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On the calibration of elastoplastic parameters at the microscale via X-ray microtomography and digital volume correlation for the simulation of ductile damage

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ABSTRACT

An identification framework is introduced herein to calibrate material parameters at the microscale in order to analyze ductile damage. It is applied to study a dog-bone sample, which is made of spheroidal graphite cast iron, loaded in tension and imaged via in situ microtomography. The region of interest is analyzed via Digital Volume Correlation (DVC) to measure kinematic fields. Finite Element (FE) simulations, which account for the studied microstructure that is explicitly meshed thanks its 3D image, are driven by Dirichlet boundary conditions extracted from DVC measurements. The plastic behavior of the ferritic matrix is calibrated via integrated DVC. The three mechanisms of ductile damage are then analyzed in view of the predictions of numerical simulations at the microscopic scale.

1. Introduction

Motivated by the constant quest for more fuel efficient and hence lighter design substantial progress has been made in understanding and modeling failure of ductile materials over the last decades (Besson, 2010; Benzerga and Leblond, 2010; Pineau et al., 2016). Yet, some questions still remain open and robust ductile damage models that would be able to correctly predict fracture loci $\varepsilon_f(\eta, \mu)$ under arbitrary loading paths are still lacking (Cao et al., 2014, 2015; Thomas et al., 2016), where ε_f denotes the fracture strain, η the stress triaxiality and μ the Lode parameter. One of the main reasons is an incomplete understanding of ductile damage mechanisms at lower scales. The current work is motivated by the idea of having more realistic macroscopic calculations thanks to physical models directly calibrated at the microscale when analyzing two of the three steps of ductile damage, namely, void growth and coalescence. To achieve this aim, the feasibility of an experimental-computational framework allowing for validation *and* identification of the material properties at the microscale is shown in the following work. To the authors' knowledge, it is the first time that such type of study is reported.

Damage models are useful to optimize the forming processes when dealing with metals and alloys and to predict the in-service life of structures (Lemaitre and Desmorat, 2005; Voyiadjis, 2014). The first models, which are known as macroscopic postulates, were written at the scale of the volume element in continuum mechanics. They allow damage occurrence and the softening toward fracture to be described (Kachanov, 1958; Rabotnov, 1963; Lemaitre, 1992). However, these models are known to have limited predictive capabilities for complex loading paths and are not easy to calibrate (Cao et al., 2015).

An alternative to the previous constitutive postulates is to derive the macroscopic response from microscopic formulations (Gurson, 1977; Needleman and Tvergaard, 1984). The first propositions were based on closed-form derivations (Gurson, 1977). Numerical simulations were also proposed to enhance the initial propositions (Needleman and Tvergaard, 1984). Over the years, many improvements were proposed to enlarge the validity domain of the developed models (Benzerga and Leblond, 2010; Voyiadjis, 2014; Pineau et al., 2016). However, it is worth noting that the calibration of such models still is a (very) difficult task (Cao et al., 2014). All such simulations were never probed against experimental results, in particular the behavior of the matrix, which is usually described by very simple constitutive postulates (*e.g.,* Ludwik's power law). This calls for advanced observation, simulation and

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identification techniques.

On the experimental side, computed microtomography was used to directly monitor damage in various materials (Baruchel et al., 2000; Maire et al., 2003; Salvo et al., 2003; Maire and Withers, 2014). Physical damage variables such as porosity were observed experimentally thanks to 3D imaging techniques (Babout et al., 2004; Bouchard et al., 2008; Ueda et al., 2014; Hannard et al., 2016). It is possible to study individually inclusions and voids with manual (Ueda et al., 2014) or automatic (Hannard et al., 2016) procedures. The three ductile damage mechanisms, namely, void nucleation (Landron et al., 2010, 2012), growth (Bontaz-Carion and Pellegrini, 2006; Maire et al., 2008; Landron et al., 2011) and coalescence (Martin et al., 2000; Babout et al., 2001; Salvo et al., 2003; Weck et al., 2008) were analyzed and quantified thanks to computed microtomography.

Simulations are needed to experimentally relate observed quantities such as total strain, porosity and the number of fractured/debond inclusions to internal variables (*e.g.,* stresses) to derive criteria for nucleation and coalescence (Torki et al., 2017). Averaged damage models were derived by such simulations. The microscale calculations were usually performed with idealized microstructures and constitutive behavior (Benzerga and Leblond, 2010; Voyiadjis, 2014; Pineau et al., 2016). Moreover, uniform kinematic or static boundary conditions were prescribed. Such conditions cannot capture the local strain and stress states that inclusions and voids are subjected to due to their random shapes and distributions (Babout et al., 2004; Morgeneyer et al., 2009; Tang et al., 2013; Hannard et al., 2016; Shakoor et al., 2017a). The effect of the three-dimensional random distribution of voids on softening was also studied (Fritzen et al., 2012) using different void volume fractions. It was concluded that it is desirable to work with realistic microstructures.

From the acquired tomographies, real microstructures can be meshed (Zhang et al., 2005; Young et al., 2008). The level set (LS) method (Osher and Sethian, 1988) is useful to describe interfaces in FE computations when large deformations and complex topological events occur (Sukumar et al., 2001; Roux et al., 2014; Quan et al., 2014). When FE simulations were run with such interfaces, image processing was directly carried out on FE meshes, thereby making such procedures applicable thanks to parallel implementations (Shakoor et al., 2015a).

Once such microstructures were generated, the next step was to start validating the numerical simulations. One key aspect is to be able to perform and monitor in situ mechanical tests (Buffière et al., 1999, 2010). Combined with digital volume correlation, displacement fields can be measured within the bulk of imaged materials. The early developments of DVC (Bay et al., 1999; Smith et al., 2002; Bornert et al., 2004; Verhulp et al., 2004) consisted of *independently* registering small interrogation volumes in the considered Region of Interest (ROI). Global approaches (Roux et al., 2008) perform registrations over the whole ROI by measuring kinematic fields that are, for instance, based on FE discretizations, which assume displacement continuity. Such DVC approaches were directly linked with numerical simulations of mechanical problems (Rannou et al., 2010; Bouterf et al., 2017). They were also used in a numerical framework to partially validate simulations at the microscale (Buljac et al., 2017; Shakoor et al., 2017a).

The previously introduced experimental-computational framework (Buljac et al., 2017; Shakoor et al., 2017a) is further extended herein to perform the calibration of material parameters at the *microscale* via 4D mechanical correlation for nodular graphite cast iron. Up to now, such approaches were only performed at the macroscopic level (Hild et al., 2016). Once such calibration has been achieved, the next step is to analyze the development of ductile damage. The proposed framework to calibrate material parameters at the microscale is based on the following steps (Fig. 1):

1. X-ray microtomography to get 3D images of an in situ test in a lab equipment. By post-processing the reconstructed volume in the reference configuration, the morphology of the microstructure is obtained. The interest of using tomography instead of laminography is that the whole sample cross-section can be imaged. Consequently, measured load data will also be used in the present analyses to be compared with predicted resultant forces. Such data were not available in the in situ experiments reported so far on the same material for the analyzed volume of interest (Buljac et al., 2017;

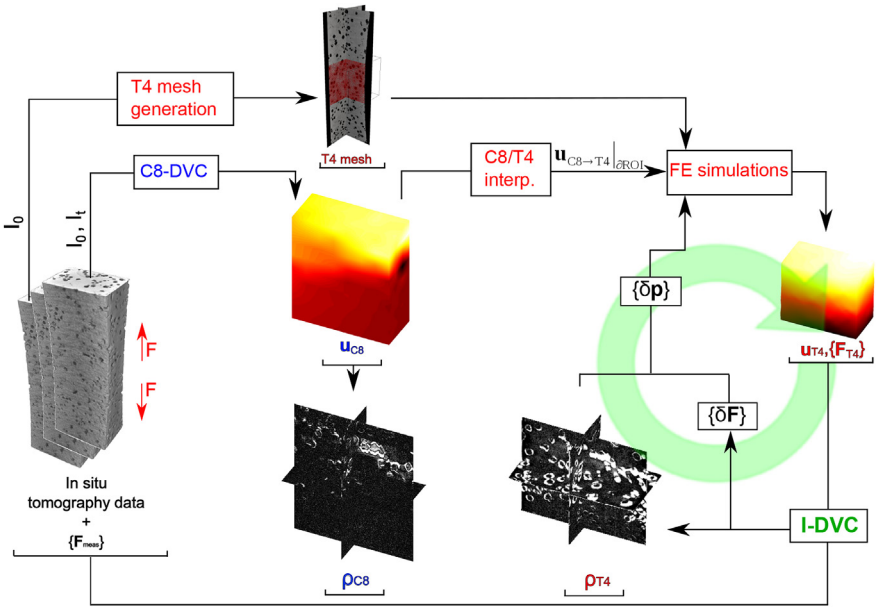

Fig. 1. Schematic representation of the methods used in the present paper for calibrating material parameters via numerical simulations at the microscale. Global DVC based on 8-noded elements (C8-DVC) is run to register a series of reconstructed volumes I_t with respect to the reference configuration I_0. Such analyses provide the gray level residuals ρ_{C8}, and the measured displacements $\boldsymbol{u}_{C8}$, which are interpolated on a mesh made of 4-noded tetrahedra (T4). From the reference volume I_0, a T4 mesh is adapted to the underlying microstructure. Finite element simulations are then run to determine, for any given set of material parameters $\{\boldsymbol{p}\}$, the displacement fields $\boldsymbol{u}_{T4}$ and the reaction forces $\{\boldsymbol{F}_{T4}\}$ to be used in an integrated DVC (I-DVC) approach to compute global equilibrium residuals $\{\delta\boldsymbol{F}\} = \{\boldsymbol{F}_{meas}\} - \{\boldsymbol{F}_{T4}\}$, and gray level residuals ρ_{T4}.