Micromechanical simulations and analyses based on synchrotron 3D imaging for nodular cast iron tested under different stress states

Thilo F. Morgeneyer, Ante F Buljac, Modesar Shakoor, Jan Neggers, Marc Bernacki, Pierre-Olivier Bouchard, Lukas Helfen, François Hild

Micromechanical simulations and analyses based on synchrotron 3D imaging for nodular cast iron tested under different stress states

Thilo F. Morgeneyer[a] , Ante Buljac[a,b], Modesar Shakoor[c], Jan Neggers[b], Marc Bernacki[c], Pierre-Olivier Bouchard[c], Lukas Helfen [d,e], François Hild [b]

[a] MINES ParisTech, PSL Research University, Centre des Matériaux, CNRS UMR 7633, France
[b] Laboratoire de Mécanique et Technologie (LMT), ENS Paris-Saclay/CNRS/Univ. Paris-Saclay, France
[c] MINES ParisTech, PSL - Research University, CEMEF, CNRS UMR 7635, France
[d] ANKA/Institute for Photon Science and Synchrotron Radiation Karlsruhe Institute of Technology (KIT), Germany
[e] European Synchrotron Radiation Facility (ESRF), France

Abstract

A combined computational–experimental framework is introduced herein to validate numerical simulations at the microscopic scale. It is exemplified for a flat specimen with two machined holes hole made of cast iron and imaged via in-situ synchrotron laminography at micrometer resolution during a tensile test. The region of interest in the reconstructed volume, which is between the two machined holes, is analyzed by digital volume correlation (DVC) to measure kinematic fields. Finite element (FE) simulations, which account for the studied material microstructure, are driven by Dirichlet boundary conditions extracted from DVC measurements. Gray level residuals for DVC measurements and FE simulations are assessed for validation purposes. The influence of the used boundary conditions, from FE simulations or from DVC measurements, on the predicted void growth is assessed for a case with two small machined holes in the flat sample that localize strains in the ligament between them.

Introduction

The main objective of the current work is to enable for more realistic microscopic calculations thanks to physical models calibrated directly at the microscale to analyze the three steps of ductile damage, namely, void nucleation, growth and coalescence. To achieve such goal, a first step consists of developing a numerical framework enabling for such validation and identification. The proof of concept of such validation framework is the topic of the present work. The studied material is nodular cast iron, which at the microscale features a ferritic matrix and graphite nodules, with no significant porosity in the initial state. Then, under tensile loading, ductile fracture is mainly driven by a very early debonding of the nodules from the matrix, growth of the nucleated voids and coalescence [Dong 1997, Hutter 2015]. Evidence in the literature [Dong 1997, Zhang 1999, Hutter 2015] suggests to model the nodules as voids, as their load carrying capacity is very low under tensile loading. This assumption is made herein and at the microscale the material is considered as a two-phase microstructure with a ferritic matrix and voids.

The final objective of the present work includes enabling for discussions regarding such assumptions, thanks to accurate and local error measurements directly at the microscale. This would help the development of experimentally probed microscopic models that could then be used to improve the common knowledge and understanding of ductile fracture, and deduce more accurate macroscopic responses. In particular, the ultimate aim is to set up a framework that allows failure and coalescence mechanisms and criteria such as internal necking or coalescence via nucleation of voids on a second population of particles to be assessed numerically.

The methodology proposed to obtain these local comparisons between experimental analyses and numerical simulations is based on the following steps (see figure 1):

- X-ray laminography to get 3D pictures of an in situ test in a synchrotron facility. By post-processing them, one may get, for instance, a first estimate of the morphology of the two-phase microstructure.
- Global digital volume correlation (DVC) to measure displacement fields whose kinematic basis is made of the shape functions of 8-noded elements. These displacement fields serve two purposes. First, they correspond to the kinematic data of the test. Second and more importantly, they will be used as Dirichlet boundary conditions of Finite Element (FE) simulations at the microscale.
- The FE simulations at the microscale explicitly account for the morphology of the studied two-phase material. Therefore the mesh made of 4-noded P1+/P1 tetrahedra elements is adapted to the microstructure with Level-Set (LS) functions and body-fitted mesh adaption.
- FE simulations are run with an elastoplastic constitutive equation to model the nonlinear behavior of the matrix.
- Comparisons between experimental measurements and numerical simulations are carried out for the displacement fields and correlation residuals.
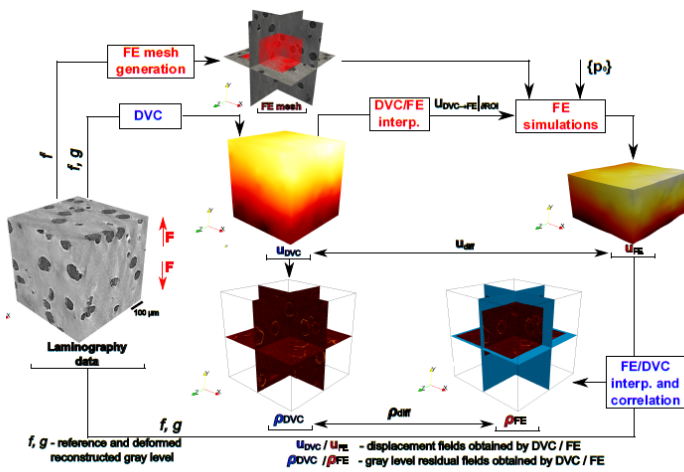
Figure 1 framework for micromechanical simulations based on synchrotron 3D imaging and comparison with volume field measurements (DVC) [Buljac 2017]

Results

For a case of a flat specimen with two machined holes arranged at 45° with respect to the loading direction, DVC measurements have been performed and simulations have been made using the measured boundary condition for the simulations. Figure 2 shows the comparison of the two approaches in terms of equivalent plastic strain. Local strain concentration can be seen where a high density of graphite nodules is found. The distribution of the strain fields is qualitatively in good accordance between the measurement and the simulation. The difference in strain magnitude is here due to the fact that in the measurement only an incremental field is shown whereas in the simulation the total strain is shown.
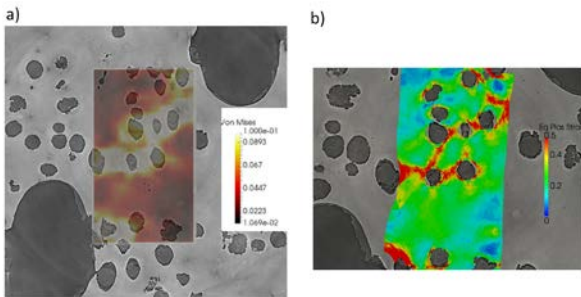

Figure 1 comparison of the equivalent strain field for a) an incremental DVC correlation and b) the total strain field for a micromechanical simulation using measured boundary conditions

Using such kind of simulations, the effect of boundary conditions on the void growth can be assessed. Here the effect of three different boundary conditions is assessed:

1. Weak FE (wFE): the boundary conditions for the ROI stemming from an elasto-plastic continuum simulation at the specimen scale.
2. Strong FE (sFE): simulation at the specimen scale with meshed nodules in the ROI during the simulation where the rest of the sample obeys an elasto-plastic material law.

3. DVC-FE: simulation of the ROI only using boundary condition measured by DVC.

The result of the simulations and also the measurement of the void volume fraction can be seen in figure 3.

It can be concluded that the simulations driven by the DVC measurement yield the best results even though the void growth is somewhat overpredicted.
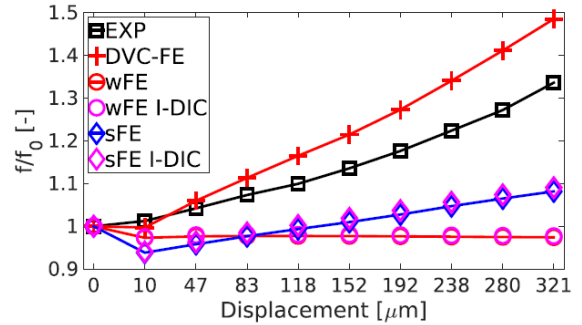

Figure 3 Comparison of the predicted void growth with different boundary conditions and the measured void volume fraction [Shakoor 2017]

References

[Dong 1997] Dong MJ, Prioul C, François D (1997) Damage effect on the fracture toughness of nodular cast iron: part I. Damage characterization and plastic flow stress modeling. Metall Mater Trans A 28(11):2245–2254

[Hutter 2015] Hütter G, Zybell L, Kuna M (2015) Micromechanisms of fracture in nodular cast iron: from experimental findings towards modeling strategies—a review. Eng Fract Mech 144:118–141

[Zhang 1999] Zhang K, Bai J, François D (1999) Ductile fracture of materials with high void volume fraction, Int J Solids Struct 36(23):3407–3425

[Buljac 2017] Buljac, A., Shakoor, M., Neggers, J., Helfen, L., Bernacki, M., Bouchard, P.-O., Morgeneyer, T.F., Hild, F., 2017. Numerical validation framework for micromechanical simulations based on synchrotron 3D imaging. Comput. Mech. 59(3):419–441, 2017

[Shakoor 2017] M. Shakoor, A. Buljac, J. Neggers, F. Hild, Thilo F. Morgeneyer, L. Helfen, M. Bernacki, and P.-O. Bouchard. On the choice of boundary conditions for micromechanical simulations based on 3D imaging, Int J Solids Struct 112:83–96, 2017