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Effective properties of nodular cast-iron: A multi-scale computational approach

F.D. Carazo [a,*], S.M. Giusti [b], A.D. Boccardo [b], L.A. Godoy [c]

[a] Universidad Nacional de San Juan – IMA-IDIA, CONICET, Av. Lib. San Martín (Oeste) 1109, J5400ARL – San Juan, Argentina
[b] Universidad Tecnológica Nacional, Facultad Regional Córdoba – GIDMA, CONICET, Maestro M. López esq. Cruz Roja Argentina, X5016ZAA – Córdoba, Argentina
[c] Universidad Nacional de Córdoba, FCEFyN, CONICET, Avda. Vélez Sarsfield 1611, Ciudad Universitaria, X5016GCA – Córdoba, Argentina

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ABSTRACT

A numerical approach based on a computational constitutive multi-scale model is used in this work to predict the effective Young's modulus and Poisson's ratio of a pearlitic nodular cast iron. The Representative Volume Element (RVE) is defined based on a set of micrographs acquired from an optical device. For each micrograph, two RVE with different shape, rectangular and hexagonal, are defined. The volume fraction of graphite and metal matrix and the boundary of each object were identified on each RVE by using a procedure of image enhanced and segmentation. The set of RVE obtained was meshed with triangular finite elements. The numerical results obtained with rectangular and hexagonal RVE are compared with results obtained by means of an analytical expression. The influence of graphite fractions, aspect ratios and nodularity are investigated. The results show that graphite fraction has the largest influence on the effective modulus E. This feature is independent of the external shape of the RVE. Only one multi-scale model show a good agreement with the analytical expression in the effective modulus E. Also, the influence of the graphite volume fraction on the effective Poisson's ratio is investigated by means of multi-scale simulation.

1. Introduction

Cast irons are a Fe–C–Si alloy with 3.0–4.3%C and 1.3–3.0%Si. The high carbon content determines the mechanical properties based in the retained carbon in the solid solution at room temperature, while silicon promotes the precipitation of carbon in the form of graphite.

At present, cast irons are manufactured in larger quantities than any other type of cast alloy [33], and in some applications they have replaced steel castings. This is mainly due to their lower melting point and higher carbon content which improves, the castability and fluidity during the pouring process. Other important properties of cast irons are the lower levels of defects produced during the filling of a mold and a wide range of mechanical properties as indicated in [1]. There are two main factors that control these properties: *(a)* type, size, and size distribution of graphite nodules; and *(b)* type of matrix and defects present: ferrite/pearlite relation, their own characteristics and the presence of microstructural defects.

The goal of the metallurgist is to design a process producing a microstructure which yields the expected mechanical properties. This requires knowledge of the relations between microstructure and mechanical properties as well as the identification the defects presents in the microstructure that affect these relations.

A Representative Volume Element (RVE) is commonly used in the context of micro-mechanics to determine the effective properties of materials. Thus, a proper choice of the RVE may become decisive to predict the effective properties of different alloys.

In general terms, a RVE should be: *(a)* statistically representative of the macroscopic response of the continuum, and *(b)* its dimension must be larger than the minimum size of the heterogeneity that characterizes the microstructure of the material. However there are numerous definitions of RVE in the literature [14,16,21,23,24,44,45], but there is a general agreement that a RVE can be considered as the minimum volume of material whose behavior is equivalent to a volume of a homogeneous fictitious material. From an engineering point of view, the main applications and uses of RVE are: *(a)* modeling and study of the influence of heterogeneities at the nano, micro and meso-structural level (localization), and *(b)* evaluation of the effective properties based on the properties of the individual micro-constituents (homogenization).

There are two prevailing philosophies for generating the RVE for heterogeneous finite element modeling: first, synthetic microstructures, usually obtained by means of computer algorithms,

* Corresponding author. Tel./fax: +54 264 4210277.
E-mail addresses: fcarazo@unsj.edu.ar (F.D. Carazo), sgiusti@civil.frc.utn.edu.ar (S.M. Giusti), aboccardo@mecanica.frc.utn.edu.ar (A.D. Boccardo), lgodoy@com.uncor.edu (L.A. Godoy).

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and second, microstructures obtained directly from experiments conducted in the laboratory. Most papers in research fields related with multi-scale theories and effective properties of alloys are based on RVE obtained from synthetic techniques. Therefore, the microstructures are characterized by periodic idealized micro-geometries, such as classical arrays composed of cubic spheres embedded in a homogeneous matrix and idealized form of cylinders with varying aspect ratios [7,36,37,43,47]. A RVE obtained by this way is applicable only in cases where the microstructure consists of periodic arrays characterized by homogeneous, uniform and one size heterogeneities. However, in alloys (including a large number of composite materials) the microstructure does not satisfy such requirements. A clear example is the alloy studied in this paper, spheroidal graphite cast iron (SGI). Fig. 1 shows two micrographs corresponding at two different points of a melted SGI's part, which have different cooling rates. There is a non-uniform distribution of the *spheres* of graphite (which correspond to the black color phase in both figures); further, their size and shape are not uniform. These variables are of great importance in evaluating the effective properties of a continuous medium [8,12].

On the other hand, there are many publications in which the RVE are obtained from micrographs [5,17,20,26,27,42], but none of them correspond to metallic alloys.

In the case of SGI, the importance of employing an adequate RVE from the micrographs is evidenced by observing and comparing the micrographs shown in Fig. 1(a) and (b). There are several differences in the size distribution of graphite nodules, the presence of micro-pores, and graphite nodules of low quality. All these properties affect the quality of the alloys by contributing to generate crack initiation zones and concentrations of stresses and strains at the micro-level.

In this paper the concept of RVE is used in the sense of *statistical volume element* [32]. Another interpretation from which the RVE proposed in this paper can be considered periodic, is given by [14], where the RVE can be considered as the volume element for which the macroscopic constitutive properties are precise enough

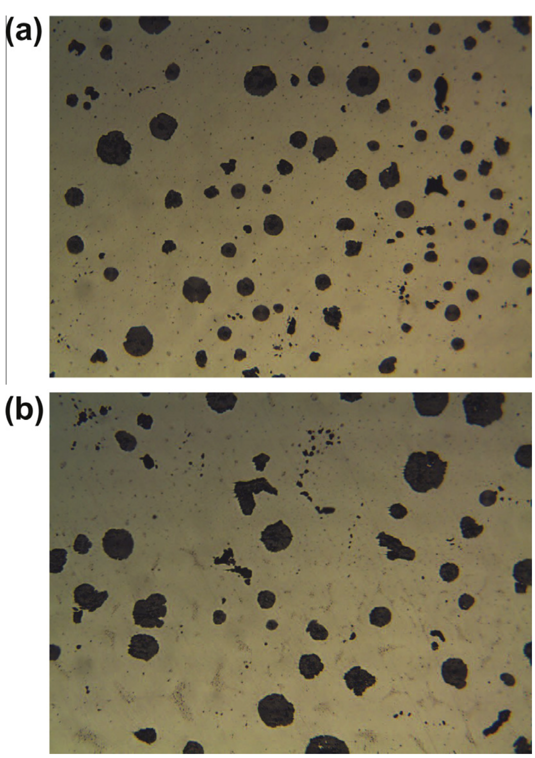

Fig. 1. Micrographies of pearlitic-ferritic SGI (×100).

to represent the overall constitutive response of the continuum medium. Then, a RVE can be considered valid if the moduli values are within the 5% of the value of the module given at macroscopic level. Thus, the evaluation of upper and lower bounds in effective properties calculated from RVE has great significance.

This work presents a comprehensive methodology to determine the effective properties in a heterogeneous continuum medium from micrographs, which involves the combination of digital image processing and quantification and characterization of microstructure. The main scope of this paper is to compare the results obtained from numerical simulations carried out with two RVE shapes: rectangular and hexagonal. To achieve this objective, a computational constitutive multi-scale model is presented to predict elastic constants such as Young's modulus and Poisson's ratio of a pearlitic SGI by taking into account the influence of graphite, matrix volumetric phase fractions, and nodularity of samples used in the study. The multi-scale models used in this work are based on the concept of the volume average of the strain field over a RVE. Such models have been widely used in the literature to simulate material behavior and predict effective properties at macroscopic level [31,34,38,46]. Numerical values are compared with results obtained from an analytical formula [6].

This paper is organized as follows: Section 2 describes the multi-scale model used in the simulations. The analytical expression for the effective Young's modulus of a pearlitic nodular cast iron is presented in Section 3. The experimental and numerical procedures developed to obtain the rectangular and hexagonal RVE are described in detail in Section 4. The results for a rectangular and hexagonal RVE are presented in Section 5 and Section 6, respectively. The paper ends with a comprehensive discussion of the results (Section 7) and and concluding remarks (Section 8).

2. Multi-scale modeling

This section presents a summary of the multi-scale constitutive theory upon which the estimation of the macroscopic elasticity properties is based. This family of (now well established) constitutive theories has been formally presented in a rather general setting in [18] and later explorated, among others, in [29,30] in the computational context. When applied to the modeling of linearly elastic periodic media, it coincides with the asymptotic expansion-based theory described in [4,38].

The starting point of this family of constitutive theories is the assumption that any point $\boldsymbol{x}$ of the macroscopic continuum is associated to a local RVE whose domain Ω_μ, with boundary $\partial\Omega_\mu$, has characteristic length l_μ, much smaller than the characteristic length l of the macro-continuum domain Ω, as shown in Fig. 2. For simplicity, we consider that the RVE domain consists of a matrix, Ω_μ^m, containing inclusions of different materials occupying a domain Ω_μ^i (see Fig. 2), but the formulation is completely analogous to that presented here if the RVE contains voids instead. Hereafter, symbols $(\cdot)_\mu$ denote quantities associated to the micro-scale.

An axiomatic variational framework for this family of constitutive theories is presented in detail in [10,11,41]. Accordingly, the entire theory can be derived from two basic principles: *(a)* the strain averaging relation and *(b)* the Hill-Mandel Principle of Macro-Homogeneity, which ensures the energy consistency between the so-called micro and macro-scales of the material.

The first basic axiom, the strain averaging relation, states that the macroscopic strain tensor $\boldsymbol{\varepsilon}$ at a point $\boldsymbol{x}$ of the macroscopic continuum is the volume average of its microscopic counterpart $\boldsymbol{\varepsilon}_\mu$ over the domain of the RVE, that is:

$$\boldsymbol{\varepsilon} := \frac{1}{V_\mu}\int_{\Omega_\mu} \boldsymbol{\varepsilon}_\mu dV \tag{1}$$