

Finite Element Modeling of Porous Nickel Base Cast Alloys with Representative Volume Elements

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Abstract: In order to quantify the influence of pores on the deterioration of cast alloys, a micromechanical finite element model using Abaqus/Standard is introduced. Python scripting is employed to automate the pre- and post processing of the microstructure generation, the finite element meshing and the model predictions.

The mechanical response upon loading of the micromechanical model is studied by volumetric homogenization and quantile evaluations of stress and strain distributions. In order to obtain reliable results it is important to ensure that the micromechanical models are representative. Varying the size of the modeled microstructural volume element and keeping the geometric parameters and the volume fraction of the pores constant enables to determine the smallest micromechanical model size that can be considered representative.

Key Words: representative volume element; micromechanical modeling,

Introduction

A fundamental goal of the aeronautical industry is to increase the specific thrust of gas turbines while keeping emissions to a minimum. One way to reach this goal is to reduce safety factors and thus the mass of the engine. This necessitates a thorough understanding of the mechanical behavior of the materials. In the high temperature sections of turbines, advanced nickel base alloys are used [1]. In this work attention is paid to the nickel base cast alloy MAR-M247. The material properties of MAR-M247 are governed by its microstructure, which contains finely dispersed pores in regions where the feeding of liquid metal is constricted during casting and solidification. Also carbides are found in the nickel matrix. The heterogeneous nature of the microstructure has a significant influence on the observed macroscopic material behavior [2]. As described in [3] pores give rise to stress peaks. Carbides also cause local stress peaks due to their resistance against deformation. Such inhomogeneities are important factors determining the fatigue lifetime of cast components. In the following, the term inclusion will be used when referring to both pores and carbides. Quantifying the effect of inclusions on the overall mechanical properties enables a sharpening of the design rules and thus a more advanced component layout. Over the last decades considerable effort has been invested into experimental and theoretical investigations of the microstructures' influence on the mechanical materials behavior. A comprehensive overview of various analytical and numerical methods available for this task is given for example in [4].

In this paper we present a finite element approach to study the influence of the microstructure on the mechanical behavior. A crucial criterion for such is to ascertain the convergence of the finite

element model models in order to obtain reliable results. This necessitates a sufficiently fine mesh as well as a minimum size of the modeled microstructural volume element. The influence of the mesh density and the size of the modeled microstructural volume element is investigated by convergence studies.

Finite element modeling

The finite element (FE) method is a powerful tool to study and quantify local effects triggered by inclusions. At the micro-scale level, there are two common types of geometry model: Real microstructure phase arrangements derived from 3D computed tomography (CT) and micrographs, and computer-generated geometries. An advantage of computer generated microstructure models as pursued in this work over geometries derived from the real microstructure is that the former enable parametric studies.

Microstructural model generation

In order to achieve reliable results it is important for the microstructure model to represent the relevant characteristics of the real structure. We restricted ourselves to the accumulated volume of the inclusions, the shape of single inclusions in terms of their aspect ratio, as well as the spatial distribution of the inclusions in the sampled volume. These characteristics can be obtained from detailed studies of micrographs and 3D CT images of nickel base cast alloy samples. The aspect ratios and volumes of single inclusions are statistically characterized utilizing truncated normal and lognormal distributions with minimum and maximum thresholds, respectively. The pore topologies in the model are based on a Boolean union of parameterized ellipsoids with their major axis arranged perpendicular around their common geometric center. This accounts for the ramification of interdendritic pores and ensures a realistic representation of the materials microstructure.

The algorithm to construct the microstructure model is implemented in Python. This requires the experimentally determined distributions or the shape and volume of the inclusions as well as the pore volume fraction as input parameters. The generated geometry is designed to be suitable for the periodic microfield approach (PMA) as described in [4]. PMA assumes that the whole material exhibits a geometric periodicity corresponding to a periodic arrangement of the modeled microstructural volume element. Once the topology of the microstructure is constructed, a finite element mesh has to be generated. The default element size is a fraction of the smallest ligament length (shortest distance between two inclusions) within the model. This ensures that ligaments are resolved by a minimum number of finite elements over their cross section, which is vital to obtain reliable FE results. To mesh the microstructure model the quadratic tetrahedral elements C3D10M [5] were used in order to avoid locking effects. Figure 1 shows the mesh at the pore surface of an exemplary geometric microstructure model.

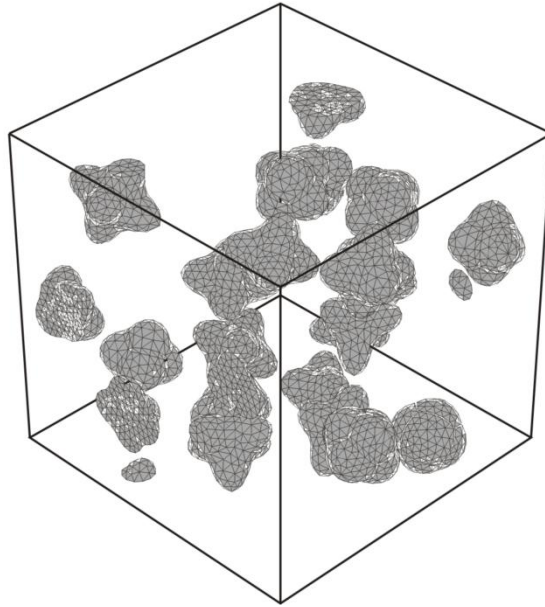


Figure 1: Micromechanical finite element model exhibiting a pore volume fraction of 10%. The mesh on the surface of the pores is shown, whereas the matrix is transparent. Note be seen that the pores vary in size and shape.

Comparison of real- and modeled microstructure

Figure 2 shows a comparison of a real and a computer-generated microstructure. The micrograph of the computer-generated microstructure was derived from a cross section of a three-dimensional finite element model using Abaqus/CAE.

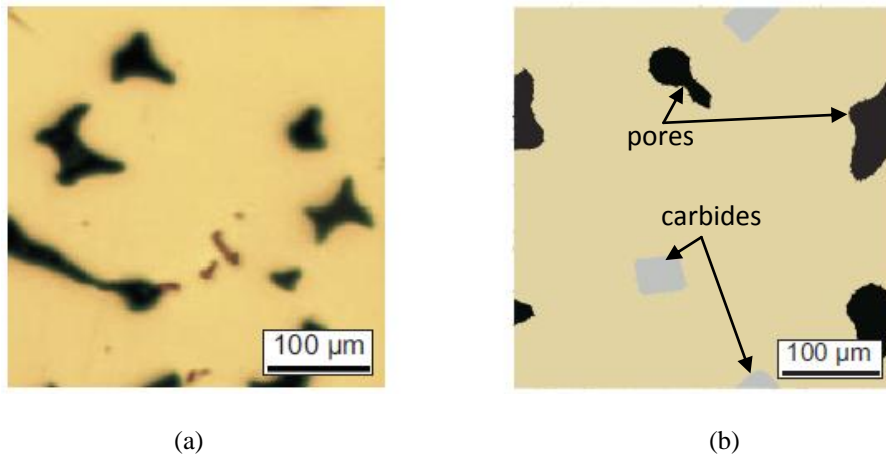


Figure 2: (a) Cross sectional light optical micrograph of a sample containing 4,9% porosity and 0,78% carbides (by volume); (b) Cross sectional image of a computer-generated microstructure containing 5,0% porosity and 0,8% carbides.

Obviously, the images are not congruent. However, the accumulated pore and carbide volumes, minimum pore sizes and the minimum ligament length of the real and the computer-generated microstructures match. The parameters derived from the real and computer-generated microstructures as well as the input parameters for the model generation are listed in Table 1.

Only the maximum pore sizes deviate significantly. This is due to the maximum pore volume defined as an input parameter to generate the microstructure model. Pores larger than 400.000 μm^3 are treated as macroscopic defects and thus are not considered in the micromechanical model. The remaining parameters derived from the model correspond well with the real microstructure. The small deviations are due to the statistical modeling approach.

Table 1: Some characteristic parameters of the real and computer generated microstructure

Model	Accumulated pore volume fraction [%]	Accumulated carbide volume fraction [%]	Single pore volume min/max [μm^3]	Minimum ligament length [μm^3]
Real microstructure	4,9	0,78	6.570/1.876.450	10
input parameters	4,9	0,78	6.570/400.000	10
exemplary model geometry	5,0	0,8	6.894/375.000	13

Convergence study

In order to obtain reliable results, the FE models have to be examined for mesh and property convergency. Due to the low carbide volume fraction, only pores are considered in this study. Both periodic as well as uniform displacement boundary conditions were applied to study the convergency behavior of the micromechanical volume element models. The periodic boundary conditions (PBC) can be written as

$$x^+ - x^- = F(X^+ - X^-),$$

where x^+ and x^- denote corresponding points on opposing faces of the micromechanical volume element model in the current configuration, X^+ and X^- denote the reference configuration of these points, and F is the homogenized deformation gradient imposed upon the micromechanical volume element. The uniform displacement boundary conditions (UD-BC) can be written as

$$x = F X,$$

where x is an arbitrary point on the surface of the micromechanical volume element model in the current configuration and X is its reference configuration. A more detailed description of the boundary conditions can be found in [4]. To test the convergency of the microstructure models the stress and strain fields within the matrix material, as shown in Figure 3, are evaluated using volumetric homogenization as well as quantile evaluations. The homogenization of any quantity $A(x)$ over a specific region Ω can be written as

$$\langle A \rangle = \frac{1}{V_{\Omega}} \int_{\Omega} A(x) d\Omega ,$$

where V_{Ω} is the volume of the region and $\langle A \rangle$ is the homogenized quantity. The homogenized properties obtained from the microstructure model mimic the macroscopic material behavior. In contrast to the homogenized material behavior local effects like the onset of fracture can be studied by quantile evaluations.

In the present work, we defined mesh convergency as reached, if the homogenized response of the micromechanical model does not change by more than 2% when doubling the number of elements used to mesh the microstructural finite element model.

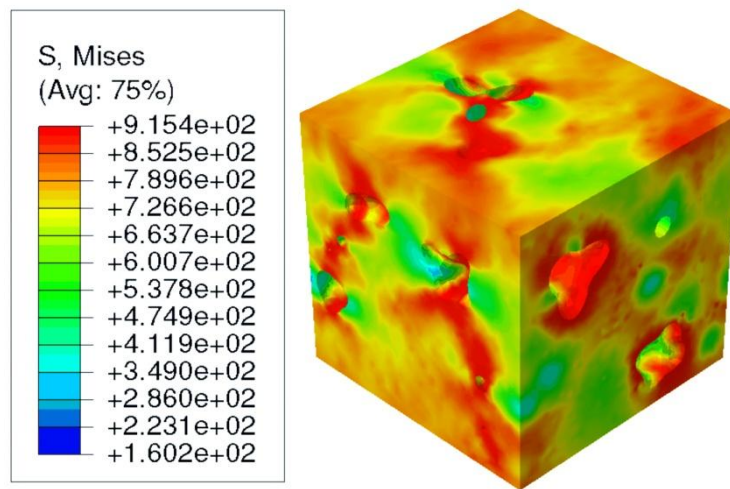


Figure 3: Von Mises stress distribution in the matrix material. The unit cube exhibits a pore volume fraction of 10%. The highest stresses occur in the vicinity of the pores.

To identify the volume element of minimum size exhibiting property convergency and thus being considered a representative volume element (RVE), different volume element sizes were studied. The largest volume element models used within this study have an edge length of 200 μ m and contain on average 20 pores, whereas the smallest models have an edge length of 50 μ m and contain only 1 pore. For each micromechanical model size the mean value and standard deviation of the Young's modulus and the 98% quantile of the plastic equivalent strain is evaluated from 100 simulations, Figure 4. We define property convergency as reached, if the mean of the Young's modulus and the mean of the 98% quantile of the plastic equivalent strain do not change by more than 1% when increasing the edge length of the volume element model by 50 μ m. In Figure 4 these restrictions are indicated by the RVE bounds. Clearly, a minimum size of the unit cell is needed in order to obtain viable results. If the micromechanical model is too small, the results are strongly influenced by the boundary conditions. This is especially critical for the quantile evaluation of the plastic equivalent strain as shown in Figure 4 (b). The difference between the mean values of the smallest and the largest tested cells is 17%. The increase of the mean value of the 98% quantile of the plastic equivalent strain is due to the

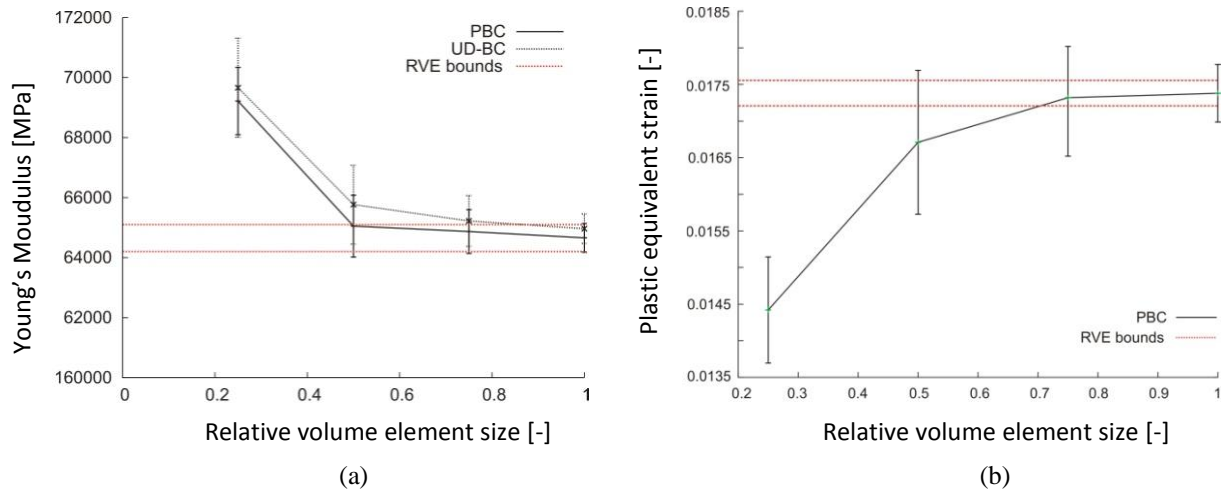


Figure 4: Convergence study. The finite element models evaluated for this study exhibit a pore volume fraction of 10%. Each data point represents 100 simulations. (a) shows the effective elastic response; (b) shows the 98% quantile of the plastic equivalent strain depending on the unit cell size is shown.

higher complexity of the interaction of the increased number of inclusions in larger micromechanical finite element models. As can be seen, the results obtained from the micromechanical model largely depend on the representativeness of the volume elements. In the conducted study a minimum edge length of the micromechanical models of 150 μ m was determined as sufficiently large.

The largest finite element models used for the convergence study presented above contain approximately 80000 to 110000 finite elements. For the simulations the iterative solver from Abaqus/Standard was used. The total CPU time to perform one calculation is between 3000 and 5000 seconds using an Intel Xeon X5550 CPU with a clock speed of 2.66GHz on a system with 12 GB RAM. The high degree of automation of the modeling approach in combination with the acceptable calculation time allows determining the required minimum volume element size with reasonable effort.

Summary

The proposed approach provides a fast and robust way to create computer generated microstructure models. These models enable studying and quantifying the influence of the pores on the overall mechanical behavior. The results shed light on the local stress and strain distribution in the vicinity of inclusions. Particularly, the use of Abaqus/CAE and python scripting for the pre- and post processing allows for a high degree of automation and thus for the generation and evaluation of a statistically relevant set of microstructure models. This provides a useful basis both for addressing scientific questions and industrial problems.

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