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Thermo-mechanical analyses of heterogeneous materials with a strongly anisotropic phase: the case of cast iron

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ABSTRACT

This work presents a systematic study of thermo-mechanical behaviour of macroscopically isotropic heterogeneous materials with anisotropic constituents based on microstructural modelling. As an example, lamellar cast iron is considered, whose microstructure is composed of spatially interconnected anisotropic graphite particles embedded in ferrite/pearlite matrix. The complex three-dimensional microstructure of lamellar cast iron is represented here by an idealised unit cell model which captures in a simplified manner the main morphological features of the material. The thermal, mechanical and thermo-mechanical response of the unit cell incorporating the highly anisotropic phase is analysed by comparing the results for the equivalent unit cell with the isotropic constituents and considering both fully fixed and loose interface conditions. The major conclusion drawn from these analyses is that the anisotropy of microstructural phases plays crucial role in determining both the effective as well as local response of the material. The simplifying isotropy assumption leads to significantly different predictions at both scales.

1. Introduction

Many advanced high performance materials are heterogeneous at a certain scale, with complex microstructures composed of two or more constituents exhibiting different mechanical and physical properties. This microstructural complexity makes the engineering and performance prediction of such materials a challenging task. Furthermore, it requires a good understanding of the microscale phenomena and a proper multi-scale approach to extract the macroscopic material response.

Cast iron is a typical example of such a material, which presents a complex heterogeneous microstructure composed of anisotropic graphite inclusions embedded in a ferrite/pearlite matrix. According to the morphology of the graphite inclusions, cast irons can be classified as: *Flake or Lamellar Graphite Iron (FGI)*, *Compacted or Vermicular Graphite Iron (CGI)* and *Spheroidal, Nodular or Ductile Graphite Iron (SGI)*. The graphite morphology plays a decisive role in the resulting mechanical and physical properties of cast iron (Rundman, 2001). In particular, the complex 3D connectivity of the graphite network found in FGI and CGI, combined with the graphite shape and its local anisotropy are important microstructural factors. For example, nodular cast iron (SGI) contains spherical inclusions dispersed in a metal matrix, which results in a relatively high strength and ductility, but its thermal conductivity is close to that of steels. On the contrary, lamellar cast iron (FGI) contains graphite inclusions in the form of lamellas or flakes that form a 3D interconnected network. An example of the lamellar cast iron microstructure is shown in Fig. 1a. Although the sharp graphite edges act as local stress concentrators, leading to an overall strength decrease, the 3D interconnected network of graphite results in a material with a high thermal conductivity and a relatively low thermal expansion coefficient. In between nodular and lamellar cast iron is compacted cast iron (CGI). In CGI, the 3D interconnected graphite network is also present, however the flake type inclusions are replaced by vermicular worm shaped ones leading to a coral like morphology. This type of microstructure results in mechanical and physical properties that are intermediate between FGI and SGI (Sjögren, 2005; Holmgren et al., 2006; Velichko et al., 2009). This makes lamellar and compacted cast irons a popular option for heavy-duty thermo-mechanical applications (e.g. truck engines).

The complex microstructure of cast irons makes the estimation of their effective properties a challenging task. In the literature several papers can be found in which analytical models are used to predict the elastic (Dryden et al., 1987; Dong et al., 1997; Cooper

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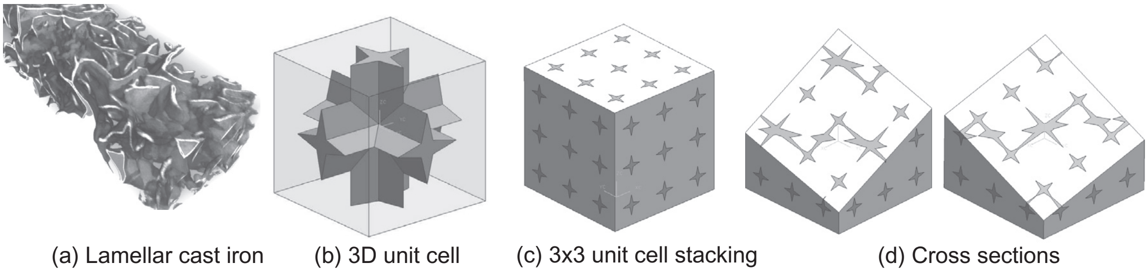

Fig. 1. Lamellar cast iron unit cell: (a) CT-scan of the lamellar cast iron microstructure, (b) 3D unit cell, (c) 3 × 3 × 3 periodic unit cell stacking, (d) 3 × 3 × 3 periodic unit cell model cross sections; dark – graphite, light – steel matrix.

et al., 2002; Boccaccini, 1997; Gaudig et al., 2003) and thermal properties (Helsing and Grimvall, 1991; Holmgren, 2005) of cast irons. The different approaches considered range from simple Reuss and Voigt bounds, to the more advanced Hashin–Shtrikman bounds and self-consistent methods. In general, in these (semi)-analytical methods, cast irons are considered as two phase materials composed of isotropic or anisotropic graphite inclusions embedded in an isotropic metal matrix, in which the influence of the shape of the particle is taken into account through the particle aspect ratio. The main drawbacks of the (semi)-analytical methods is that no interaction between individual particles is considered and a perfect adhesion between graphite particles and metal matrix has to be assumed. The lack of interaction between particles is not a problem in nodular cast iron, where the graphite inclusions are nearly isolated nodules, but this does not hold for lamellar and compacted cast irons where the graphite inclusions form a 3D interconnected network.

In the particular case of nodular cast iron, several finite element unit cell models have been introduced in the literature to study the mechanical response of the material within elastic and elasto-plastic regimes (Dong et al., 1997; Collini and Nicoletto, 2005; Bonora and Ruggiero, 2005; Kuna and Sun, 1996). However, to the best of our knowledge this approach has not been used to study lamellar and compacted cast irons. For the analysis of the isothermal mechanical response of compacted cast iron a direct discretization of 2D micrographs (Fukumasu et al., 2005; Mohammed et al., 2011) or a model of slender ellipsoids (Gaudig et al., 2003) has been used. These approaches do not include the 3D interconnectivity and are therefore not applicable to transport properties and coupled effects. Recently, Velichko et al. (2009) have used FIB-tomography images in a FEM analysis to obtain the overall thermal and electrical conductivity of lamellar cast iron. Although the tomography based model is a geometrically exact representation of a small part of the microstructure, it becomes prohibitively computationally expensive if anisotropic and/or non-linear material properties are to be included.

In this work, a microstructural model for lamellar cast iron is introduced to study the response of the material under mechanical and thermo-mechanical loading conditions. To this end, the coupling between the mechanical and thermal fields and the influence of temperature on the mechanical and thermal properties of the microconstituents are incorporated. The complex microstructure of lamellar cast iron, is represented here by an idealised unit cell model that captures the main morphological features of the material, such as the sharpness and the 3D connectivity of the graphite inclusions. This simplified representation of the microstructure makes it possible to investigate the influence of different microstructural features (i.e. matrix/graphite interface, graphite anisotropy, matrix nonlinear material behaviour, etc.) and complex mechanical and thermo-mechanical loads on the local and macroscopic response of the material. Even though this paper focuses on lamellar cast iron as a case study, the methodology and results presented are applicable to a broader class of heterogeneous materials with complex 3D interconnected microstructures composed of anisotropic constituents under thermo-mechanical loads.

This paper is composed of five parts. In Section 2 the microstructural model is introduced. The mechanical analysis is presented in Section 3. Here, the influence of graphite anisotropy and the interface condition is evaluated. Then, in Section 4, the thermo-mechanical analysis is discussed, in which a uniform temperature distribution over the microstructural unit cell is considered. The influence of graphite anisotropy on the material thermal expansion is studied. In Section 5 the heat transfer and the fully coupled thermo-mechanical analyses are discussed. Finally, in Section 6 the main conclusions are summarised.

2. Microstructural model

2.1. Geometry

Among the different methods for solving the governing equations in a direct 3D microstructural analysis, the finite element method (FEM) is used here since it is well suited for complex geometries and non-linear material behaviour. To create a 3D FE model of the microstructure, in general two approaches can be followed. In the first approach, the material microstructure can be obtained experimentally from tomography analyses and exported to FEM (Velichko et al., 2009). A geometrically precise description of the microstructure can be obtained in this way. However, because of the large number of voxels required to provide a good representation of the microstructure, the problem becomes computationally very expensive. Moreover the use of advanced material (e.g. anisotropy, non-linear mechanical and thermal properties) or interface models to describe the behaviour of the micro-constituents can significantly increase the computational cost of the many degree-of-freedom model (Velichko et al., 2009). The second approach is to build a more compact 3D FE model based on an idealised geometry that is sufficiently representative of the actual material microstructure. This model needs to include all relevant features of the material microstructure that may have a significant impact on the overall response. In spite of the fact that the geometrical representation of the microstructure no longer exactly resembles that of the real material, the underlaying complex material response of the micro-constituents still apply. This enables a feasible analysis of certain complex mechanisms, like the combination of the plastic deformation, temperature dependent material properties, thermal cycling and residual stresses, which is otherwise not at reach with a fully detailed 3D model. This second approach is therefore adopted here.

Departing from the concept of local periodicity, that is by now well established in computational homogenisation (Saavedra Flores and de Souza Neto, 2010), a unit cell is introduced in Fig. 1b, which is a representation of the idealised material