Digital microstructures matching statistical distributions of features in real materials - Example of forgings

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Digital microstructures matching statistical distributions of features in real materials – Example of forgings

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Various analytical rules of mixture are commonly used to take into account heterogeneous features of a material and to derive global properties. But, with such models, one may not be able to fulfil the requirements for separating appropriately the different lengthscales. This might be the case for some issues such as strain localisation, surface effect, or topological distributions. At an intermediate lengthscale, which we refer to as the mesoscopic scale, one can still apply continuum mechanics. So why not perform calculations using the finite element method on volumes of material to obtain the response of Representative Elementary Volumes (R.E.V.). The construction of digital microstructures for such calculations is performed in two steps.

First, a series of R.E.V.s with statistics of features of real materials should be defined. Then, finite element meshes should be produced for these R.E.V.s and updated when calculations involve large strains. Powerful automatic three-dimensional mesh generators and remeshing techniques prove necessary for this latter task.

This strategy is applied to create digital R.E.V.s which match statistical features of forgings. Measurements provide micromechanical parameters of each subvolume. As an example of calculations, numerical simulations provide the anisotropic fatigue properties of forgings.

Key words: Statistical similar microstructures, Digital Material, Forging

Introduction

Over the last decades, micromechanics models [1] have been developed in order to approximate the material behaviour by taking into account explicitly the heterogeneous nature of materials. Today, explicit representations of microstructures are commonly constructed for allowing calculations meant to determine local variables and fields such as strains or stresses. Such representations require an important investment in terms of computing power to the quantity of elements to obtain a Representative Elementary Volumes (R.E.V.) which would be statistically representative of the real material organization. Several methods have been reported in the literature to generate microstructures by means of topological mappings [2][3][4]. Rigorous statistical approaches are needed to perform such realistic microstructures. Data needs to be determined from fairly intensive experimental analyses so as to obtain the needed mechanical characteristics of each constituent and local geometrical features. The first part of this work describes the panel of different experimental methods which were performed. The second part provides an overview of numerical tools used to perform numerical computations on R.E.Vs. The third part presents the link between values and fields obtained at different microstructure scales to simulate fatigue properties of a forging component.

Microstructure characterization

In a first approach, two main categories of microscopic constituents are often defined and used to describe a metallic microstructure : grains and inclusions (or voids). Scanning Electron Microscopy (S.E.M.) together with Electron Back-Scattered Diffraction (E.B.S.D.) analyses were performed to determine the statistics of morphological characteristics of the microstructure and of all constituents which are known to be the key parameters governing the fatigue behaviour of the material. Note that some of these features are known to have a bigger impact on fatigue behaviour than others.

E.B.S.D. analyses of the grains of the matrix for the material of interest in this study display a fairly random crystallographic texture. Therefore, the anisotropic mechanical response of the R.E.V. and of the component is assumed to be induced by the presence and the organisation of inclusions in a matrix, and the crystallographic nature of the grains is not taken into account in the R.E.V. representation.

Forging processes are known to induce orientations of particles which cause the final material anisotropy. And indeed, several analyses and tests on the material of interest for this work have showed that the anisotropy of the final component was essentially due to the orientation of inclusions clusters, mainly MnS (manganese sulfide) inclusions. Statistical studies were performed in order to determine all parameters meant to generate a realistic R.E.V. The shapes of the inclusions were approximated as ellipsoids which match the statistics of the real morphology of MnS inclusions. Note that these inclusions are gathered in cluster **(Figure 1).**
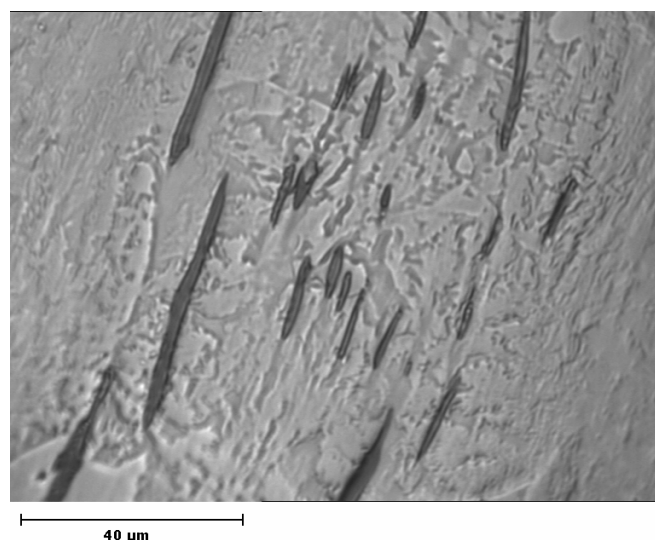

Figure 1. Example of a MnS cluster (S.E.M.)

The method of the "Localized cluster" [4] was chosen to generate the cluster by controlling the number of inclusions and their widths. Each parameter follows a Gaussian (Euler orientation) or a log-normal distribution (length, width, thickness, number …) [5]. An example of stochastic data about the length and the orientation of the inclusions is represented in **Figure 2** : statistical distributions are in good agreement with experimental results. Precise statistics were determined for components at each of the forging stages for an industrial sequence. To apply such distributions and to take into account all stochastic parameters, a specific algorithm has been developed [5] [6]. Numerical statistical selections were performed using a Box-Müller method [7] with random sampling carried out with the "mersenne twister" algorithm [8].

Figure 3 shows an example of such a digital cluster. Each inclusion is separated using its specific topology in order to define it independently from the other inclusions. A robust and automatic 3D mesher (MTC) was used in order to refine the mesh in the vicinity of each inclusion [9]. The meshing operation (global meshing and the size of all elements) allows to control the local refinement of the topology in the vicinity of each interface. The interface of each inclusion can then be refined and, overall, an 'anisotropic' (in the sense of an anisotropic metrics of the finite elements) mesh is produced. This anisotropic mesh prevents numerical stress discrepancy which could be due to finite element methods with linear approximation of the constitutive law near the interfaces.
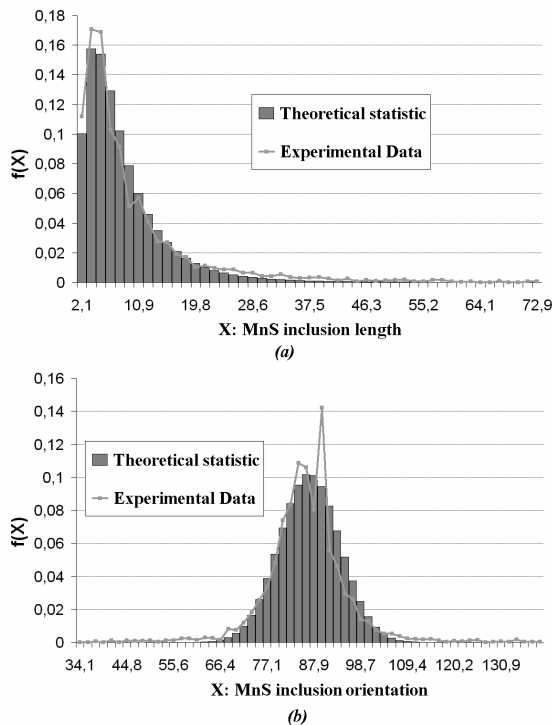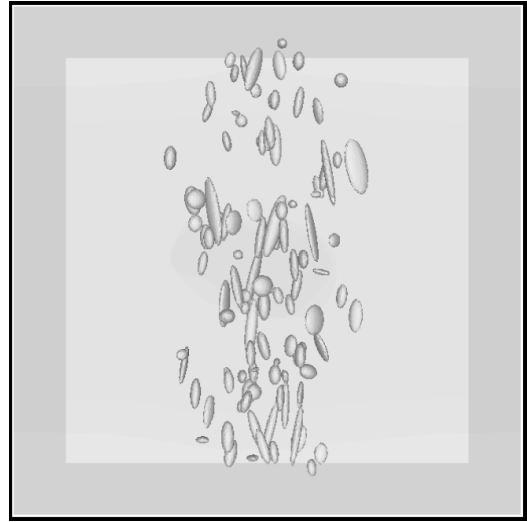

Figure 3. Numerical generation of a MnS cluster

An example of such an anisotropic mesh is given in **Figure 4**. Near the inclusions, the size of the mesh is significantly refined. This method allows to obtain a very high efficient mesh in terms of mechanical calculation with a limited number of finite elements for the global R.E.V. mesh.
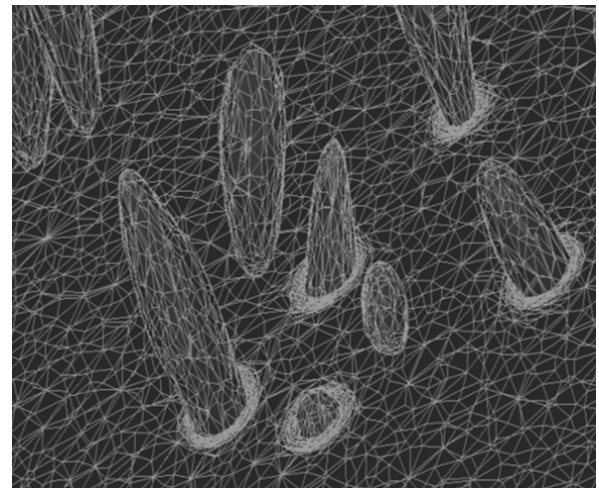

Figure 4. Mesh adaptation near inclusions using MTC Mesher.

Computation of the mechanical response of a R.E.V.

An elastic-plastic or viscoplastic finite element computation can then be performed in order to study the influence of particles distribution and morphology on the stress field throughout the R.E.V. Inclusions are assumed – and this is checked later on- to remain in the elastic regime. A log-normal statistical distribution of the Young's moduli for the MnS inclusions was determined by nano-indentation. Then, a value of Young's modulus is associated to each inclusion. The matrix is considered to follow a standard plastic Hollomon law. Interestingly, the role of MnS inclusions on the global response was found not to be significant on the global intensity during a forming operation. And the parameters of the Hollomon law could therefore

(a)

(b)

Figure 2. Examples of statistic representation of MnS inclusions

be determined from standard tensile tests in the longitudinal direction.

In order to assess the role of each morphological parameter of inclusions in a standard high cycle fatigue simulation, a total of 150 R.E.Vs were constructed and studied under different loading modes. The analyses of the calculations concentrated on different characteristics. **Figure 5** describes an example of such simulations. The fatigue criterion used was Papadopoulos criterion [5][6][10] which gives a critical domain under which the structure is found to be safe. Each parameter had to be carefully assessed to provide, statistically, this critical domain at the mesoscopic scale.
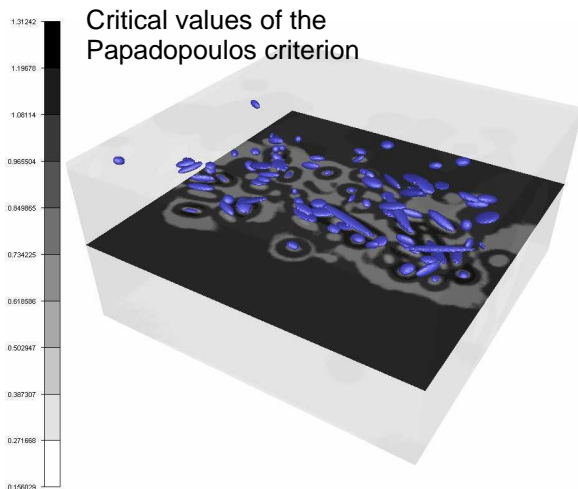

Critical values of the Papadopoulos criterion

Figure 5. Numerical simulation of a tensile fatigue test for a specific loading direction

Linking lengthscales in a forming process analysis

The morphology of the particles depends essentially on the strains undergone by the material during the forging process. Two macroscopic parameters are commonly used to assess the impact of such forming history :
- the kneading rate, defining the deformation undergone by the part during forming [5] ;
- the direction of microstructural flow orientation given by a fiber vector [5][6].

In our approach, morphological characteristics at the microscopic scale are described with these two parameters. For instance, the orientation of inclusions can be associated to the fiber vector, and the shape and organisation of a cluster is connected to the kneading rate.

The industrial case chosen in this study is a suspension component described in **Figure 6**. Various virtual fatigue tests at the microscopic scale were performed on R.E.Vs with different kneading rate and anisotropy orientation (fiber vector) distributions.
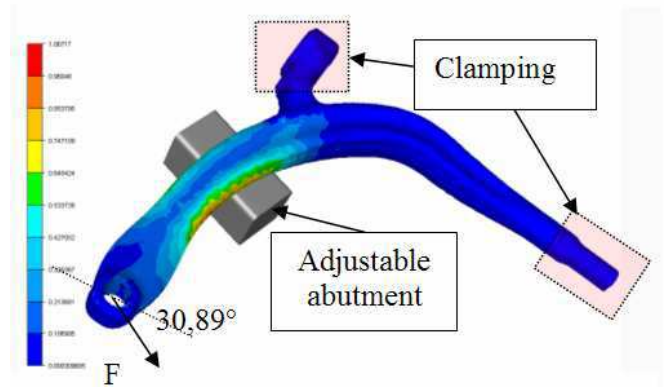

Figure 6. Experimental fatigue test bench on the real component

These fatigue simulations at the microscopic scale were needed to determine two material parameters in the anisotropic Papadopoulos criterion [10]. Indeed, the only mean to obtain these coefficients without experimental tests (expensive and difficult to perform) is to simulate several digital cases. **Figure 7** shows the endurance limits, which were used to determine these Papadopoulos coefficients, for different configurations of R.E.V.s and relying on macroscopic results of the forging component.
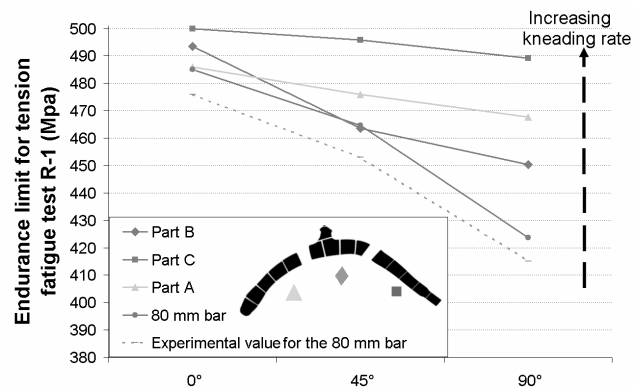

Figure 7. Determination of the fatigue limit evolution from different calculations of various digital R.E.Vs with MnS clusters.

The values of the two Papadopoulos coefficients are necessary to perform high cycle fatigue tests on the real components. Moreover, this multi-scale approach gives not only one value, but a distribution of these coefficients.

A numerical testing campaign for various Papadopoulos coefficients provided standard deviation prediction of the endurance limit for real forgings (**Table 1**.)

	Endurance limit force (N)	Standard deviation (N)
Experimental	11 083	204
Without statistic	11 153	. . .
Statistic selection	11 280	276.2

Table 1. Example of predictions of endurance limit forces

Critical areas in terms of fatigue resistance can then be determined in the thickest area of the suspension arm.
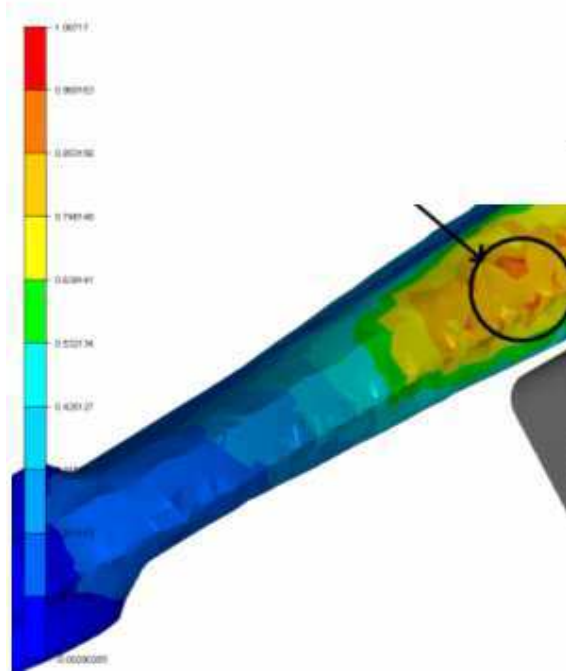
Figure 8. Most critical area predicted by the modified Papadopoulos criterion

Numerical predictions are in good agreement with experimental results, quantitatively and qualitatively.

Conclusion

A multi-scale pragmatic approach for high cycle fatigue computation was presented and applied to forging applications. Microstructural flow orientation and kneading rate have been taken into account in order to perform fatigue analyses. This approach consists in describing the microstructure morphology and rheological characteristics of the main microstructure constituents in order to create numerically adapted elementary volumes. Fatigue simulations were then performed on different statistically representative morphologies to obtain material coefficients of the Papadopoulos criterion which allows to describe the anistropy of the material. Results seem to be more conservative than experimental endurance limits but they remain within the standard deviations. It is also possible to obtain, at the end of the forging process, anisotropic characteristics which can be linked to material coefficients obtained statistically from calculations on elementary volumes. Endurance limits obtained for the real forged components are quantitatively and qualitatively close to the experimental results.

Perspectives

This method is being confronted to R.E.Vs obtained from tomography imaging. The reconstruction from different cross sections gives a more realistic description of the material. As an example of such representation, **Figure 9** shows a R.E.V. reconstructed from experimental data.
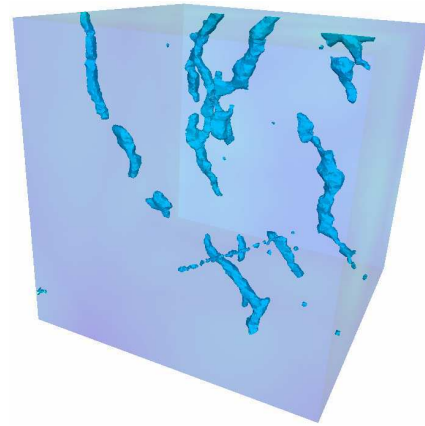

Figure 9. Numerical reconstruction of a R.E.V. from imaging obtained by tomography.

And it is possible to perform simulations on such R.E.V.s following the same approach as previously described.

Acknowledgement

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