Micro-macro modeling of spheroidal cast iron: parameters identification by inverse analysis

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ABSTRACT: In a previous study, a generic micro-macro mechanical model based on the coupling of an incremental mean-field model [1, 4, 5] with the Gurson-Tvergaard (GT) porous plastic law [2, 6] has been developed for the prediction of the mechanical properties of multiphase materials with a large volume fraction of voids. This model has been used in the framework of the FP6 PROHIPP European project to investigate the link between the microstructure and the mechanical properties of spheroidal cast iron. In this contribution, experimental results are presented and an inverse analysis procedure is proposed to adjust the parameters of the model.

KEYWORDS: Inverse Analysis, Homogenization Scheme, Plasticity, Porosity, Cast Iron

1 INTRODUCTION

Depending on the thermomechanical treatment and the alloying elements, the microstructure of spheroidal cast iron can vary from fully ferritic to fully pearlitic matrix with a maximum graphite nodules volume fraction of 13%. In the present work, the focus is set on spheroidal cast iron with low pearlite volume fraction. In this case pearlite is modeled as a dispersion spheroidal inclusions. Moreover, it is observed that the graphite nodule are weakly bound to the ferrite matrix. As a consequence, the ferrite+graphite sub-system can be seen as a porous plastic phase in the case of positive stress triaxiality loading conditions.

A multi-scale mechanical model was thus proposed to describe the overall cast iron properties taking into account the microstructural features [4, 5]. In this model, the mechanical behaviour of the ferrite+graphite system is modeled using the Gurson-Tvergaard (GT) porous plastic law with a yield surface equation given by:

$$\phi(\boldsymbol{\sigma}, f, \overline{\sigma}) = (\frac{\sigma_0}{\overline{\sigma}} - 1) + 2q_1 f cosh(\frac{-3}{2} q_2 Tr) - (q_1 f)^2 \quad (1)$$

where $\boldsymbol{\sigma}$ is the stress tensor, $\overline{\sigma}$ is the von Mises equivalent stress in the ferrite matrix, $Tr = -\sigma_m/\overline{\sigma}$ is the stress triaxiality ratio with σ_m the hydrostatic pressure. f is the void volume fraction while q_1 and q_2 are parameters introduced by Tvergaard in order to better fit the results of a FE unit cell model. σ_0 is the yield stress of the ferrite matrix which obeys the J2 plasticity theory with a Ramberg-Osgood hardening law:

$$\frac{\overline{\sigma}}{\sigma_y} = (\frac{\overline{\sigma}}{\sigma_y} + \frac{E}{\sigma_y} p)^n \quad (2)$$

where p is the accumulated plastic strain in the matrix, σ_y is the initial yield stress and n is the hardening exponent.

The overall cast iron properties are predicted using a mean field homogenisation scheme in which the matrix phase (the ferrite+graphite subsystem) is modeled by the GT law and the inclusions (representing the pearlite grains) are modeled using the J2 plastic theory with a Ramberg-Osgood hardening law (equ.2). Several homogenization schemes are available. In a previous study, it was shown that the incremental formulation of the Mori-Tanaka mean field homogenization scheme lead to a poor description of the stress partitioning between the phase. Therefore, an original multi-level homogenization scheme was proposed to improve the results [3, 4].

The multi-scale model contains free parameters to be adjusted in order to reproduce the phases properties: the parameters of the hardening law for the ferrite and pearlite phases and the Tvergaard parameters for the GT model. It is important to note that the homogenization scheme does not contain such free parameters, but, once the mechanical properties of the phases identified, it is a parameter by itself. In this study, the homogenization is performed using a two step approach coupling the isostrain and Mori-Tanaka models to compute the stress and strain partioning.

In a first step, an experimental study was performed in order to characterize both the microstructure and the mechanical behaviour of the spheroidal cast iron. In a second step, the experimental results were used: i) identify the model parameters using an home build optimization loop, ii) to predict the behaviour of the spheroidal cast iron.

2 EXPERIMENTAL WORK

Tensile tests and optical microscopy studies have been performed in order to explore the relationship between the microstructure and the mechanical behaviour of spheroidal cast iron and indentify the model paramaters. To this purpose, a serie of tensile specimens with three typical microstructures have been studied (M1: ferrite+graphite, M2: M1+few pearlite, M3: pearlite+graphite).

The effect of stress triaxiality on the mechanichal properties is studied using three specimen geometries with different notch radius (G1: no notch, G2: r=1mm, G3: r=6mm) inducing different average stress triaxiality within the notch (G1: Tr=$1/3$, G2: Tr=1, G3: Tr=0.5). Three samples are used for each microstructure and geometry in order to check the results variability.

Traction tests up to rupture have been performed. During the tests, the force and the displacement were recorded. The resulting 'traction curves' are used as reference data for the identification of the mechanical model parameters.

The broken specimens were cut along the longitudinal direction in order to allow observation of their internal microstructure. For each nominal microstructure and specimen geometry, 10 pictures of the microstructure were taken with an optical microscope. Figure 1 contains typical snapshots for microstructures M1, M2 and M3. The pictures were analysed using the free software 'ImageJ' in order to measure the volume fraction of ferrite, pearlite and graphite. The measured volume fraction of graphite is equal to $8 \pm 2.$% in M1, M2 and M3. The measured pearlite volume fraction in the three microstructures are M1: 2.5±1.3%, M2: 30.3±2.8%, M3= 93.2±2.1%.

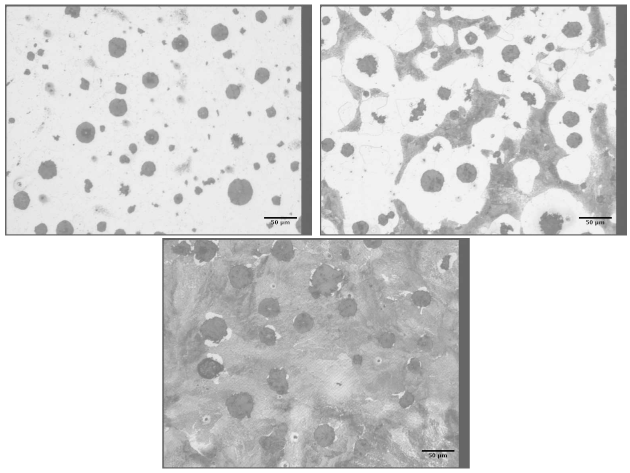

Figure 1: Picture of microstructures M1(top), M2(middle) and M3(bottom). The white and light grey zones are ferrite and pearlite respectively. The graphite nodules appear as dark disks.

3 INVERSE ANALYSIS PROCEDURE

3.1 Description

An inverse analysis method is developped to identify the free parameters of the model. The aim is to find the parameters set giving the best fit of the experimental traction curves for all the geometries. As the triaxiality of the first geometry (G1) is uniform in the zone of interest, the developped constitutive law can be used as is. On the contrary, an heterogeneous mechanical response is observed in the notch of G2 and G3. Therefore, the traction tests must be simulated using a finite element model in Abaqus. To this purpose, the proposed micro-macro mechanical model has been coupled with Abaqus through a dedicated UMAT interface. The parameter identification is performed using a generic optimization software called 'MAX' developped at CENAERO. MAX is based on genetic algorithms coupled with surrogate models allowing to reduce the calculation time. Genetic algorithms allows to find the parameters set corresponding to the global optimum of a given function. In the present study, the function (ϕ) is defined on the basis of the mean square distance (MSD) between the model and the experimental traction curves. In order to capture both the stress level and the hardening effects, the fitness function is the weighted sum of the force and force derivative MSD defined as :

$$MSD(F) = \frac{1}{N}\sum_{j=1}^{N}(F(j)^{Model} - F(j)^{Exp.})^2 \quad (3)$$

$$MSD(\frac{dF}{dU}) = \frac{1}{N}\sum_{j=1}^{N}(\frac{dF}{dU}^{Model} - \frac{dF}{dU}^{Exp.})^2 \quad (4)$$

where N is the number of points in the traction curve. U, F and $\frac{dF}{dU}$ are the displacement, the force and the derivative of the force with respect to the displacement, respectively. In order to separate the effects of void growth from the matrix strain hardening, the fitness function is defined as the arithmetic mean of the MSD evaluated for the three tensile specimen geometries.

3.2 *Identification of the parameters of the GT model for the ferrite+graphite system*

The parameters of the GT model for the ferrite+graphite system are obtained from the inverse analysis of the traction curves of microstructure M1. The identified parameters are:

- the yield stress and hardening exponent of the ferrite phase $\sigma_y^{ferrite}$ and $n^{ferrite}$,
- the initial void volume fraction f_0: due to the large variability of the graphite phase characteristics, the initial void volume fraction is considered as a free parameter. The range of variation for this parameter corresponds to the experimentally observed range of initial graphite volume fraction ([0.06,0.1]).
- The Tvergaard parameters $q1$ and $q2$.

The optimized values of the parameters are given in Table 1. The 'identified' traction curves are compared to the experimental ones in Figure 2. Good agreement is observed.

Table 1: Values of the parameters of the micro-macro mechanical model identified for microstructures M1 and M3.

Parameters	M1(ferrite+graphite)	M3(pearlite)
E(GPa)	210	210
ν	0.3	0.3
$\sigma_y^{ferrite}$(MPa)	228.7	272.1
$n^{ferrite}$	0.1454	0.2611
$q1$	1.69	N/A
$q2$	0.938	N/A
f_0	0.071	N/A

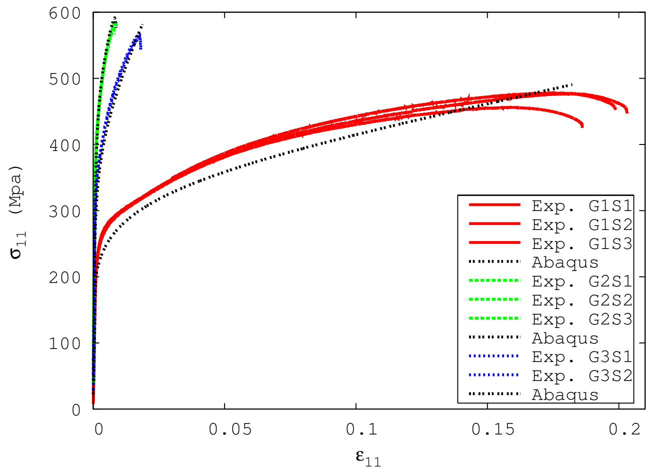

Figure 2: Comparison of the experimental identified true stress-true strain curves for microstructure M1. The parameters used in the Gurson model are given in Table 1

3.3 *Identification of the parameters of the hardening law for the pearlite phase*

The parameters of the Ramberg-Osgood model for the pearlite phase are obtained from inverse analysis of the traction curves of microstructure M3. This is justified by the experimental observation that the graphite present in microstructure M3 does not lead to void growth. The Gurson model does not need to be used to describe the mechanical properties of the phase which is mainly driven by the plastic behaviour of the pearlite phase. The adjusted parameters are the yield stress and the hardening exponent of the ferrite phase $\sigma_y^{pearlite}$ and $n^{pearlite}$.

The optimized values of the parameters are given in Table 1. The 'identified' traction curves are compared to the experimental ones in Figure 3. Here again, good agreement is observed.

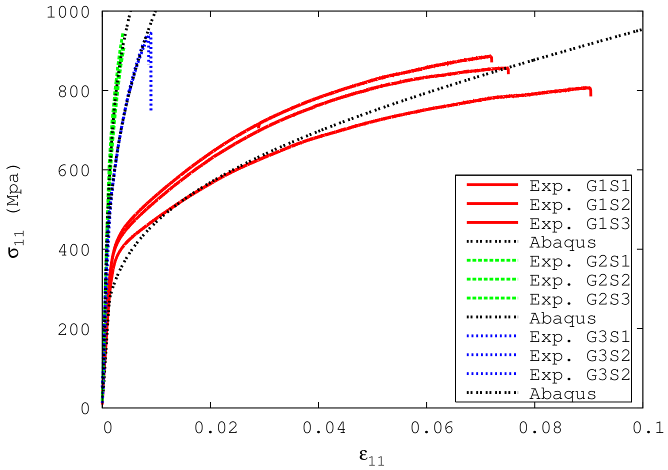

Figure 3: Comparison of the experimental and identified true stress-true strain curves for microstructure M3. The parameters used in the Ramberg-Osgood model are given in Table 1

3.4 *Validation of the multi-scale mechanical model for the spheroidal cast iron (ferrite+graphite+pearlite)*

The experimental traction curves for microstructure M2 are compared with those obtained with the multi-scale model using the parameters sets previously identified for both the ferrite+graphite and the pearlite phase. Several homogenization schemes are compared for the case of G1 in Figure 4. It is observed that the home-build multi-level homogenization scheme leads to the best results as compared to the results of the simple Mori-Tanaka scheme. This scheme give very good results for the tensile specimen geometry G2.

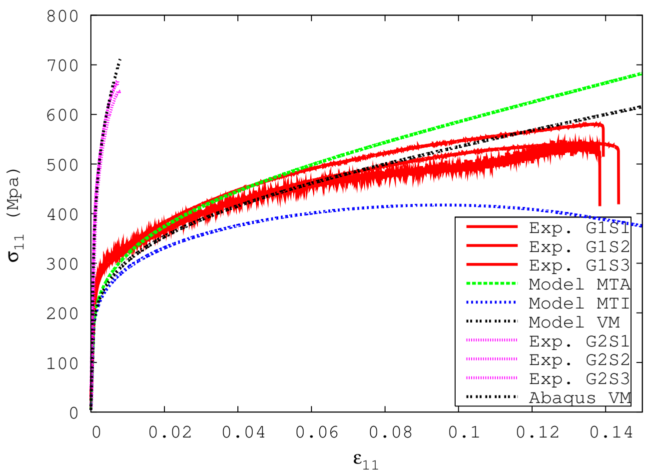

Figure 4: Comparison of the experimental and identified true stress-true strain curves for microstructure M2. Several homogenization schemes are compared for the case of G1. VM is the multi-level (recursive) homogenization scheme. MTA and MTI are the Mori-Tanaka schemes with the anisotropic and isotropic descriptions of the matrix respectively.

4 CONCLUSIONS

In a previous study, a multi-scale mechanical model for multi-phase material with high void volume fraction was proposed. In the present study, the free parameters of the model have been identified in order to reproduce the mechanical properties of the spheroidal cast iron. To this purpose, an inverse analysis method based on genetic algorithm optimization coupled with finite element simulations of experimental tensile tests has been developped. In a first step, mechanical testing and microstructural characterization have been performed. In a second step, inverse analysis has been used to identify the constitutive behaviour of the phases. The adjusted parameters have been used in the multi-scale model to predict the mechanical response of the spheroidal cast iron containing the two phases. Good agreement has been found.

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