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Numerical modeling of ductile fracture at the microscale combined with X-Ray laminography and digital volume correlation

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Abstract. Predicting ductile fracture for complex loading paths is essential within the framework of metal forming processes. Most models are developed and used at the macroscopic scale and do not account explicitly for material microstructures. This paper describes a methodology aiming at understanding and modeling ductile damage mechanisms at the microscale. This methodology relies on (i) the acquisition of X-Ray laminography pictures during in-situ tensile tests, (ii) digital volume correlation (DVC) to measure 3D displacement and strain fields in the bulk and (iii) 3D finite element (FE) modeling of the heterogeneous microstructure including ductile damage mechanisms. The methodology is illustrated on nodular graphite cast iron. FE simulations of the heterogeneous microstructure are conducted and compared with DVC results and the influence of boundary conditions is discussed.

INTRODUCTION

From an industrial point of view, predicting ductile fracture during metal forming processes is a top priority. This is why numerous scientific studies were conducted over the last 50 years in order to be able to predict the initiation of ductile fracture for various manufacturing conditions. Despite all these studies, there is no universal theory and predicting ductile failure is still challenging. This is due to the complexity of the thermomechanical and metallurgical mechanisms occurring during forming processes, namely, the material can be submitted to large plastic strains under multiaxial and non-proportional loading conditions, and thermal effects together with plastic strains can lead to microstructure changes. At the component scale, the prediction of ductile fracture is usually addressed using uncoupled failure criteria, coupled continuum damage mechanics approaches or damage models based on porous-plasticity theory (See Ref. [1] for a comparison of such approaches for cold metal forming applications). These approaches do not explicitly account for the material microstructure and phenomena such as the influence of elongated particles on damage anisotropy or nucleation/coalescence mechanisms are difficult to address.

The objective of this work is to study the intimate interaction between plasticity and damage mechanisms at the micrometer scale during ductile failure in the material bulk for different levels of stress triaxialities and Lode angles, and to understand the underlying physical mechanisms. To achieve this goal, three modern techniques are seamlessly coupled, namely, laminography to image in situ tested large flat samples made of ductile materials [2], digital volume correlation (DVC) to measure 3D displacement (and strain) fields in the bulk [3], and 2D/3D finite

element simulations using the experimental information on multiple length-scales [4]. In this paper, the overall methodology will be presented first to show how these three techniques can be combined. The second part will then focus on the application of this methodology to nodular graphite cast iron, and the last part will finally show some results comparing FE simulations driven by DVC boundary conditions and laminography pictures.

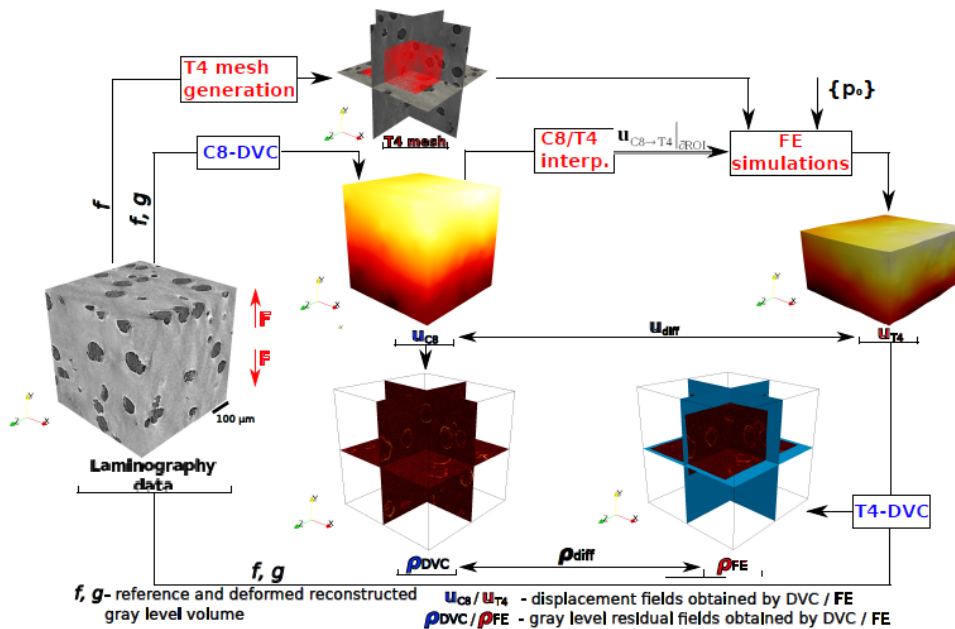
METHODOLOGY

The final goal of this study is to be able to define and calibrate nucleation and coalescence criteria based on real in-situ observations of these mechanisms. This requires images of the microstructure at different stages of the test as well as numerical tools able to mesh the microstructure and to model the mechanisms of ductile fracture. These simulations are performed on a Region of Interest (ROI) containing multiple graphite nodules from which voids will grow and eventually give rise to coalescence mechanisms. However, if one wants to understand coalescence mechanisms and calibrate criteria, the appropriate boundary conditions need to be applied on this ROI.

The methodology developed for obtaining local comparisons between experimental analyses and numerical simulations is therefore based on the following steps:

- X-ray laminography to get 3D pictures of an in situ test in a synchrotron facility [2, 3]. The ability to use flat specimens is of particular interest in the field of mechanics of materials since sheet-like samples allow for a wide range of engineering relevant boundary conditions.
- Global DVC to measure displacement fields whose kinematic basis is made of the shape functions of 8-noded elements [5]. It consists in minimizing gray level residuals over the whole ROI and in using kinematic fields based on FE discretizations.
- FE simulations at the microscale explicitly accounting for the morphology of the studied two-phase material [4, 6].
- Comparisons between experimental measurements and numerical simulations based on displacement fields and correlation residuals [7].

This methodology is summarized in **FIGURE 1** where it can be seen that an interpolation is required between DVC fields, obtained using trilinear hexahedral elements, and FE simulations using linear tetrahedral elements (mixed velocity-pressure P1+/P1 elements). All details about the methodology and the accuracy assessment can be found in Ref. [7].



APPLICATION TO NODULAR GRAPHITE CAST IRON

Studied material

The studied material is a commercial nodular graphite cast iron (EN-GJS-400), and specimens were supplied by M. Kuna, L. Zybell and M. Horn from TU Bergakademie Freiberg. At the microscale, this material features a ferritic steel matrix and graphite nodules with no significant porosity in the initial state. Then, under tensile loading, ductile fracture is mainly driven by very early debonding of the nodules from the matrix, and coalescence of the subsequent growing voids. Evidence in the literature [8] suggests modeling the nodules as voids, as their load carrying capacity is very low under tensile loading. This simplifying assumption is made herein and the material is considered as a two-phase microstructure with a ferritic matrix and voids. The ferritic matrix is considered as elastic-plastic and described using a power-law hardening

$$\sigma_0(\bar{\varepsilon}) = \sigma_y + K(\bar{\varepsilon})^n$$

where $\bar{\varepsilon}$ is the equivalent plastic strain, σ_y the yield stress, K the plastic consistency and n the hardening exponent. An immersed approach is used hereafter, which means that voids are meshed and defined as a purely elastic material with very low Young's modulus with respect to the matrix. A sensitivity analysis showed that a ratio of 1000 between this modulus and that of the matrix was sufficient [7]. The properties of the matrix are deduced from stress/strain curves given in Ref. [9], namely, $E = 210$ GPa, $\nu = 0.3$, $\sigma_y = 290$ MPa, $K = 382$ MPa and $n = 0.35$.

Tensile test on sample with two machined holes

The application shown herein is based on a tensile sample with two machined holes oriented at 45° with respect to the loading direction. This tensile specimen (see **FIGURE 2**) is tested in-situ. A ROI is meshed and studied under boundary conditions coming either from macroscopic FE simulations or from DVC data [10]. For this reason, the FE meshed domain (cyan in **FIGURE 2**) must always be embedded within the DVC domain (blue in **FIGURE 2**).

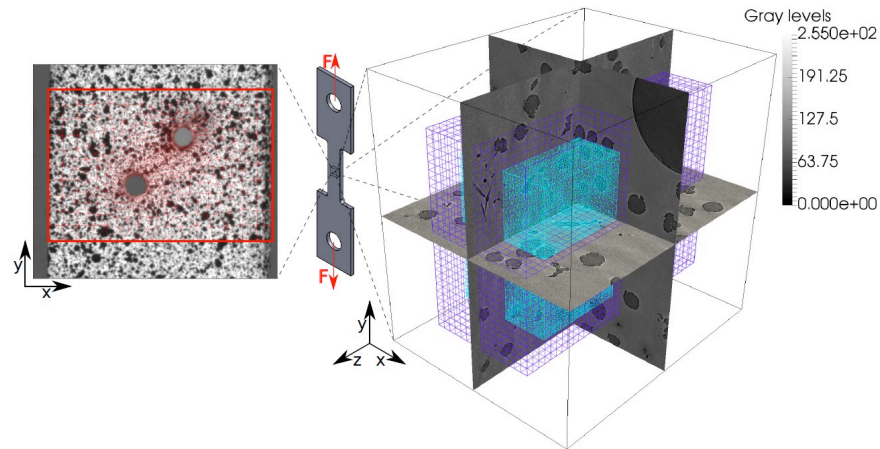


FIGURE 2. Schematic view of the sample with the definition of DVC (blue) and FE (cyan) meshes plotted over the corresponding cast iron microstructure in isometric view [10]

FE modeling

The first step consists in the definition and meshing of real microstructures based on X-ray laminography pictures. This step is facilitated by the use of level-set functions to represent interfaces between phases and by a dedicated body-fitted mesh adaption technique that also addresses volume conservation issues. Topological mesh adaption is applied automatically during mesh motion to reach large plastic strains while maintaining an appropriate discretization and preventing element flip [4]. In a more general framework, failure can be modeled for the void nucleation and coalescence stages. Stress-based criteria are used for particle failure and particle/matrix debonding whereas coalescence can be activated either through a local damage parameter or a minimum distance between neighboring voids. The finite element framework described above enables for the dynamic insertion of cracks during the computation and their remeshing throughout void growth. This technique also allows accounting for complex topological events such as void coalescence. In the following, since nodular cast iron is considered as a two-phase microstructure with ferritic matrix and voids, only void growth will be studied.

RESULTS

In the following, real microstructures were meshed on a given ROI as shown in **FIGURE 2**. A sensitivity analysis to RVE sizes was carried out in [6] for 2D and 3D configurations with random voids distribution. While such analysis is easily conducted for random distributions, it is hardly applicable to real microstructures. The region of interest we use in this work is a mesh of the whole observable microstructure, with respect to X-ray images. Accessing a larger region of interest would require larger specimens, and a larger field of view in the experiments, which is not possible with current imaging techniques. Nevertheless, the number of voids in the region of interest is rather big (~100) and we expect it to be representative of the material.

Influence of boundary conditions

FE results strongly depend on applied boundary conditions. In Ref. [10], a comparison was made between different ways of applying boundary conditions on the ROI. Since Direct Numerical Simulation (DNS) is too costly, three different approaches were compared:

- Weak FE coupling (w-FE): a first macroscopic simulation is conducted at the specimen scale in which the material is considered as homogeneous (**FIGURE 3.a**). The displacement field between each consecutive loading step where 3D X-ray scans were acquired is stored in the reference configuration. These displacements are then interpolated at the boundaries of the ROI during a second FE simulation at the microscale by means of linear interpolation.
- Strong FE coupling (s-FE): a single FE simulation is carried out at the specimen scale, but the heterogeneous ROI is embedded in this mesh by means of local mesh refinements (**FIGURE 3.b**).
- DVC driven boundary conditions (DVC-FE): as detailed in Ref. [7], DVC provides displacement fields that can be interpolated and used as boundary conditions on the ROI boundaries. In that case, computations are carried out only on the ROI (see **FIGURE 4**).

The comparison showed the limitations of both w-FE and s-FE approaches and the advantage of the DVC-FE framework with respect to void growth prediction [10].

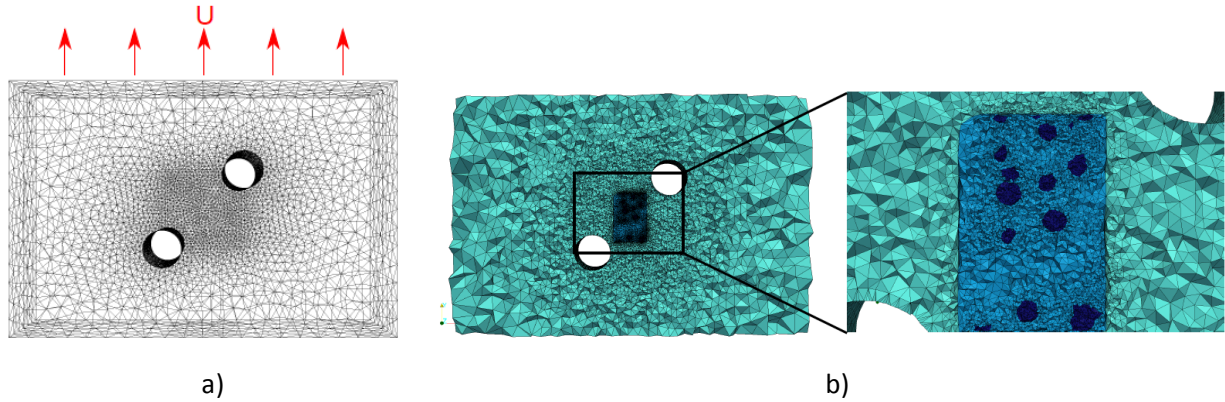


FIGURE 3. a) Mesh used at the specimen scale for the w-FE approach and b) inside view of the mesh used for the s-FE approach with detailed view of the heterogeneous ROI.

Void growth and plastic strain localization

In the following, the DVC-FE approach is adopted. **FIGURE 4** shows a 3D view of the RVE where both void growth and plastic strain are observed. At the end of these simulations, an acceleration of displacement gradients in the top-right corner of **FIGURE 4**'s last picture is an indication of coalescence mechanisms occurring before final failure.

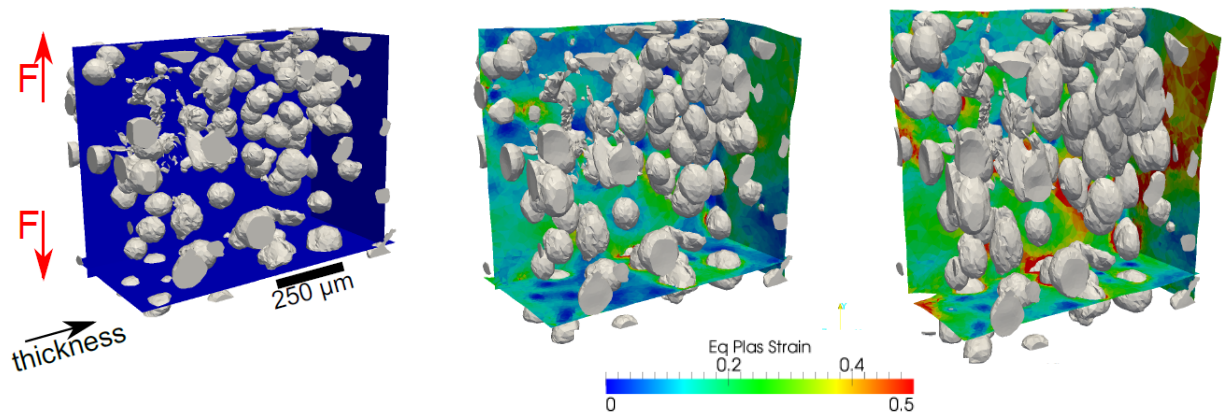


FIGURE 4. ROI calculation results using the DVC-FE approach and showing void growth and plastic strain for three different states during the tensile test.

Computed void growth can be compared with experimental void growth obtained from different laminography scans acquired during the tensile test [10]. FE local strains are also compared with DVC computed strain and final strain localizations between nodules are analyzed with respect to the coalescence mechanisms leading to final fracture (**FIGURE 5**). In **FIGURE 5.c**, FE strain localizations can be observed. These strain localizations are in good agreement with the failure path observed at the last stage before complete fracture (**FIGURE 5.d**).

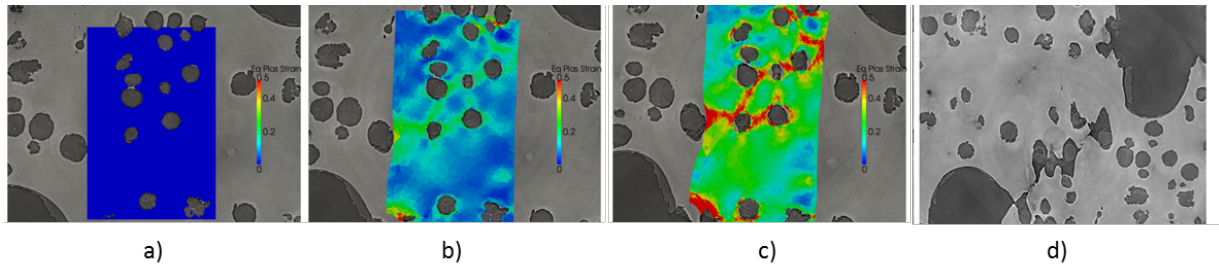


FIGURE 5. a), b) and c) Superposition of strain fields and X-ray laminography pictures at different stages of loading. d) Final coalescence mechanisms.

CONCLUSION

An innovative methodology combining in-situ X-Ray laminography, integrated DVC technique and FE modeling of heterogeneous microstructures was presented. This methodology, which is described in more details in Refs. [6, 7, 10], is a promising approach for getting a better understanding of nucleation, growth and coalescence mechanisms of heterogeneous microstructures for complex loading paths. By using DVC measurements as boundary conditions for FE simulations, this approach can also be used to calibrate nucleation and coalescence criteria and could therefore be an interesting way of feeding more physical macroscopic damage models used in material forming processes.

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