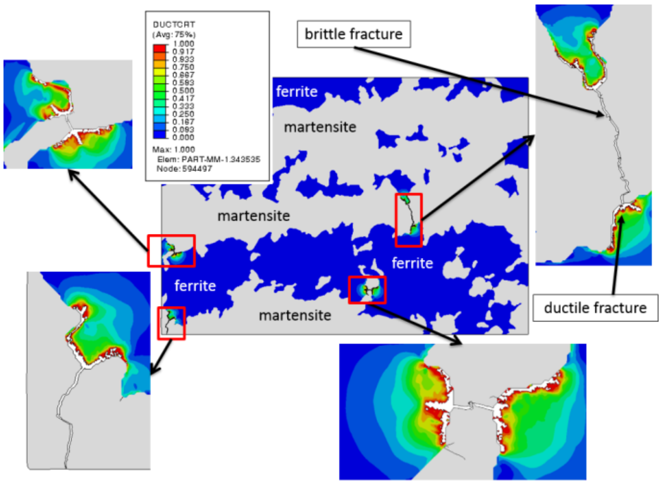

Figure 7: Brittle-ductile fractures propagating across martensite and ferrite.

5 CONCLUSIONS

- DMR model allow to take into account microstructural inhomogeneities, which have large influence on damage behaviour in DP steel.
- The representativeness of the DP DMR models is not strongly related to the size of the model, but mainly depends on proper replication of martensite volume fraction.
- Minimum number of finite elements used for the discretization of the DP DMR models should be approximately 224 000 FE elements peer 100 μm^2 to minimize mesh sensitivity effect during calculations.
- The use of the proposed method for modelling fracture in DP steels provides the possibility to take into account all relevant mechanisms of fracture: brittle fracture in

martensite phases, decohesion between martensite-ferrite phases and ductile failure in ferrite.

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