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NUMERICAL ANALYSIS OF DATA TRANSFER QUALITY IN THE MULTI-SCALE UNCOUPLED CONCURRENT MODEL

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Abstract

The main goal of this paper is an analysis of a quality of obtained results from a multiscale, concurrent modeling based on combination of macro and micro finite element models. Particular attention is put on an influence of different number of data transfer nodes between micro and macro scales on a material behavior predicted by a micro model. Results in form of equivalent strain distribution, homogenized stress-strain curves and samples shape changes are presented and discussed.

Key words: multiscale model, digital material representation, finite element method

1. INTRODUCTION

Numerical models based on a Digital Material Representation (DMR) become more and more popular in many research works and are used to describe evolution of material morphology under complex loading conditions. The concept of the DMR was proposed recently and is constantly evolving. The definition according to (Senkov et al., 2004) states that the Digital Material Representation is a material description based on measurable quantities that provides the necessary link between a simulation and an experiment.

Such approach makes it possible to directly include inhomogeneities in polycrystalline material, in the form of, e.g. different grain sizes, crystallographic grains orientations, inclusions or precipitates, unlike in conventional models, which are based on closed-form equations, where material is treated as homogenous in whole specimen volume. As a results, DMR models enable to improve the quality of obtained numerical results.

The DMR is expected to create a possibility for analyzing material behavior in difficult, or in some cases, impossible to monitor experimentally conditions at the present state of research equipment. Thus, the DMR approach is mainly used for modeling materials characterized by highly elevated properties, which are the result of sophisticated and complex microstructures with combinations of different microscale features, e.g. for modern steel grades (TRIP – TRansformation Inducted Plasticity steel, CP – Complex Phase steel, DP – Dual Phase steel, etc.).

Generation of microstructure morphology with its specific features and properties is one of the most important algorithmic parts of systems based on the DMR. There are several experimental and numerical methods that can provide accurate representation of microstructure morphology, e.g. based on microscopy imaging (optical microscopy, Scanning Electron Microscopy etc.) (Uchic et al., 2006; Uchic et al., 2007; Yazzie et al., 2012) or on less time consuming computer methods (e.g. Voronoi tessellation, voxel method, cellular automata, sphere growth, inverse

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analysis or Monte Carlo methods tec.) (Danielsson et al., 2007; Madej et al., 2011a; Baxter & Behringer, 1991). The problem of proper generation of the DMRs with various algorithms was extensively studied by one of the co-authors in (Madej et al., 2009; Madej, 2010) and is not addressed in the present work.

The second step of preparing DMR model is connected with a FE mesh generation, necessary for further numerical calculations. Based on the obtained DMR morphology, the generation of the non-uniform triangular or quadratic mesh (2D or 3D) is performed using the DMR_mesh software developed in (Madej et al., 2012) (figure 1). This approach enables obtaining coarse mesh inside microscale features and fine at its boundaries, what accelerates numerical calculations and maintain good quality of numerical results.

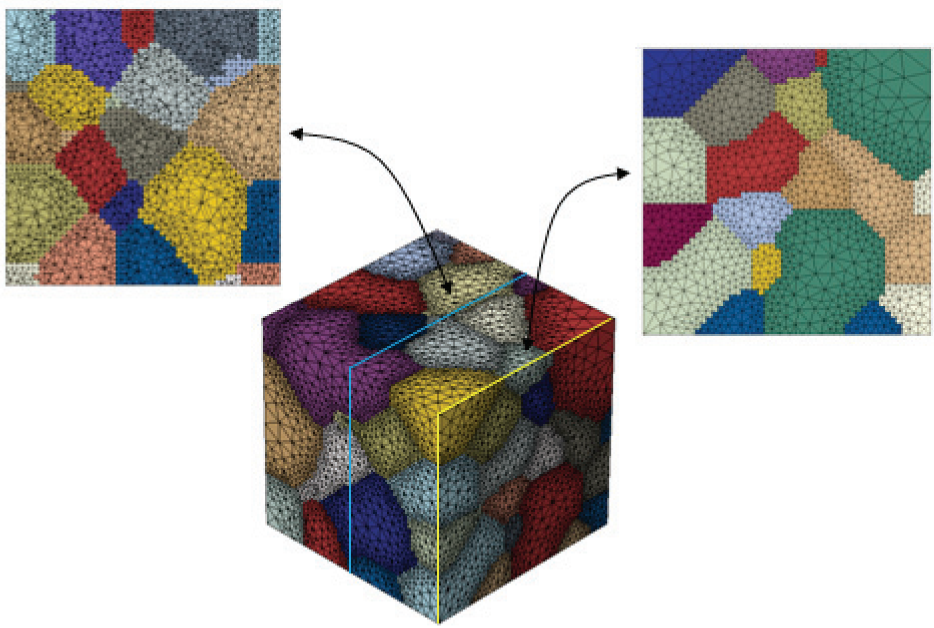


Fig. 1. Digital microstructure with non-uniform FE mesh obtained using DMR_mesh software (Madej et al., 2012).

Assignment of material properties to subsequent features is the next step of generation of digital microstructures. Two approaches are commonly applied. The first includes assignment of crystallographic orientations to each microstructure element and then use crystal plasticity models (Kilian et al., 2011; Devincre & Kubin, 2010). The second, simplified approach, is based on defining the appropriate flow stress models, which describes particular features of the investigated microstructure.

Finally, the last step of the DMR model is an incorporation of such digital model, with DMR morphology, FE mesh and material properties into a commercial FE software.

The digital material model can be treated as a Representative Volume Element (RVE) or a Unit Cell (UC) during numerical calculations. The difference between the RVE and the UC is related to a type of information required during investigation, local or global. The RVE is a model of the material to be used to determine the corresponding effective properties for the homogenised macroscopic model. The RVE should be large enough to contain sufficient information about the microstructure in order to be representative for a large volume of the investigated material. However it should be much smaller than the macroscopic body (Gitman et al., 2007; Hashin, 1983). Unlike the RVE, Unit Cell is not representative for the whole numerical model and enables obtaining results accurate for particular part of the specimen. Unit Cell is a small section of the RVE and enables analyzing material behavior in some interesting locations (e.g. crack initiation along the inclusion), without focusing on the rest of the model. It is commonly assumed that several Unit Cells can be considered as the RVE. However, both of presented approaches can have a simplified or detailed shape of microstructure features. In a simplified model e.g. only volume fraction of particular phase is considered, while geometry of this phase is not regarded. Such digital model can provide representative global material response, while morphology is simplified and gives results only statistically similar to real specimens (Brands et al., 2011; Brands et al., 2010; Rauch et al., 2011). Study on representativeness aspects of the DMR model can be found in earlier authors work (Szyndler & Madej, 2014).

As mentioned, the DMR approach becomes increasingly popular and is applied in many research works focused on different, new and modern materials, e.g. metals, composites or heterogeneous structures (Ivanov et al., 2009; Piezel et al., 2012; Flores et al., 2011; Xue et al., 2010; Madej et al., 2011b; Larsson et al., 2011; Różański & Łyżba, 2011; Zeman & Sejnoha, 2007; Liu, 2004; Simonovski & Cizelj, 2007; El Houdaigui et al., 2006; Gurgul et al., 2013a; Gurgul et al., 2013b; Goik et al., 2013; Sieniek et al., 2011). These digital microscale models are often used in multiscale solutions that predict global material behavior as well as can analyze microstructure changes during deformation in some critical/interesting locations, e.g. where the material failure or delaminating can be observed.

There are various approaches to multi scale modeling, that can be classified into two groups: upscaling and concurrent approaches as seen in figure 2.

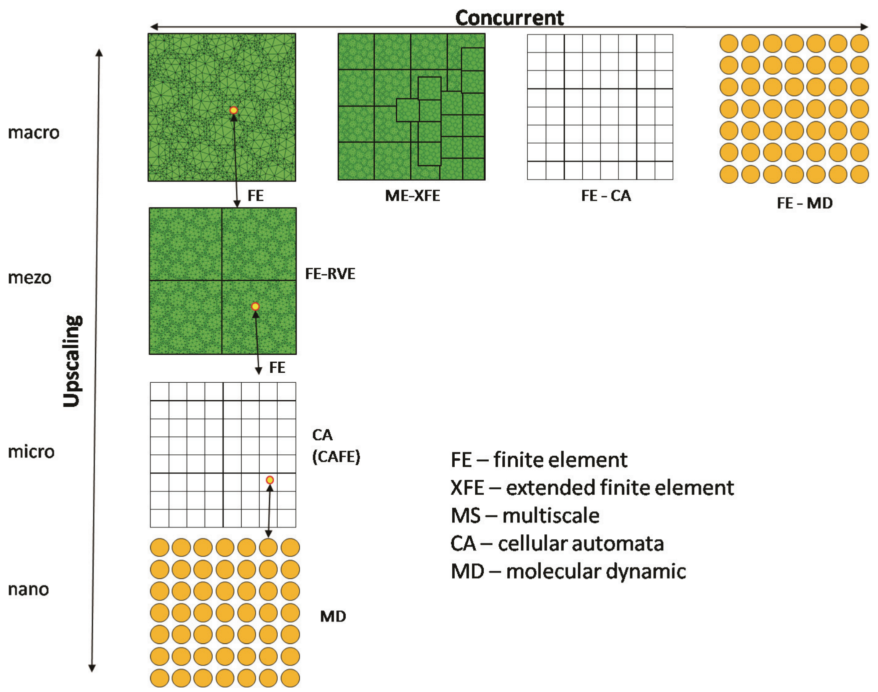


Fig. 2. Schematic representation of the concurrent and upscaling multiscale model.

In the upscaling class of methods, constitutive models at higher scales are constructed from observations and models at lower, more elementary scales. The idea of the representative volume element is employed here. By a sophisticated interaction between experimental observations at different scales and numerical solutions of constitutive models at increasingly larger scales, physically based models and their parameters can be derived at the macro scale, see for example (Da et al., 2002). Methods of the computational homogenisation, e.g. (Mieche, 2003), are considered to belong to this group of methods. In these approaches solution at the micro scale level usually is insensitive to the mesh density at the macro scale as these micro models are connected to particular integrations points.

In concurrent multiscale computing one strives to solve the problem simultaneously at several scales by an *a priori* decomposition. Two-scale methods, whereby the decomposition is made into coarse scale and fine scale, have been considered so far. Contrary to the upscaling approaches, mesh density at the macro scale can have an influence on micro scale results as several elements in the macro scale are used to transfer data into the micro scale model. However, information on errors introduced during the data transfer in these models is limited in scientific literature.

Such multiscale models are presently used in many research works, e.g. for parametric study on the fracture behavior of a crack in functionally graded materials where crack-driving forces are evaluated (Chakraborty & Rahman, 2009). Similar example of work based on the concurrent multiscale approach is (Wen & Zabaras, 2012), where a multiscale model reduction scheme based on the bi-orthogonal KLE (Karhunen–Ločve Expansion) is presented. The basic idea was to decompose the location-specific random microstructure field into a few orthogonal modes in different (macro and meso) scales. Another interesting work (Farrugia & Cheong, 2009) presents a methodology which combines mechanical testing and modelling that has been developed to account for local microstructural heterogeneities of low ductility steels. A 5-step modeling approach from macroscale damage criteria to meso scale elastoplastic and viscoplastic constitutive material models combined with microscale FEMs of inclusion behavior has been developed to deal with aspect of physical length scale.

Such multiscale models are not only used for different metallic materials but also for non metallic structures like bone tissue, for which biomechanical behavior of the complex hierarchical structure can be investigated (Coelho et al., 2011). However, as already mentioned there is a relatively small amount of works connected with an investigation of an influence of a data transfer procedure between these different scales.

Thus, the issue of data transfer in the multi scale concurrent model based on a combination of macro scale finite element model and micro scale finite element digital material representation solution is addressed within the present work.

The main aim of this paper is determination of the amount of FE nodes in the macroscale model, which enables accurate data exchange between scales, and would not affect the quality of material behavior in the microscale model. To investigate this issue series of numerical tests with different number of data transfer-nodes between scales was conducted for the two case studies with different level of complexity: simple channel die test and vertical bending test, respectively. Previously developed DMR methodology (Madej et al., 2012) was used during this investigation and obtained results are summarized below.

2. MICRO AND MACRO DATA TRANSFER

As mentioned, the multiscale approach used in the research enables to use coarse FE mesh in a global macroscale model and fine FE mesh in a micro scale model. The combined model provides general information concerning inhomogeneities in strains, stresses, etc. at the macro scale level and at the same time detailed information about microstructure behavior at the micro scale level.

This approach improves the quality of obtained results in some specific, *a priori* selected parts of the sample. The general concept of the multiscale approach used in the present work is shown in figure 3.

The data from the macroscale model can be transferred into the microscale by series of FE nodes located at the boundaries of these models, respectively. Thus, the key aspect in this approach is to ensure that an appropriate partitioning strategy is used in the macro model for extracting the steady state boundary conditions to be imposed in the micro scale model (figure 4).

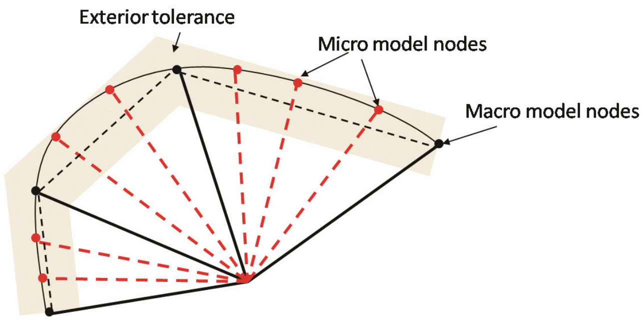


Fig. 4. *Illustration of the data transfer e.g. displacement boundary conditions, between macro and microscale models.*

As seen in figure 4 the microscale nodes are connected with macroscale by an interpolation method within the exterior tolerance zone. As can be expected the quality of obtained results mainly depends on number of transfer nodes at the macro scale level as coarse mesh is used in this case (figure 5). Micro scale model is usually discretized with very fine mesh, and large amount of boundary nodes is available. Thus, the main aim of this work is to

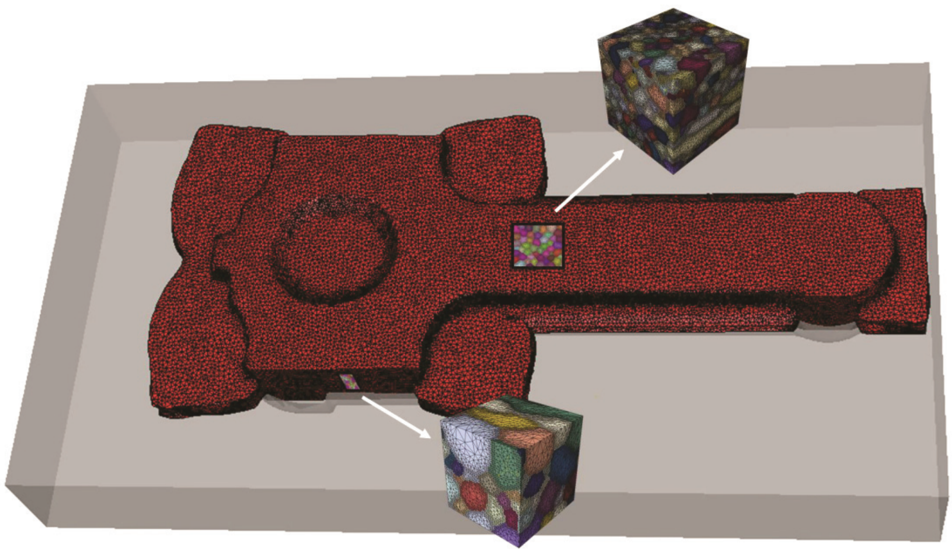


Fig. 3. *Illustration of the concept of the multi scale concurrent method based on the digital material representation.*

evaluate the influence of different number of macro scale nodes on the quality of obtained results at the microscale.

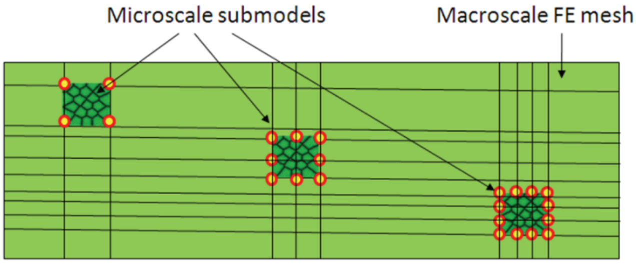


Fig. 5. *Schematic representation of the multiscale model for different number of data transfer nodes between micro and macro scales for a) 2, b) 3, c) 4 nodes on one side of the micro model.*

To analyze mentioned issue a concurrent multiscale model was developed, with different number of data transfer nodes at the macroscale, namely 2, 4, 6, 11, 21 and 41 nodes. The amount of boundary nodes at the micro scale remains constant on every edge and is equal to 45 nodes. Numerical simulations with specified deformation conditions were carried out in the commercial finite element program Abaqus. The triangular mesh with 3 Gaussian points was used during simulation (element type: CPE3 – a 3-node linear plane strain triangle). The Digital Material Representation model of a ferritic sample (300×300μm) was obtained using the methodology described earlier and was attached to the center of the macro scale sample (10×50 mm). As stated, the analysis is based on the two case studies with a different level of complexity. The first is the simple channel die test where the DMR is subjected only to loading in a one direction. In the second case the DMR sample is subjected to bending and severe changes in the shape are expected due to additional shearing stresses.

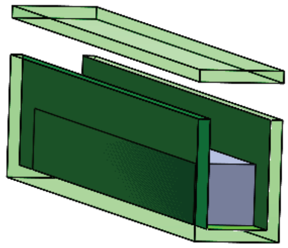
3. MULTISCALE CHANNEL DIE TEST

The channel die test is a simple compression test, where additionally flow of the material is constrained by a channel. As a result plain strain conditions are obtained. Schematic illustration of the test is presented in figure 6.

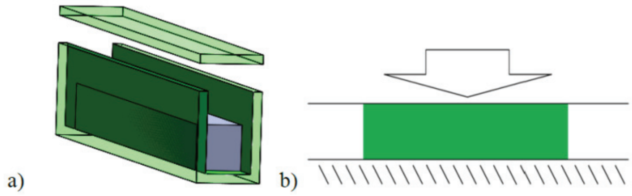
During the test the macro model has uniform material properties characteristic for a ferritic steel (figure 7). Due to the fact that cold deformation conditions are considered, the simple flow stress model was selected. Coefficients of this model were chosen to match experimental data from (Delannay et al., 2007). The flow stress model is defined as:

$$\sigma_p = K(\varepsilon_i + E_{bp})^n \qquad (1)$$

where: σ_p – flow stress, ε_i – equivalent plastic strain, K, E_{bp}, n – model coefficients with the values, 700, 0.008 and 0.08 respectively.



a)



b)

Fig. 6. *Schematic illustration of the a)3D, b) 2D channel die test.*

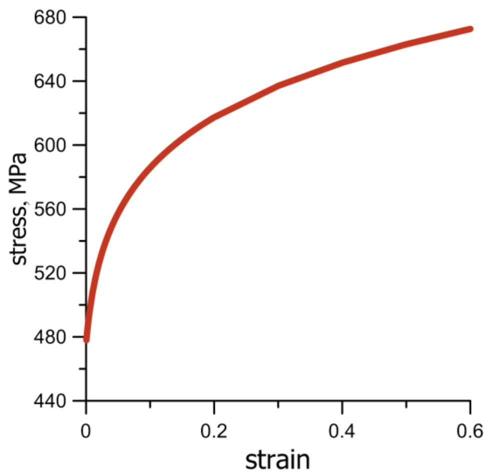


Fig. 7. *Stress/strain relationship plot (Delannay et al., 2007).*

The developed DMR model that was attached in the center of the macro sample contained 20 grains. To take into account differences in the properties of subsequent grain e.g. due to various crystallographic orientation, a slightly different flow stress models were assigned to particular microstructure features.

These different flow behaviors were obtained by diversification of the K parameter by Gaussian distribution.

height. Shapes as well as equivalent strain distributions obtained for the macro scale model with different mesh densities are presented in igure 8.

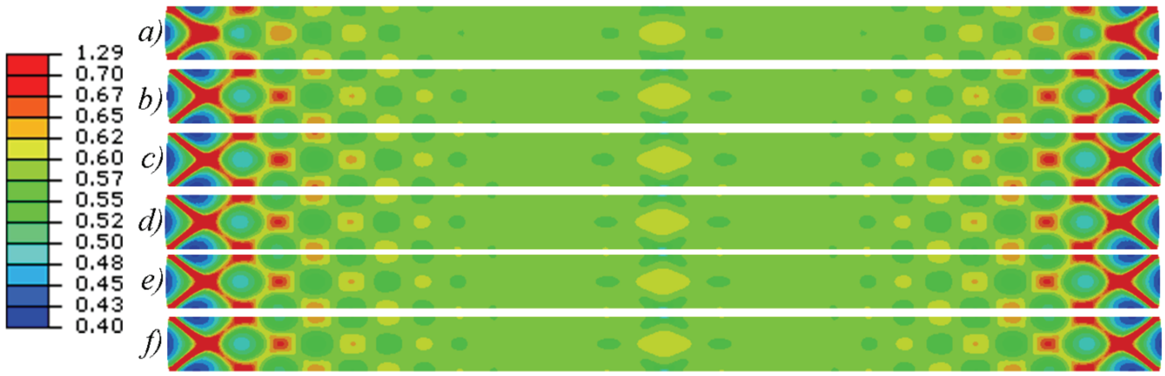


Fig. 8. *Equivalent strain distribution for macro models with a different mesh density after channel die test. The density of the FE mesh was selected to obtain expected data transfer nodes between macro and micro scale: a) 2, b) 4, c) 6, d) 11, e) 21, f) 41, respectively (see Figure 5).*

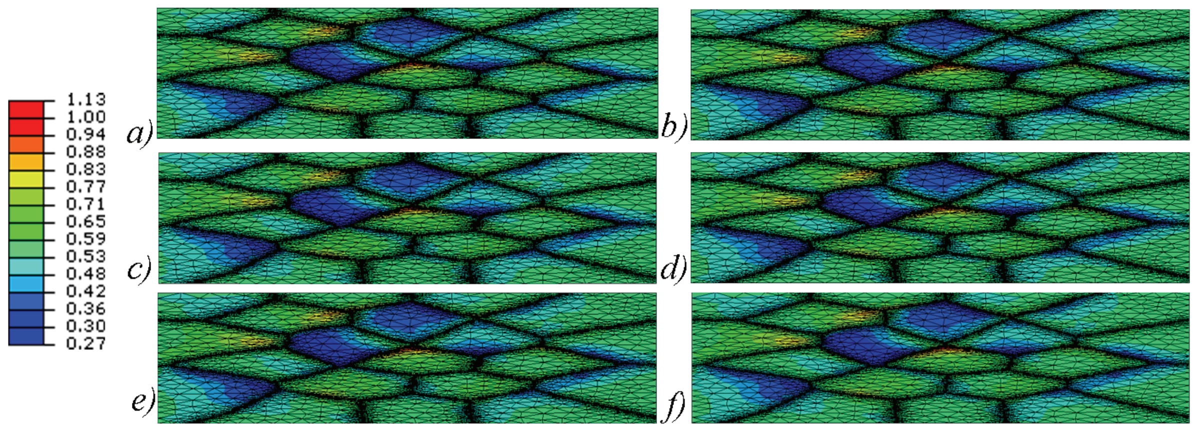


Fig. 9. *Equivalent strain distribution results in a microscopic scale for a)2, b)4, c)6, d)11, e)21, f)41 data transfer nodes on every sample edge after channel die test.*

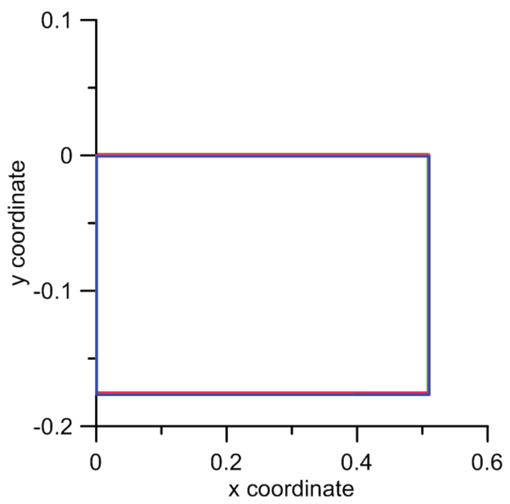


Fig. 10. *Micro models shapes after the channel die test,*

A schematic representation of the developed numerical model is presented in figure 6b. Samples were deformed up to 40% of their initial

Corresponding results for micro scale DMR models are shown in figure 9. As seen in figure 8 and 9, results in the form of equivalent strain distribution in macro and micro scales are repetitive. Also shapes of the sample in the micro models are the same after channel die test (figure 10). Obtained results indicate that different number of data transfer nodes do not have any visible influence on results in form of strain distribution and sample shapes.

Additionally, a homogenization procedure was performed in order to get global information on stress/strain relationships based on the local results obtained by subsequent micro scale models (figure 11):

$$\sigma_j^{macro}(t) = \frac{1}{V}\int_v \sigma_i^{micro}(t)\,dV_i \tag{2}$$

$$\varepsilon_j^{macro}(t) = \frac{1}{V}\int_v \varepsilon_i^{micro}(t)\,dV_i \tag{3}$$

where: σ_i^{micro} – local value of the equivalent stress in each integration point, ε_i^{micro} – local value of the equivalent strain in each integration point, σ_j^{macro} – global value of the equivalent stress, ε_j^{macro} – global value of the equivalent strain, V – volume.”

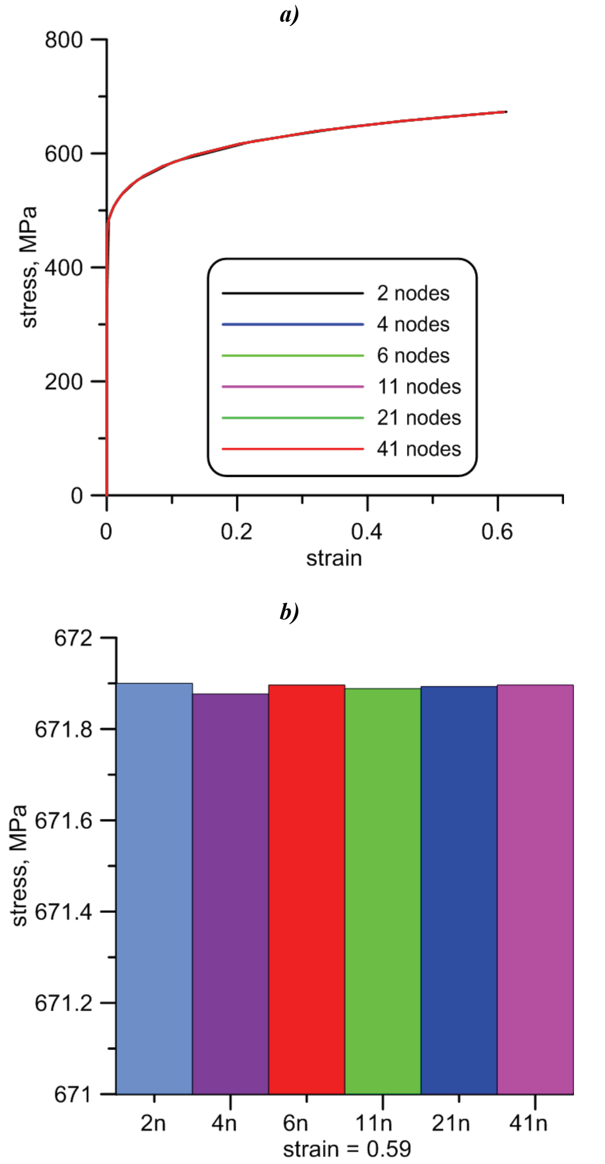


Fig. 11. *Comparison of a)homogenized flow stress curves, b)flow stress value for 0.59 strain obtained from models with different number of data transfer nodes.*

As presented in figures 9, 10 and 11, in the case of simple deformation mode, increasing number of data transfer nodes at the macro scale has a hardly visible effect on material behavior at the microstructure level. The geometry of DMR models after deformation remain exactly the same. Moreover, stress-strain relationship curves proves current conclusions.

4. MULTISCALE VERTICAL BENDING TEST

To have comparable results to the first case study, the same geometry and properties of the macro and micro scale models where used in the case of the vertical bending. Schematic illustration of the applied boundary conditions at the macro scale model in the bending test is shown in figure 12.

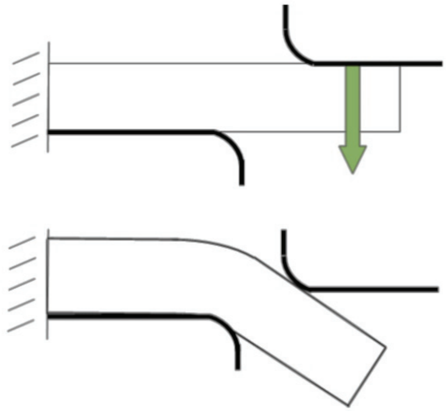


Fig. 12. *Schematic representation of a bending test model.*

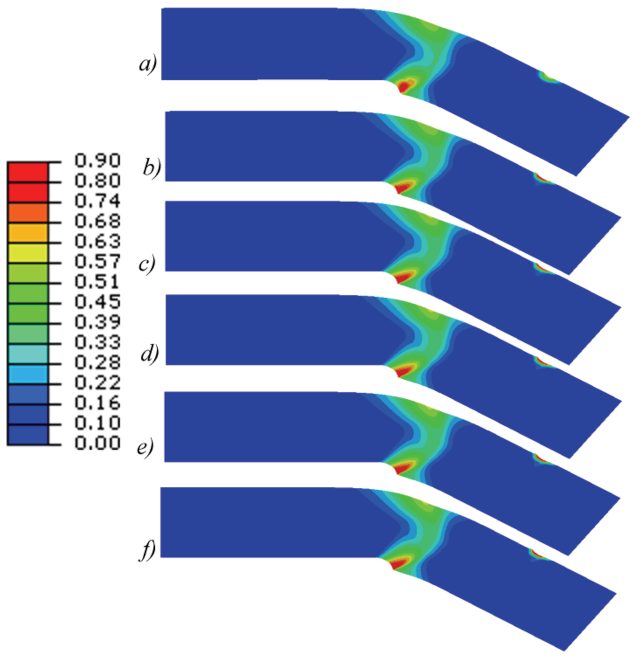


Fig. 13. *Equivalent strain distribution for macro models with a different mesh density after the bending test. The density of the FE mesh was selected to obtain expected data transfer nodes between macro and micro scale: a) 2, b) 4, c) 6, d) 11, e) 21, f) 41, respectively (see figure 5).*

Samples were bended with the displacement value of 15 mm in a vertical direction. Results in the form of equivalent strain distribution in a macro model clearly indicates strain inhomogeneities in the middle of the sample, where DMR model is located (figure 13).

Corresponding results obtained at the micro scale level in form of equivalent strain distribution for different number of macroscale transfer nodes are presented in figure 14.

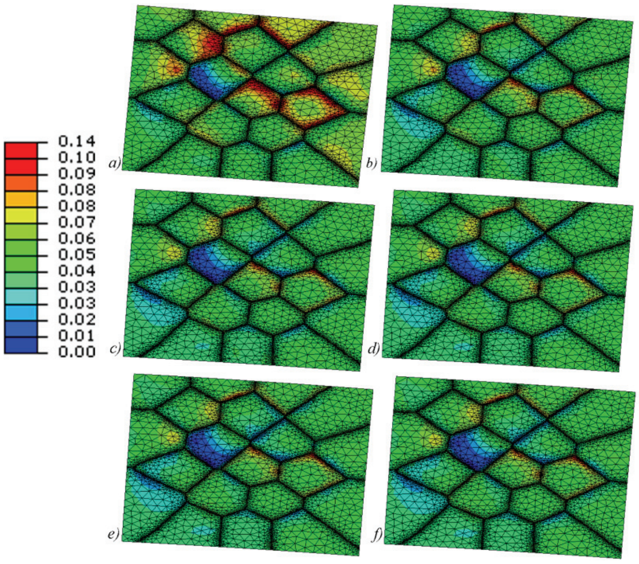


Fig. 14. Equivalent strain distribution in microscale models after the vertical bending test for a) 2, b) 4, c) 6, d) 11, e) 21, f) 41 data transfer nodes.

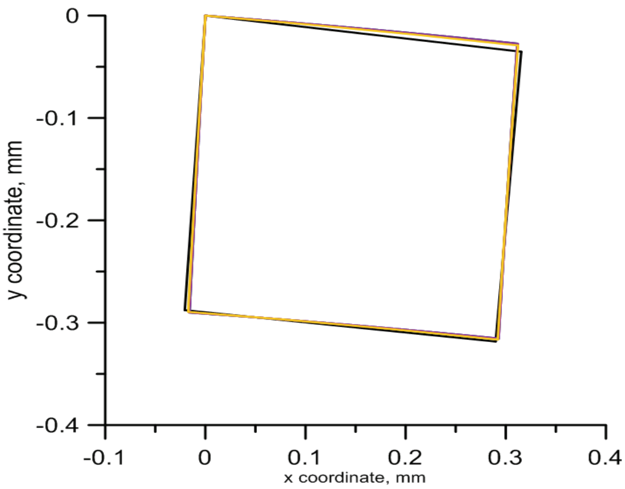
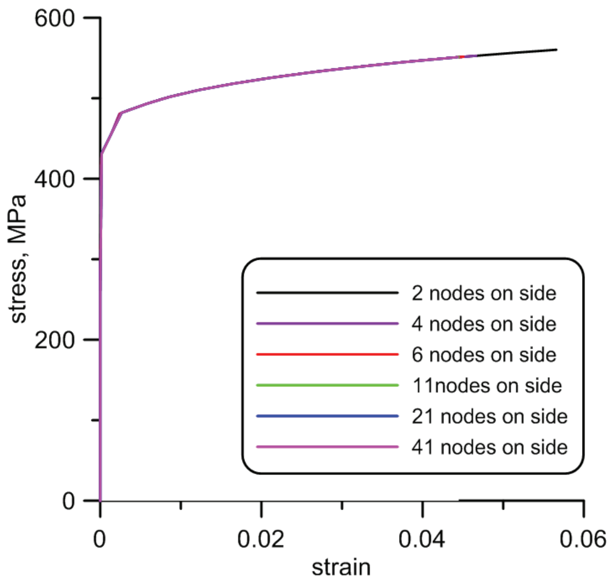


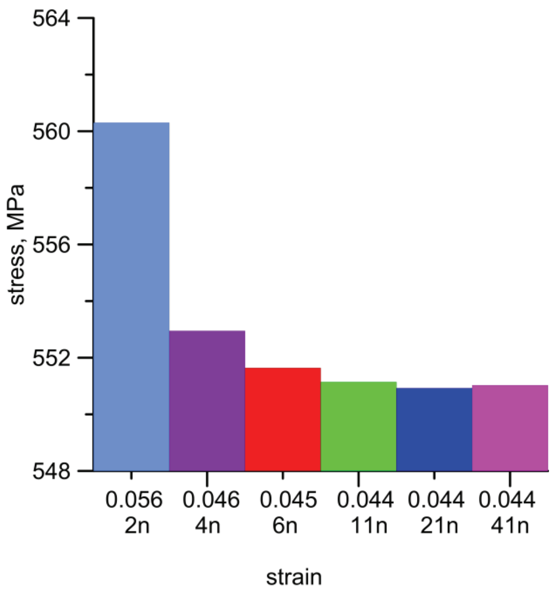
Fig. 15. Micro models shapes after the bending test.

As seen in figure 14, only the first model, with the smallest number of data transfer nodes, differs from other results obtained after bending. Zones with localized strain along grain boundaries can be observed in figure 14a. This is the results of insufficient data transfer of displacement boundary conditions between macro and micro scale models. This, behavior is even better visible when final positions of the DMR model in the macro mesh is compared as seen in figure 15.

As presented, cases with 4, 6, 11, 21 and 41 nodes behaves very similar to each other and only the first model with 2 data transfer nodes does not math. This behavior is also pronounced in the homogenized flow stress model as seen in Figure 16a. Analysis based on particular flow stress values for similar strains for investigated cases proves this observation (figure 16b).



a)



b)

Fig. 16. Comparison of a) homogenized flow stress curves, b) flow stress value for selected strain obtained from models with different number of data transfer nodes.

As presented in figures 14-16, in the case of more complex deformation mode, the increasing number of data transfer nodes at the macro scale has some visible effect on material behavior at the microstructure level. The geometry of DMR models after deformation is repetitive for cases with more than 2 data transfer nodes. Obtained result indicates that 4data transfer nodes case gives satisfying results and very similar to the case with 41 nodes. Reduction of data transfer nodes to 4, gives the possibility to obtain satisfying quality of results in a microscale model, while maintaining acceptable time computations.

5. CONCLUSIONS

The aim of this paper was to determine the minimum number of data transfer nodes between micro and macro scale models in the developed concurrent multiscale model, that does not have an influence on quality of obtained results at the micro scale. Two kinds of deformation case studies with different number of data transfer nodes at the macro scale were presented. As a result of this study it can be concluded that:

- In case of simple deformation mode it can be clearly seen that the different number of data transfer nodes between scales does not have visible influence on the quality of obtained results in the micro model located in the middle of the macro sample. Thus, only two nodes are enough to obtain satisfying results in form of strain distribution and gives a possibility to significantly accelerate numerical calculations.
- In case of more complex deformation modes like in the bending test, it can be concluded that two nodes are not enough and do not give satisfying results. In this case slight increase in number of data transfer nodes significantly improve outcome from interpolation. As seen four and more data transfer nodes between macro and micro scale models provides very similar and repetitive results in micro model. Thus, application of only four nodes is sufficient and also enables to accelerate computation time.
- Finally, it can be summarized that the more complex deformation mode the more data transfer nodes should be used to guarantee the quality of obtained results in micro model.

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ANALIZA NUMERYCZNA WPŁYWU JAKOŚCI TRANSFERU DANYCH NA WYNIKI MODELOWANIA WE WSPÓŁBIEŻNYM MODELU WIELOSKALOWYM

Streszczenie

Celem pracy jest określenie jakości uzyskanych wyników podczas stosowania współbieżnego modelu wieloskalowego, bazującego na kombinacji modeli elementów skończonych w skali makro i mikro. Szczególną uwagę poświęcono wpływowi zróżnicowanej ilości węzłów przekazujących dane między skalami mikro i makro na zachowanie się materiału w skali mikro. Wyniki przedstawiono w formie rozkładu odkształceń, krzywej płynięcia materiału i zmian w kształtach próbek w skali mikro.

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