Available online at www.eccomasproceedia.org
Eccomas Proceedia UNCECOMP (2017) 419-425

ECCOMAS
Proceedia

UNCECOMP 2017
2nd ECCOMAS Thematic Conference on
Uncertainty Quantification in Computational Sciences and Engineering
M. Papadrakakis, V. Papadopoulos, G. Stefanou (eds.)
Rhodes Island, Greece, 15–17 June 2017

CONSTRUCTION OF STATISTICALLY SIMILAR RVES FOR THE QUANTIFICATION OF UNCERTAINTY ASSOCIATED WITH THE MATERIAL'S MICROSTRUCTURE MORPHOLOGY

Daniel Balzani[1,2], **Niklas Miska**[1], **and Stefan Prüger**[1]

[1]Institute of Mechanics and Shell Structures
Technische Universität Dresden
August-Bebel-Str. 30, 01219 Dresden
e-mail: {daniel.balzani, niklas.miska, stefan.prueger}@tu-dresden.de

[2] Dresden Center for Computational Materials Science
01062 Dresden

Keywords: Uncertainty Quantification, Statistically Similar Representative Volume Elements, Morphology, Microstructure, Dual Phase Steel.

Abstract. *Various engineering applications require the use of modern materials. In particular with view to automotive applications, where increased safety standards at reduced weight are important, multiphase steels are advantageous. These steels make use of a pronounced microstructure in order to achieve a high ductility with high strength. The morphology of these microstructures varies over the location in the macroscopic part and over different specimen. As the macroscopic response of the steel is governed by the microstructure morphology, the randomness of the microscopic morphology implies uncertainties regarding the macroscopic material response. We propose to create statistically similar representative volume elements (SSRVE) to enable access to the incorporation of these uncertainties in numerical computations. The SSRVEs are obtained by minimizing a least-square functional consisting of higher order statistical measures, which describe the morphology of the microstructure. The resulting geometries are significantly less complex than the real microstructure and exhibit an advantage regarding meshing and computing the problem. Aside from these advantages, the method also provides a basis to construct various SSRVEs which are within predefined bounds regarding the microstructure statistics. These bounds may be obtained from measurements performed by analyzing the microstructures at different locations in one material. Based on this variety of applicable SSRVEs multiple Finite Element (FE) simulations can be performed to obtain the homogenized response and thus, to quantify statistics regarding macroscopic material parameters. In order to automatize these numerical simulations the Finite Cell Method (FCM) can be applied such that a conforming FE mesh for each of the SSRVEs is not needed to be constructed.*

Peer-review under responsibility of the organizing committee of UNCECOMP 2017.
doi: 10.7712/120217.5380.16923

1 Introduction

Many modern materials make use of a pronounced microstructure to achieve advantageous properties. Advanced high strength steels (AHSS) for instance combine high strength with high ductility and are therefore used e.g. to create light-weight car bodies whilst enhancing the crash-safety. As the macroscopic behavior depends on the morphology of the microstructure, the variation of the morphology of the microstructure over different specimens or different locations in one specimen leads to an uncertainty of the material's response on the macroscale. Thus, it may be necessary to consider this uncertainty in computations of AHSS (among other uncertainties, e.g. implied by variation of the material parameters). Nowadays most approaches to quantify the uncertainty regarding the microstructure use stochastic approaches, e.g. [10, 4], where Monte Carlo simulations are connected with extended finite elements (XFEM) to quantify uncertainties in effective properties or [6], in which random microstructures are combined with model reduction methods. For such analysis a large number of microstructures all representing possible real microstructures is required. The question in this context is how to obtain these microstructures, in particular with view to the fact that they will in most cases not be experimentally accessible. So far, most approaches make use of a rather random generation of artificial and idealized microstructures without taking into account the statistics of the real microstructure morphology. Therefore, here we propose a method based on such statistics which are experimentally measured to enable a suitable and representative set of microstructures. For this purpose we exploit the idea of statistically similar RVEs (SSRVEs) [1], which are obtained by minimizing a least-square functional defined in terms of differences of statistical measures evaluated for the real microstructure and the SSRVE. This contribution is organized as follows: Section 2 briefly introduces the concept of direct micro-macro-computations, before Section 3 describes the method to create the set of microstructures. In Section 4 a simple computational example is provided, Section 5 concludes this paper.

2 Micro-Macro Modeling of DP-Steel

In this contribution we focus on DP steel, whose microstructure consists of a ferrite matrix in which martensite inclusions are embedded. The ferrite matrix with its relatively low yield stress is responsible for the high ductility respectively good formability whilst the martensite inclusions with a higher yield stress act as a reinforcement and increase the strength of the DP steel. Since the different elasto-plastic properties of the microscopic constituents and their interaction govern the macroscopic response, it is advantageous to include the micro-heterogeneity in the modeling. A suitable direct micro-macro approach is the FE^2 scheme, cf. e.g. [9]. In this scheme, the evaluation of the material law at every integration point of the macroscopic problem is replaced by homogenizing the microscopic stress distribution, which is in turn obtained by numerically solving a microscopic boundary value problem based on a representative volume element (RVE) in terms of Finite Elements. When suitable boundary conditions are applied to the RVE, the stresses and tangent moduli can be homogenized by

$$\overline{\mathbf{P}} = \frac{1}{V}\int_B \mathbf{P} dV \quad \text{and} \quad \overline{\mathbf{A}} = \frac{1}{V}\int_B \mathbf{A} dV - \frac{1}{V}\mathbf{L}^T\mathbf{K}^{-1}\mathbf{L},\ \mathbf{L} = \int_B \mathbf{B}^T\mathbf{A} dV, \tag{1}$$

cf. [12, 13] for further details. Herein, the microscopic 1st Piola-Kirchhoff stresses are denoted by $\mathbf{P}$ and the associated moduli are $\overline{\mathbf{A}} = \partial_F \mathbf{P}$ with the deformation gradient $\mathbf{F}$. The macroscopic counterparts are denoted by an overline. $\mathbf{K}^{-1}$ is the inverse of the global stiffness matrix of the microscopic boundary value problem, $\mathbf{B}$ is the classical Finite Element B-matrix.

Although the FE^2 scheme replaces a constitutive material law for the composite material, constitutive material laws for the individual microscopic phases are still required to solve the microscopic boundary value problem. Here, we consider a classical finite strain elasto-plasticity formulation with isotropic exponential hardening [14], which is implemented in the material setting following [5]. This model is adjusted to experimental data obtained from mechanical tests, which were performed for the individual phases.

3 Method for the Quantification of Microstructure-Related Uncertainty

This section is devoted to the proposed method for the quantification of microstructure-based uncertainties of the DP steel properties. The method makes use of statistically similar representative volume elements such that variations regarding the morphology of microstructures can be taken into account.

The direct incorporation of the microstructure in FE simulations described in section 2 creates an additional problem: the complex geometry of the microstructure requires many elements to create a sufficient mesh, so that every microscopic boundary value problem ends in an expensive numerical computation with large demands not only with respect to the computing time but also with respect to the required memory. This is particularly important for any problem where a large number of microscopic boundary value problems has to be solved, i.e. for FE^2-simulations, but also for Monte-Carlo uncertainty quantification. A possible way out is proposed in [1, 11], where an artificial microstructure, the SSRVE, is constructed which is as similar as possible in a statistical sense to the real microstructure. This SSRVE is characterized by a less complex morphology, which therefore requires fewer degrees of freedom for the Finite Element discretization. The SSRVEs are obtained by optimizing a least square functional $\mathcal{L}$, which is given by

$$\mathcal{L}(\gamma) := \sum_L \omega_{(L)} \left(\mathcal{P}^{\text{real}}_{(L)} - \mathcal{P}^{\text{SSRVE}}_{(L)}(\gamma) \right)^2 . \tag{2}$$

In Equation (2), the parameters characterizing the inclusions are collected in γ whereas $\mathcal{P}^{\text{real}}$ and $\mathcal{P}^{\text{SSRVE}}$ denotes a statistical descriptor evaluated for the real microstructure resp. the SSRVE. ω_L represents a weighting factor for the individual statistical descriptors. For the evaluation of the statistical measures for the real microstructure the required data can be obtained from segmenting three dimensional electron backscatter diffraction measurements, cf. [2]. For the representation of DP steel, in [1] it turns out that a parameterization with 3 ellipsoidal inclusions results in an acceptable mechanical error. Therefore, we also consider SSRVEs with 3 inclusions and incorporate the same statistical measures as in [1], namely the volume fraction $\mathcal{P}_{(\text{V})}$, the spectral density $\mathcal{P}_{(\text{SD})}$ and the lineal path function $\mathcal{P}_{(\text{LP})}$.

In principle, if unlimited data regarding the 3D microstructure was available, the uncertainties resulting from variations of the microstructure morphology can be quantified by a Monte-Carlo calculation. Then, a rather large number of 3D microstructures from either different specimens or from different locations within one specimen is simulated and the discrete probability distribution of the resulting homogenized response is obtained. However, this unlimited data is typically not available due to the high costs associated with the measurement of 3D microstructures. Therefore, a method to construct artificial microstructures, which are still in a defined interval of acceptable statistical variations, is unavoidable.
Therefore, we propose an approach based on the least square functional used for the construc-

tion of SSRVEs. We assume, that every set of parameters γ, that yields a value $\mathcal{L}$ in an interval

$$\mathcal{L} \in \Big[\min[\mathcal{L}], \mathcal{L}_B\Big], \tag{3}$$

represents an RVE with an admissible microstructure variation provided that $\mathcal{L}_B$ is suitably defined for the considered real microstructure. The acceptable range is limited by a boundary value $\mathcal{L}_B$, so that a set of statistically admissible artificial RVEs can be computed as

$$\{\gamma^{\text{SSVE}}\} = \arg[\mathcal{L}(\gamma) < \mathcal{L}_B]. \tag{4}$$

The abbreviation SSRVE stands by definition for the best solution of the least square functional and thus for the RVE best matching the statistics of the complete real microstructure. All other considered parameters lead to artificial microstructures which are thus referred to as statistically similar volume elements (SSVE). All SSVEs in this set can now be used to quantify the uncertainty of macroscopic properties by performing a Monte-Carlo calculation of the homogenized properties. In detail this means that each SSVE is discretized in terms of Finite Elements and a suitable boundary value problem representing a mechanical test is solved to obtain the homogenized macroscopic response. From this, selected macroscopic properties can be computed.

The bound $\mathcal{L}_B$ may be obtained by incorporating some additional information regarding the real 3D microstructures, e.g. a larger measurement space. For this larger microstructure first a suitable RVE defined as sub-section of the real microstructure is found by choosing a reasonable RVE size and minimizing (2), where γ solely represents the position of the sub-section. Then, $\mathcal{L}$ is computed for all possible sub-sections in order to identify $\mathcal{L}_B$, which is now the largest possible deviation from min$\mathcal{L}$. If we relate one of these sub-sections to index k, the bound is obtained by

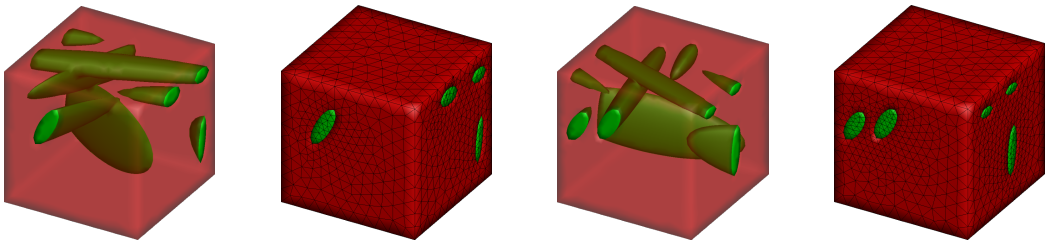
$$\mathcal{L}_B := \max\left[\mathcal{L}(\gamma_k)\right]. \tag{5}$$

If sufficient microstructure information is available such that even the probability distribution could be computed based on the real microstructure, the computational evaluation of this large set of microstructures would still be challenging. Then, the method proposed here could be used instead to enable a calculation of significantly reduced computing time. Furthermore, the probability distribution of $\mathcal{L}$ in the real microstructure could be computed and an according set of SSVEs could be constructed using the Metropolis-Hastings algorithm.

4 Example

As a simplified example we consider the real microstructure of DP steel from [1] and compute the uncertainties on the macroscopic yield stress and hardening modulus, which are considered to result from microstructure variations. Since only limited information regarding the real 3D microstructure is available, the bound is set to $\mathcal{L}_B = 0.0075$, whilst the SSRVE is obtained for $\mathcal{L} = 0.005347$. While optimizing the least-square functional (2) to obtain the SSRVE using the framework Mystic and the differential evolution algorithm, cf. [8, 7], 11 evaluations were performed in which (4) was satisfied. For simplicity, we consider these as SSVEs for the representation of some microstructure variation. Figure 1 shows the SSRVE and one example of an SSVE. As it can be seen, the morphology of the microstructure is similar.

The associated parameters are transferred to Gambit, which is used to create the geometry and the mesh of the SSVEs, which are then transferred to FEAP 8.2, which is used to solve



(a) (b)

Figure 1: Morphology and mesh of the SSRVE (a) and one exemplaric SSVE (b).

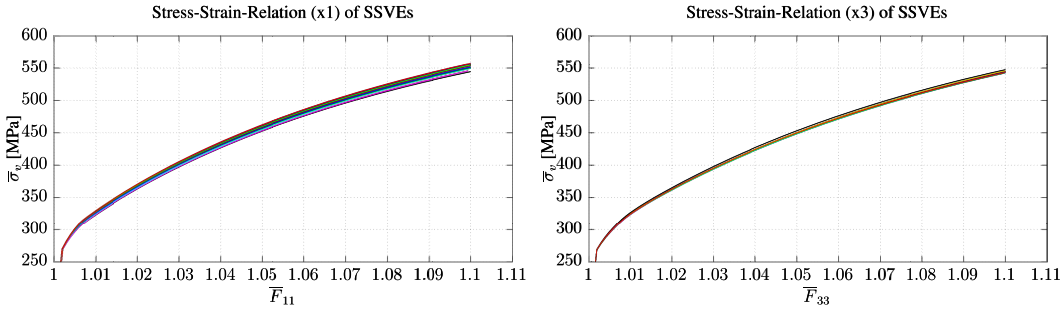


Figure 2: Stress-strain-relation for tensile test in x1 (left) and x3 (right) direction

the boundary value problem using periodic boundary conditions. All meshes are in the range of 25,000 to 30,000 elements and can thus be calculated rather efficiently. Here, only a macroscopic tension test in two different spatial directions is considered. The computations are strain driven and carried out until 10 percent elongation. Figure 2 shows the VON MISES stress plotted against the deformation gradient component in tensile direction. The curves splay in the hardening region due to the different morphologies. There is no spreading in the elastic regime, as the material model for the individual phases shares the same elastic properties and differs only in the hardening parameters. Additionally, the expected tiny degree of anisotropy as typically observed in DP steel is obtained. On the basis of the resulting stress strain curves effective material properties on the macroscale are computed. First, we analyze the effective yield stress $R_{p,0.2}$, whose histograms are displayed for both tensile tests in Figure 3. Note that due to the intuitively chosen bound $\mathcal{L}_B$ the obtained uncertainty is rather small, i.e. in a range of only a few MPa. Appearently this bound is not realistic for DP steels, however, it shows the principle

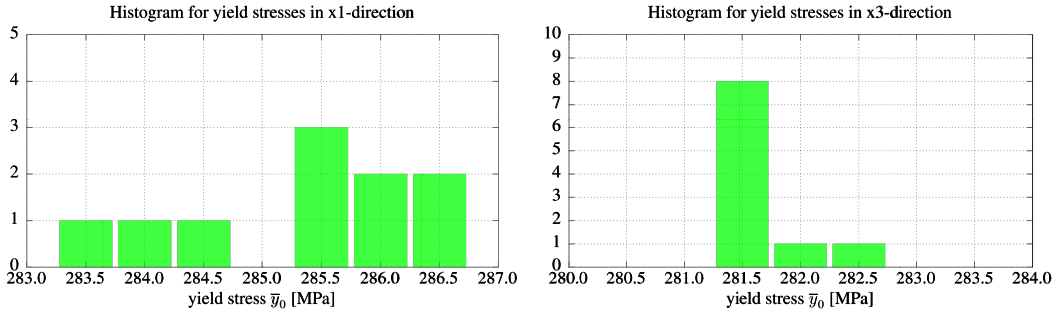


Figure 3: Histogram of resulting initial yield stress in x1 (left) and x3 (right) direction

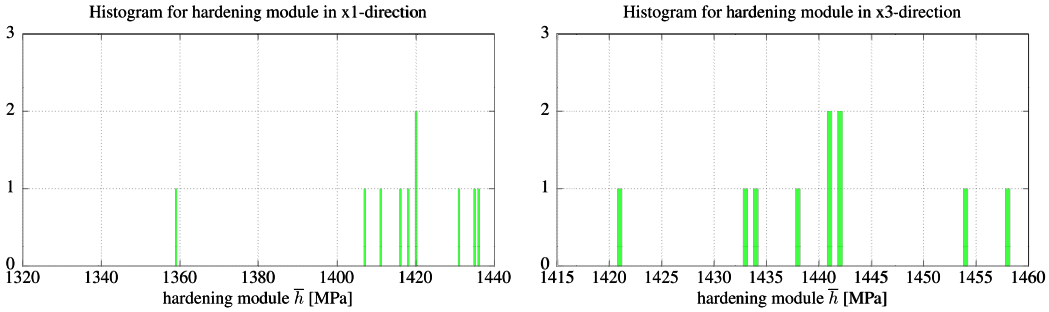


Figure 4: Histogram of resulting effective hardening moduli in x1 (left) and x3 (right) direction

procedure proposed here. With the consideration of additional real microstructures and a larger bound a greater variance in the material parameters is expected. The same effect is noticeable for the hardening modulus at the macroscopic strain $\overline{F} = 1.1$, for which the histogram is shown in Figure 4. A slight uncertainty is also found here due to the chosen bound.

5 Conclusion

In this paper a method was proposed, that is capable to quantify uncertainties of the material's response due to variations in the microstructure morphology. It makes use of artificial RVEs, so that the demand of additional scans of the microstructure is reduced to a minimum. Here, a simplified example was considered in the sense that only few SSVEs were taken into account in the uncertainty quantification process. For future development it is planned to implement an automatic simulation procedure based on an extended Finite Cell Method [3]. Furthermore, the statistical variation bound $\mathcal{L}_B$ was chosen rather arbitrarily and thus, the quantitative results do not represent realistic variations in macroscopic properties. More microstructure information shall also be included, so that the bound can be extended to more realistic values. However, the example was able to demonstrate the principle procedure of the proposed approach which enables the construction of a statistically matching set of artificial microstructures to be used in the uncertainty quantification.

Acknowledgements

The authors greatly appreciate financial funding by the German Science Foundation (Deutsche Forschungsgemeinschaft, DFG) as part of the priority program "Polymorphic uncertainty modelling for the numerical design of structures" (SPP 1886), project BA2823/12-1, and as part of the Institutional Strategy "The Synergetic University" at TU Dresden.

REFERENCES

[1] D. Balzani, L. Scheunemann, D. Brands, and J. Schröder. Construction of two- and three-dimensional statistically similar rves for coupled micro-macro simulations. *Computational Mechanics*, 54:1269–1284, 2014.

[2] D. Brands, D. Balzani, L. Scheunemann, J. Schröder, H. Richter, and D. Raabe. Computational modeling of dual-phase steels based on representative three-dimensional microstructures obtained from ebsd data. *Archive of Applied Mechanics*, 86(3):575–598, 2016.

[3] A. Düster, J. Parvizian, Z. Yang, and E. Rank. The finite cell method for three-dimensional problems of solid mechanics. *Computer Method in Applied Mechanics and Engineering*, 197:2768–3782, 2008.

[4] Badri Hiriyur, Haim Waisman, and George Deodatis. Uncertainty quantification in homogenization of heterogeneous microstructures modeled by xfem. *International Journal for Numerical Methods in Engineering*, 88, 2011.

[5] S. Klinkel. Theorie und Numerik eines Volumen-Schalen-Elementes bei finiten elastischen und plastischen Verzerrungen. *Dissertation thesis, Institut für Baustatik, Universität Karlsruhe*, 2000.

[6] Babak Kouchmeshky and Nicholas Zabaras. Microstructure model reduction and uncertainty quantification in multiscale deformation processes. *Computational Materials Science*, 2010.

[7] Michael McKerns, Patrick Hung, and Michael Aivazis. *mystic: a simple model-independent inversion framework*, 2009-. http://trac.mystic.cacr.caltech.edu/project/mystic.

[8] M.M. McKerns, L. Strand, T. Sullivan, A. Fang, and M.A.G. Aivazis. Building a framework for predictive science. *Proceedings of the 10th Python in Science Conference*, 2011. http://arxiv.org/pdf/1202.1056.

[9] C. Miehe, J. Schröder, and J. Schotte. Computational homogenization analysis in finite plasticity, simulation of texture development in polycrystalline materials. *Computer Methods in Applied Mechanics and Engineering*, 171:387–418, 1999.

[10] Dimitris Savvas, George Stefanou, Manolis Papadrakakis, and George Deodatis. Homogenization of random heterogeneous media with inclusions of arbitrary shape modeled by xfem. *Computational Mechanics*, 2014.

[11] L. Scheunemann, D. Balzani, D. Brands, and J. Schröder. Design of 3d statistically similar representative volume elements based on minkowski functionals. *Mechanics of Materials*, 90:185–201, 2015.

[12] J. Schröder. Homogenisierungsmethoden der nichtliniearen kontinuumsmechanik unter beachtung von stabilitätsproblemen technical report. *Bericht Nr.:I-1, Institut für Mechanik (Bauwesen), Lehrstuhl I, Universitäts Stuttgart*, 2000.

[13] J. Schröder and K. Hackl, editors. *Plasticity and Beyond Microstructures, Crystal- Plasticity and Phase Transitions*, chapter A numerical two-scale homogenization scheme: the FE2-method, pages 1–64. Springer, 2014.

[14] J.C. Simo. Algorithms for static and dynamic multiplicative plasticity that preserve the classical return mapping schemes of the infinitesimal theory. *Computer Methods in Applied Mechanics and Engineering*, 99:61–112, 1992.