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MULTISCALE MODELLING OF HETEROGENEOUS MATERIALS

MIKRO IN MAKRO MODELIRANJE HETEROGENIH MATERIALOV

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In this work an approach to solving coupled micro-macro problems was developed that enables efficient analyses of modern heterogeneous materials. It provides an efficient problem-solving tool for problems with complex microstructures, which are used in demanding structural components. An effective way of transferring the microscale information to the macroscale analysis is to use a multilevel finite-element approach-FE2. Within the FE2 framework one conducts an embedded micro-scale computation in order to extract the quantities required at a point of the macroscale finite-element mesh. The aplication of FE2 circumvents the need to construct an explicit macroscale constitution formulation, though at an increased computational cost. Here, a general method for the calculation of the consistent macroscopic stiffness matrix via a sensitivity analysis at the micro level was developed. The performance of the proposed method was studied for different microstructures with porosities and stiff inclusions.

Keywords: heterogeneous materials, multiscale analysis, macroscopic tangent computation, sensitivity analysis

V tem delu je bila razvita metoda za učinkovito reševanje vezanih mikro-makro sodobnih heterogenih materialov. Nova metoda je inovativno orodje pri reševanju problemov s kompleksno mikrostrukturo, uporabljeno pri zahtevnih inženirskih komponentah. Za prenos informacij med mikroskopskim in makroskopskim nivojem smo izbrali večnivojsko metodo končnih elementov (FE^2). V FE^2-shemi reševanja je v vsaki Gaussovi točki makroskopskega končnega elementa izvedena mikroskopska analiza, ki prispeva potrebne neznane vrednosti. Pri FE^2-metodi reševanja ne potrebujemo več makroskopske konstitutivne zveze, saj je le-ta na račun povečanega računskega časa pridobljena z natančno mikroskopsko analizo v posamezni točki makroskopskega končnega elementa. Metoda je splošen način reševanja makroskopske togostne matrike z občutljivostno analizo mikroskopskega nivoja. Lastnosti metode so bile preizkušene za različni mikrostrukturi: za porozno mikrostrukturo in mikrostrukturo s togimi vključki.

Ključne besede: heterogeni materiali, mikro-makro analize, makroskopska togost, občutljivostna analiza

1 INTRODUCTION

Materials used in engineering sciences and industrial applications prove to be heterogeneous at some scale. This heterogeneous nature, such as inclusions, pores, fibers and grain boundaries, has a significant impact on the observed macroscopic behaviour of multi-phase materials. Typical examples are metal alloy systems, various composites, porous and cracked structures, polymeric blends and polycrystalline materials. Processing and advanced forming operations force a material to undergo complex loading paths. This results in varying microstructural responses and easily provokes the evolution of the microstructure. Because of time and cost requirements, straightforward experimental measurements on a number of material samples including various phase properties, volume fractions and loading histories are highly unlikely. On the other hand, it is still impossible to discretize the macrostructure so that it accurately represents the microstructure and at the same time allows a numerical solution within a reasonable amount of time. To determine the overall macroscopic characteristics of heterogeneous structures, the effective numerical models have to be developed. Conventionally, in structural mechanics the hierarchical approach is used, especially when the scales are significantly separated. By employing micromechanical models, the material behavior at the microscale is efficiently transferred to the macroscale analysis and used for all the structural calculations. The most straightforward way is to use the multilevel finite-element method ML-FEM,[1–5] whereby the behavior of each volume element results from a finite-element computation of the microscopic structure. When analyses at both levels are made in the context of the FEM, it can be referred to as the FE^2 method.[6,7] This new type of model falls within the general category of multiscale models. The aplication of the FE^2 method removes the need to construct an explicit macroscale constitution formulation, though at an increased computational cost. The constitutive equations are written only on microscopic scale and homogenisation and localisation equations are used to compute the macroscopic strains and stresses knowing the mechanical state at the microscopic level.

The aim of this work stems from the need for a general and effective way of computing the macroscopic tangent, since this represents the main part of the FE^2

method. A conventional way of computing the macroscopic tangent in a condensation procedure necessitates the computation of a Shur complement. It inflicts for increasingly complex microstructure higher memory-allocation demands that may not be met by today's computers. Therefore, as an alternative, a tangent-computation technique based on a sensitivity analysis at the microscopic level will be presented.

2 MULTISCALE MODELING

2.1 Basic hypotheses

The material under consideration is assumed to be macroscopically homogeneous, so that continuum mechanics can be used to describe the macroscopic behavior. However, at the microlevel the material configuration is heterogeneous, consisting of many distinguishable components, e.g., grains, cavities, and hard inclusions.

In order to estimate the effective properties of a heterogeneous material, most of the micro-macro methods assume the existence of a micromechanical sample that is statistically representative of the microstructural features. The identification of such a representative volume element (RVE) is a somewhat delicate task and is outside the scope of this work. The RVE is considered both smaller enough than the macroscale media and larger enough than the heterogeneities on the micro scale, without introducing non-existing properties (e.g., anisotropy). For further issues associated with the identification procedure the reader is referred to.[8–12]

Here, the existence of an appropriate RVE is supposed. Then the problem on the RVE level can be formulated as a standard problem in quasi-static continuum solid mechanics, where kinematic, equilibrium and constitutive equations are needed.

In the computational homogenization technique, a macroscopic deformation gradient tensor ($F_{\rm M}$) is calculated for every integration point of the macrostructure. From the macroscopic deformation tensor the appropriate boundary conditions are derived to be imposed on the RVE that is assigned to this point. After the solution of the boundary-value problem for the RVE, the macroscopic stress tensor ($P_{\rm M}$) is obtained by averaging the resulting RVE stress field over the volume of the RVE. Additionally, the local macroscopic consistent tangent is derived from the sensitivity analysis of the RVE. This framework is schematically illustrated in **Figure 1**. In the subsequent sections these issues are discussed in more detail.

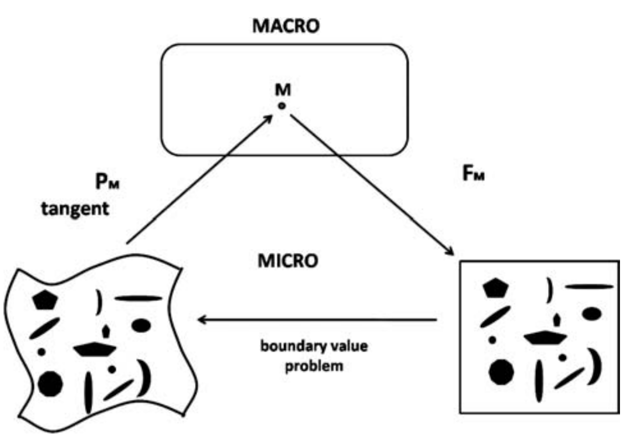

Figure 1: Shematic diagram of the FE^2 model
Slika 1: Shema FE^2-modela

2.2 Coupling of the macroscopic and microscopic levels

The actual coupling between the macroscopic and microscopic scales is based on averaging theorems. The energy averaging theorem, known in the literature as the Hill condition or macrohomogeneity condition,[12,13] requires that the macroscopic volume average of the variation of the work performed on the RVE is equal to the local variation of the work on the macroscale. Formulated in terms of a deformation gradient tensor and the first Piola-Kirchhoff stress tensor, the work criterion in differential form is written:

$$\left\langle P_{\rm m} \cdot {\rm d}F_{\rm m} \right\rangle = \left\langle P_{\rm M} \right\rangle \cdot \left\langle {\rm d}F_{\rm M} \right\rangle \qquad (2.1)$$

It is well known that this criterion is not satisfied for arbitrary boundary conditions (BCs) applied to the RVE. Classically, three types of RVE boundary conditions are used, i.e., prescribed displacements, prescribed tractions and prescribed periodicity. Periodicity here is referring to an assumption of the global periodicity of the microstructure, suggesting that the whole macroscopic specimen consists of spatially repeated unit cells. Among them the periodic BCs show a more reasonable estimation of the effective properties. This was supported and justified by a number of authors.[8–11] The periodicity conditions for the microstructural RVE are written in a general format as:

$$\begin{aligned} \vec{x}^{+} - \vec{x}^{-} &= F_{\rm M} \cdot \left(\vec{X}^{+} - \vec{X}^{-} \right) \\ \vec{p}^{+} &= \vec{p}^{-} \end{aligned} \qquad (2.2)$$

where $\vec{x}$ and $\vec{X}$ represent the actual and initial position vectors and $\vec{p}$ is the boundary traction of the RVE. In equation (2.1) the macroscopic first Piola-Kirchhoff stress tensor (PM) and the macroscopic deformation gradient tensor (FM) are the fundamental kinetical and kinematical measures, which are defined in terms of the volume average of their microscopic counterparts. Every time that the work criterion is satisfied, the volume average of the above-mentioned macroscopic measures can be obtained through a knowledge of the boundary information only.

$$F_{\rm M} = \left\langle F_{\rm m} \right\rangle_{\rm RVE} = \frac{1}{V_{\rm RVE}} \int_{\rm RVE} F_{\rm m} \, {\rm d}V = \frac{1}{V_{\rm RVE}} \int_{\Gamma} \vec{x} \vec{N} {\rm d}\Gamma \qquad (2.3)$$

$$P_{\mathrm{M}}=\langle P_{\mathrm{m}}\rangle_{\mathrm{RVE}}=\frac{1}{V_{\mathrm{RVE}}}\int_{\mathrm{RVE}}P_{\mathrm{m}}\,\mathrm{d}V=\frac{1}{V_{\mathrm{RVE}}}\int_{\Gamma}\bar{p}\bar{X}\mathrm{d}\Gamma \tag{2.4}$$

Here, V_{RVE} is the undeformed RVE, and P_{m} and F_{m} are the microscopic stress tensor and deformation gradient tensor, respectively, Γ represents the boundary of the RVE, while $\bar{N}$ represents the normal vector to the surface of the RVE.

2.3 Macroscopic tangent computation (consistent stiffness)

In the realization of the multilevel FEM approach, the macroscopic constitutive formulation is not explicitly obtained from the experimental data. Instead, the needed stiffness matrix at every macroscopic integration point has to be determined directly from the numerical relation of the macroscopic stress (P_{M}) and macroscopic deformation gradient (F_{M}) at that point.[11,14,15] The weak form of the macroscale problem in the absence of body forces and acceleration can be written in the variational form as:

$$\delta\pi=\int_{V_0}\delta F_{\mathrm{M}}\cdot P_{\mathrm{M}}\,\mathrm{d}V \tag{2.5}$$

To solve the macroscopic primal problem within the FE^2 setting, at the i-th iteration step of a standard Newton-Raphson solution scheme, the following linearization needs to be computed.

$$\begin{aligned}&\int_{V_0}\delta F_{\mathrm{M}}\cdot P_{\mathrm{M}}^{\mathrm{i}+1}\,\mathrm{d}V\approx\\&\approx\int_{V_0}\delta F_{\mathrm{M}}\cdot P_{\mathrm{M}}^{\mathrm{i}}\,\mathrm{d}V+\int_{V_0}\delta F_{\mathrm{M}}\frac{DP_{\mathrm{M}}^{\mathrm{i}}}{DP_{\mathrm{M}}}\Delta F_{\mathrm{M}}\,\mathrm{d}V\end{aligned} \tag{2.6}$$

The macrolevel element tangent stiffness matrix and the residual force vector can be obtained with the knowledge of the stress (P_{M}) and macroscopic tangent ($\partial P_{\mathrm{M}}/\partial F_{\mathrm{M}}$) obtained from the RVE analysis, since F_{M} is an explicit function of the node displacements. The (P_{M}) can be obtained directly from the RVE analysis by using averaging theorem equation (2.4), while for the determination of the macroscopic tangent a RVE sensitivity analysis is performed. For the sensitivity problem[16] the residuals and the vector of unknowns are defined as a function of the sensitivity parameters, which are in this case the elements of the tensor (F_{M}). The sensitivity problem can then be obtained from the primal problem by differentiating the response functional and the residuals with respect to the macroscopic deformation gradient (F_{M}), and the following system on the microlevel has to be solved:

$$\frac{\partial\psi_{\mathrm{m}}}{\partial a}\frac{Da}{D\phi}=\frac{\partial\psi_{\mathrm{m}}}{\partial\phi} \tag{2.7}$$

where, ψ_{m} represents the response functional on the microlevel, a is a set of unknowns (displacements), while ϕ represents an arbitrary sensitivity parameter, in our case F_{M}.

With the assembling of the macroscopic stiffness matrix, the problem on the macro level is fully described and can be solved to produce an update of the macroscopic displacement field.

Remark 1: for consistency the particular type of BC employed for the computation of K must match the type of BC employed in the computation of P.

2.4 Finite-element implementation

The multiscale algorithm has been implemented into the computer program AceFEM,[17] where a special macroscopic element can be readily defined in open-source code. The mechanical characterizations of the microstructural components are modeled as Neo-Hook isotropic hyperelastic material for which the strain-energy function takes the form:

$$W=\frac{1}{2}\lambda_{\mathrm{g}}(J-1)^2+\mu_{\mathrm{g}}\left(\frac{1}{2}(Tr[C]-3)-Ln[J]\right) \tag{2.8}$$

where $J=\det F$, C is the right Couchy-Green deformation tensor, with λ_{g} and μ_{g} as the first Lame constant and shear modulus.

The efficiency of the FE^2 method was enhanced by developing a framework that allows the micro-macro approach to be applied only at critical regions of the macrostructure, while for the other domains, the effective macroscopic properties are derived by the numerical homogenization of the micromechanical model. In order to evaluate the presented method a tree-point bending test, **Figure 2**, with a height-to-length ratio of 0.25 and unit thickness, load displacements Δ = 1 unit, under plain strain condition, has been examined. In the example two heterogeneous microstructures of a homogeneous matrix material with 6 % volume fraction of randomly distributed voids or stiff inclusions are studied. The tests were made in 2D and 3D geometry. The material parameters for the calculations are as follows: shear modulus of the matrix material and stiff inclusions are G_{m} = 77 GPa and G_{i} = 307 GPa, respectively, and the bulk modulus of the matrix material and stiff inclusions are K_{m} = 167 GPa and K_{i} = 667GPa, respectively. For the homogenized part the effective material constants are as follows: voided microstructure G = 72 GPa and K = 156 GPa, microstructure with stiff inclusions G = 90 GPa and K = 194 GPa.

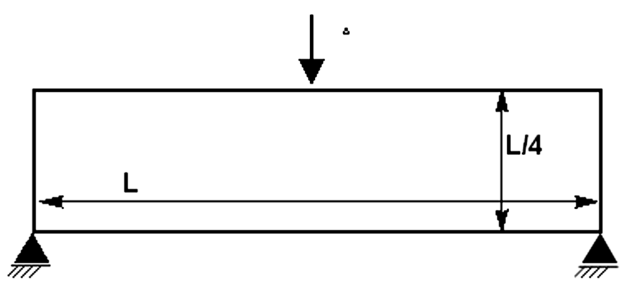

Figure 2: Three-point bending test
Slika 2: Tritočkovni upogibni preizkus

3 RESULTS – EXAMPLE OF MICRO-MACRO MODELING

Micro-macro calculations for a heterogeneous structure with voids and homogenized structure for the three-point bending test were carried out. In **Figure 3** the undeformed and deformed states of the two cases are presented. The contour plots of the equivalent Misses stress are compared. It is shown that in the case of micro-macro analysis, higher effective stresses occur than in the homogenized macrostructure.

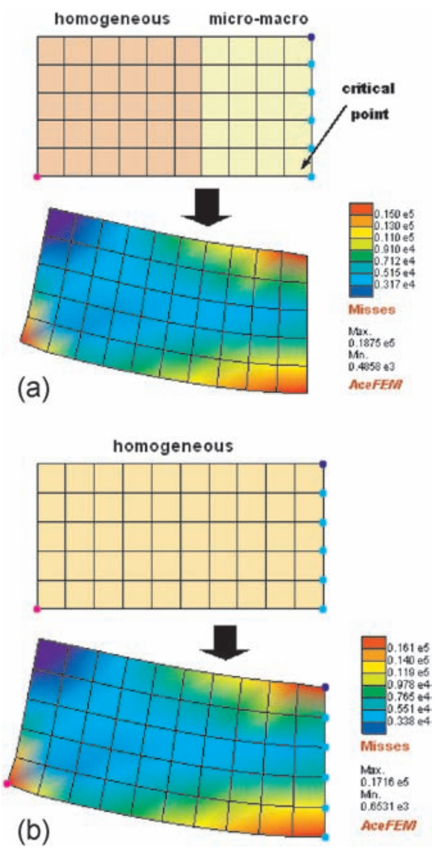

Figure 3: Macroscopic effective stress in micro-macro and homogenized problem, voided microstructure
Slika 3: Makroskopska efektivna primerjalna napetost za homogeniziran in mikro-makro problem, mikrostruktura s porami

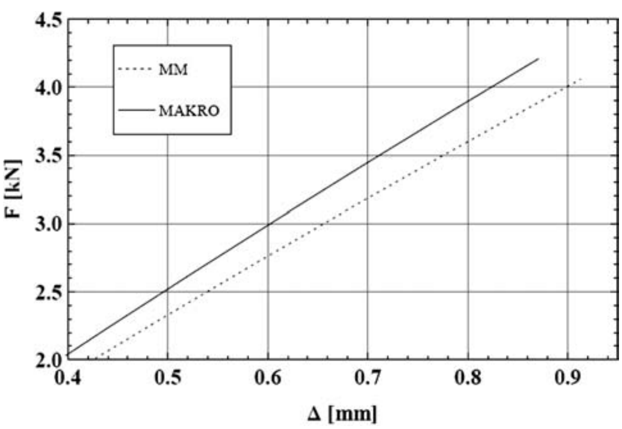

Figure 4: Loading force vs. displacement of a critical point from the micro-macro and homogenized problem, voided microstructure.
Slika 4: Sila obremenjevanja glede na pomik kritične točke za homogeniziran in mikro-makro problem, mikrostruktura s porami

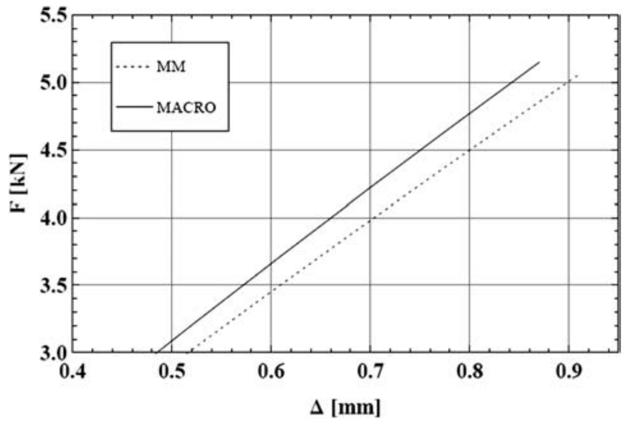

Figure 5: Loading force vs. displacement of a critical point from the micro-macro and homogenized problem, microstructure with stiff inclusions
Slika 5: Sila obremenjevanja glede na pomik kritične točke za homogeniziran in mikro-makro problem, mikrostruktura s togimi vključki

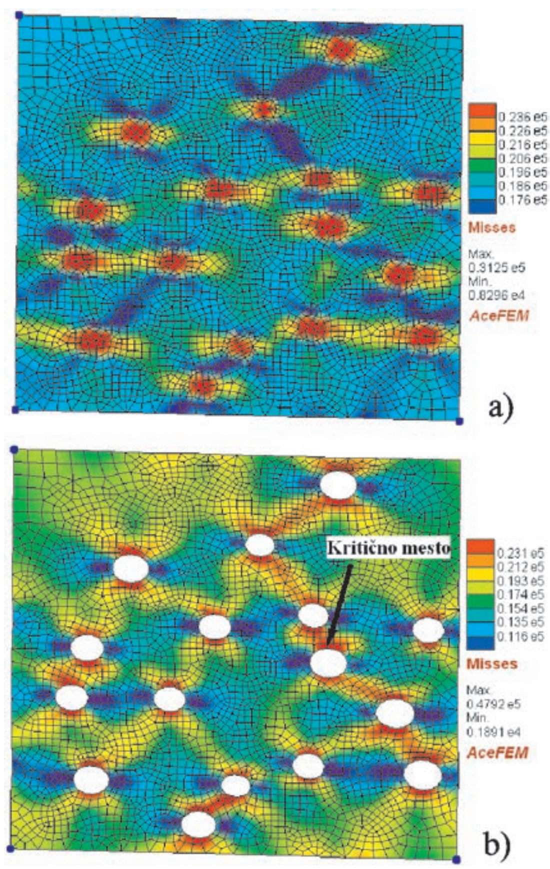

Figure 6: Effective stress in the RVE from the critical point of the macrostructure 2D a) stiff inclusions, b) voided microstructure.
Slika 6: Primerjalna napetost v RVE, vzet iz kritične točke makro strukture, a) mikrostruktura s togimi vključki, b) mikrostruktura s porami

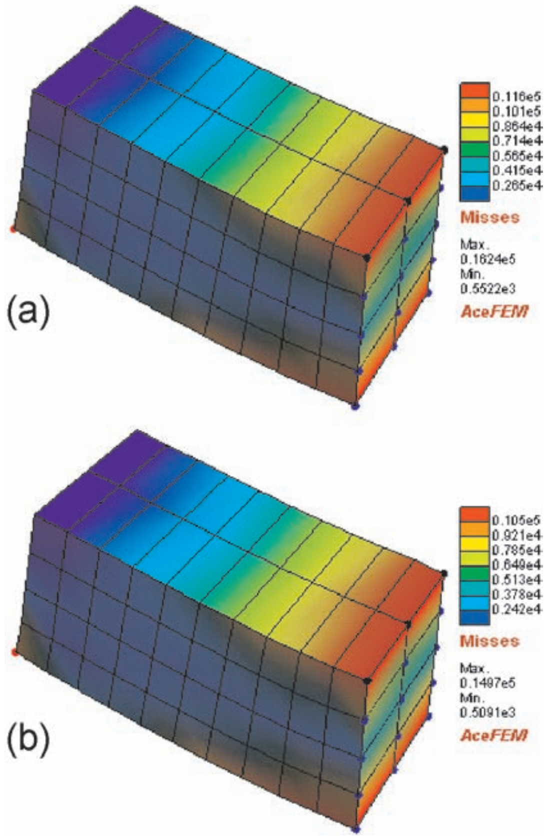

Figure 7: Macroscopic effective stress in the micro-macro and homogenized problems, voided microstructure

Slika 7: Makroskopska efektivna primerjalna napetost za homogeniziran in mikro-makro problem, mikrostruktura s porami

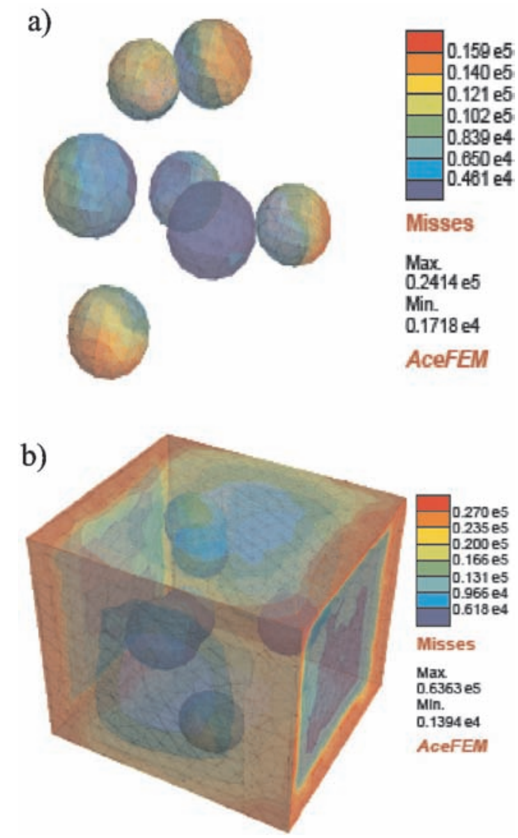

Figure 8: Effective stress in the RVE from the critical point of the macrostructure 3D a) stiff inclusions, b) voided microstructure

Slika 8: Primerjalna napetost v RVE, pripadajoč kritični točki makro strukture, a) mikrostruktura s togimi vključki, b) mikrostruktura s porami

Figure 4 shows a comparison of the load-displacement curve for micro-macro and homogenized analyses with a voided microstructure. The same situation for a microstructure with stiff inclusions is presented in **Figure 5**. The results imply that for the correct calculations, needed in precision-forming operations, the use of the micro-macro approach could provide a better estimation of the real situation. Namely, the results obtained with the micro-macro approach showed a softer response than the homogenized macrostructure.

The detailed analysis of the RVE in the critical point, the lower point in the middle of the three-point bending test, for both microstructures in 2D geometry are shown in **Figure 6**. It can be seen that the voids act as a stress concentrator and that some stress-concentration regions can be seen between the neighboring voids, **Figure 6b**. By comparing the stress field with the one in **Figure 3**, substantially higher stresses are observed. So by simultaneously examining the RVE at critical macro points, while deforming the macrostructure, a deeper understanding of the real deformation mechanisms is gained. In the case of stiff inclusions a detailed RVE analysis revealed the stress peaks in the inclusions, which can be very helpful in studying the damage mechanisms.

In addition to the 2D tests, some 3D tests were made. In **Figure 7** an effective Misses stress is shown for the two considered microstructures. By comparing the macroscopic stress field with the RVE stress field, **Figure 8**, again much higher stresses are observed.

4 CONCLUSIONS

In this work numerical models of heterogeneous materials were adapted to a multilevel finite-element framework called the FE^2 method. The key importance of this method is the efficient calculation of the macroscopic stiffness matrix, which can be done in various ways. Here, a general method for a calculation of the consistent macroscopic stiffness matrix via a sensitivity analysis of the micro level was developed. It enables a problem-solving tool for a wide variety of different micro-macro problems. Furthermore, the FE^2 method makes it possible to study easily the complex microstructural morphology and with a detailed RVE analysis it provides useful information for investigating damage mechanism at the micro level. Microstructures with stiff inclusions and voids were tested. The results showed that by using the

FE^2 method more accuracy and a deeper understanding of deformation mechanisms can be obtained.

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