Statistically Similar Reconstruction of Dual-Phase Steel Microstructures for Engineering Applications

Dominik Brands[1], **Jörg Schröder**[*], **and Daniel Balzani**
Institute of Mechanics, Department Civil Engineering, Faculty for Engineering, University of Duisburg-Essen
Universitätsstraße 15, 45141 Essen
[1]*e-mail: dominik.brands@uni-due.de*

Abstract

The focus of this contribution is to show the applicability of statistically similar representative volume elements (SSRVEs) for multiscale simulations like the FE^2-method. Such SSRVEs are characterized by a lower complexity than usual random representative volume elements (RVEs), but they represent quite accurately the mechanical response of the real material. A lower complexity of the RVE is accompanied by a reduced number of degrees of freedom of resulting finite-element discretizations and therefore, computational costs are significantly decreased. In order to demonstrate the performance of the proposed procedure we discuss the results of several representative numerical examples.

Keywords: multiscale problems, homogenization, material properties, plasticity, microstructures

1. Introduction

In many fields of steel applications, e.g. automotive engineering or aircraft construction, the optimization of material properties, e.g. with respect to stability and weight, becomes more and more one of the main challenges. At that point, one important contributor to the macroscopic (effective) properties is the microheterogeneity of the material. This requires the consideration of the microstructure during the simulation. A numerical tool for the direct incorporation of micromechanical information is the FE^2-method, also known as direct micro-macro-transition procedure (see e.g. [6], [3], [4],...). A high amount of memory and long computing time are drawbacks with respect to the application of direct homogenization methods to large random microstructures. In this context the definition of a representative volume element (RVE) plays an important role. In [2] a method is proposed for the construction of statistically similar representative volume elements (SSRVEs), which have a much lower complexity than usual random RVEs and which represent quite accurately the mechanical response of the real material.

2. Construction and Analysis of SSRVEs

A least-square functional stands at the center of our construction method. This functional takes into account differences of suitable statistical measures that characterize the inclusion morphology. In the preceding investigation [5] it is observed that the volume fraction, the spectral density and the lineal-path function are suitable measures for the characterization of two-phase materials. The corresponding least-square functional reads

$$\mathcal{L}(\boldsymbol{\gamma}) := \omega_V \mathcal{L}_V(\boldsymbol{\gamma}) + \omega_{SD}\mathcal{L}_{SD}(\boldsymbol{\gamma}) + \omega_{LP}\mathcal{L}_{LP}(\boldsymbol{\gamma}) \,, \tag{1}$$

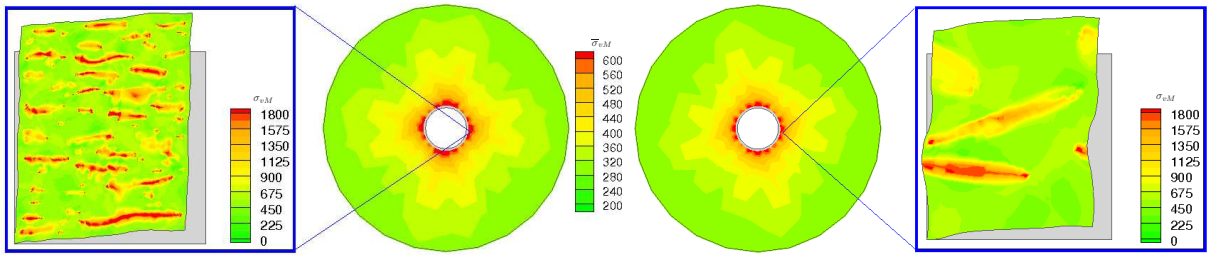
where the vector $\boldsymbol{\gamma}$ controls the parametrization of the inclusion phase morphology. $\mathcal{L}_{(\bullet)}$ denotes the individual least-square functionals for the volume fraction (V), the spectral density (SD) and the lineal-path function (LP). These functionals are defined as the difference of the respective statistical measures computed for a fixed reference target structure and the SSRVE. As an example, the appropriate equation for the volume fraction is defined as

$$\mathcal{L}_V(\boldsymbol{\gamma}) := \left(1 - \frac{\mathcal{P}_V^{SSRVE}(\boldsymbol{\gamma})}{\mathcal{P}_V^{real}}\right)^2 \,. \tag{2}$$

For the definition of a suitable RVE representing a (real) target structure the volume fraction represents a fundamental measure. The additional measures - the spectral density and lineal-path function - take into account the anisotropy of the microstructure, whereby the former measure also counts for the periodicity. Details on the individual least-square functionals, the statistical measure and their mathematical definitions can also be found in [5] and the references therein. For the parametrization of the inclusion we use splines based on three sampling points and arrange the point coordinates in the vector $\boldsymbol{\gamma}$. For the construction of the SSRVEs three different types are considered, cf. Fig.2b-d: Type A takes into account one inclusion, Type B two inclusions and Type C three inclusions. Intersections of the inclusions are not permitted. At the boundary of the SSRVE we ensure a periodic extensibility. Then the objective function (1) is minimized using the method proposed in [1]. In order to study the mechanical error we consider three different simple macroscopic virtual experiments: horizontal tension, vertical tension and simple shear. The FE^2-simulations taking into account the target structure at the microscale are compared with FE^2-simulations focusing on the constructed SSRVEs. From the deviation in each calculated stress-strain state we compute suitable mechanical errors for the three different virtual experiments, respectively. We define the mechanical error measure $r_{(*)}^{(i)} = (\sigma_i^{\text{real}} - \sigma_i^{\text{SSRVE}})/\sigma_i^{\text{real}}$ evaluated in a number of n calculated stress-strain situations i. The subscript $(*)$ identifies the main loading direction of the corresponding virtual experiments, i.e. x (horizontal), y (vertical) and xy (shear). To estimate the mechanical quality by simple identificators we define the errors $\widetilde{r}_x$, $\widetilde{r}_y$ and $\widetilde{r}_{xy}$ for the three different virtual experiments

$$\widetilde{r}_{(*)} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}[r_{(*)}^{(i)}]^2} \quad \text{with } r_{(*)}^{(i)} := r_{(*)}\left(\frac{i}{n}\frac{\triangle l_{\max}}{l_0}\right) \,. \tag{3}$$

[*]The financial support of the "Deutsche Forschungsgemeinschaft" (DFG), research group MICROPLAST on "Analysis and Computation of Microstructures in Finite Plasticity", project No. SCHR 570/8-2, is gratefully acknowledged.



a) b)

Figure 1: Results of the FE^2-simulations based on the a) target structure and b) SSRVE with the von Mises stress distributions in the deformed microstructures. The grey area behind the microstructure indicates the undeformed configuration.

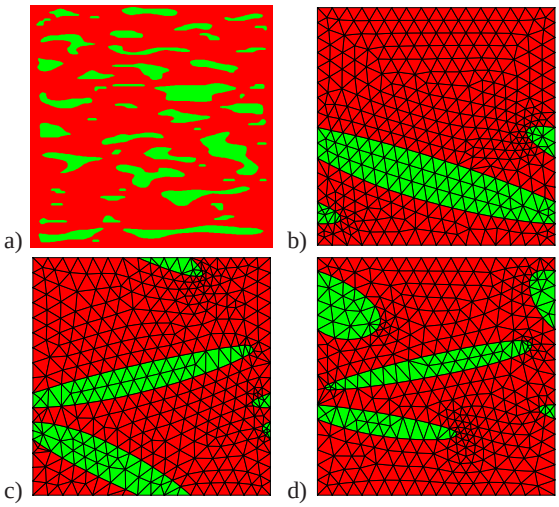
In the same manner we define the average value

$$\widetilde{r} = \sqrt{\frac{1}{3}(\widetilde{r}_x^2 + \widetilde{r}_y^2 + \widetilde{r}_{xy}^2)} \tag{4}$$

computed from the three individual errors as an overall mechanical error. The results for the three SSRVEs are tabulated in Tab. 1 and SSRVE Type C shows the best mechanical approximation with an overall mechanical error of approximately 0.91%, for further details see [5].

SSRVE	$\mathcal{L}\ [10^{-3}]$	$\widetilde{r}_x$ [%]	$\widetilde{r}_y$ [%]	$\widetilde{r}_{xy}$ [%]	$\widetilde{r}$ [%]
A	34.56	4.11	1.05	0.49	2.47
B	5.04	1.87	0.89	3.03	2.11
C	1.65	0.32	0.49	1.47	0.91

Table 1: Values of the objective function $\mathcal{L}$ and the errors $\widetilde{r}$ reulting from the optimization and the virtual experiments.



a) b) c) d)

Figure 2: a) Target structure and discretizations of the SSRVEs: b) Type A, c) Type B and d) Type C.

3. Application

To show the capability of the most suitable SSRVE with respect to the mechanical response compared to the target structure in a macroscopically inhomogeneous FE^2-simulation we consider a radially expanded circular disk with a hole, discretized by 84 triangular elements with quadratic ansatz functions and plain strain conditions. During the simulation the outer radius is extended by a radially oriented displacement $u = 1.6\,\text{mm}$. For the analysis we perform two simulations: first using the reference target structure at the microscale with 21930 degrees of freedom and second the SSRVE Type C with 3082 degrees of freedom. In Fig. 1 the macroscopic stress distributions in the disk and the microscopic stresses at one macroscopic integration point is depicted. When comparing the macroscopic response of the second simulation, where the SSRVE is considered at the microscale, with the first one based on the target structure, a qualitatively and quantitatively similar stress response is observed. The same holds for the microscopic response. This accentuates the performance of the SSRVE and shows that it seems to be possible to approximate the macroscopic response of random microheterogeneous materials by much simpler SSRVEs on the microscale. Another aspect to be emphasized is the significantly reduced computational cost due to the much lower degrees of freedom required for the discretization of the SSRVE.

References

[1] Balzani D., Schröder J. and Brands D., FE^2-Simulation of Microheterogeneous Steels Based on Statistically Similar RVEs, *IUTAM Symposium on Variational Concepts with Applications to the Mechanics of Materials*, IUTAM Bookseries, 21, pp. 15-28, 2010.

[2] Balzani D., Schröder J., Brands D. and Carstensen C., Sensitivity analysis of statistical measures for the reconstruction of microstructures based on the minimization of generalized least-square functionals, *Technische Mechanik* 30(4), pp. 297-315, 2010.

[3] Miehe C., Schröder J. and Schotte J., Computational homogenization analysis in finite plasticity. Simulation of texture development in polycrystalline materials, *Computer Methods in Applied Mechanics and Engineering*, 171, pp. 387-418, 1999.

[4] Schröder J., Homogenisierungsmethoden der nichtlinearen Kontinuumsmechanik unter Beachtung von Stabilitätsproblemen, *Bericht aus der Forschungsreihe des Institut fr Mechanik (Bauwesen)*, Lehrstuhl I, Habilitationsschrift, 2000.

[5] Schröder J., Balzani D. and Brands D., Approximation of random microstructures by periodic statistically similar representative volume elements based on lineal-path functions, *Archive of Applied Mechanics*, DOI: 10.1007/s00419-010-0462-3, 2010.

[6] Smit R.J.M., Brekelmans W.A.M. and Meijer H.E.H., Prediction of the mechancal behavior of nonlinear heterogeneous systems by multi-level finite element modeling, *Computer Methods in Applied Mechanics and Engineering*, 155, pp. 181-192, 1998.