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A computational micromechanics approach to evaluate effective properties of ductile cast iron

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Ductile iron has excellent mechanical properties. The properties of SGI are mainly controlled by the type of matrix and by the size, shape, and distribution of graphite nodules. Thus, knowledge of the relation between microstructure and mechanical properties becomes important to design parts made with SGI. Micromechanical modeling of materials is a new approach recently employed to evaluate such relations while taking the topology of the constituent phases and the properties of each into account. The macroscopic mechanical behavior of a mixed ferritic/pearlitic matrix cast iron is investigated in this work by means of a micro-mechanical model, in which asymptotic homogenization is applied to computationally generated multi-particle cells in two and three dimensions. The displacement field inside the cells is computed via finite elements. From these cells, the size of the Representative Volume Element is determined, and the effective response is obtained for this element.

Keywords: ductile iron, homogenized propertied, computational micromechanics

Introduction

Most cast metal materials are microscopically heterogeneous, being formed of different constituents and phases, which are distinguishable on an appropriate scale. The constituents of a cast material have different topologies and mechanical properties, so that the macroscopic response is actually a result of the cooperative mechanical behavior of its various elements. Since in most cases the difference between the dimensions of the macrostructure (D) and that of the forming microstructure phases and constituents (d) is large, it is not possible to make a direct representation of the microstructure on the macroscopic scale of a part. For this reason, until recently, Mechanics of Materials has only used a macroscopic characterization of the materials. According to this characterization, the material is considered to be homogeneous and the coefficients needed to describe phenomenologically the macroscopic mechanical behavior of the material are determined by testing performed on relatively large specimens. However, such description cannot explain certain macroscopic behaviors of the material without additional information of microstructure.

Extensive research has been conducted since the early nineteenth century in order to address this problem. The increase in capacity of computational calculation and the development of numerical methods of recent decades have given an important impetus to research that has extended the area of multiscale studies to different materials and different physical phenomena. In this context, the ductile cast iron, also known as nodular cast iron or spheroidal graphite iron (SGI), can be considered as an heterogeneous material formed of a metallic matrix composed of ferrite, perlite or a combination of both, in which graphite nodules are embedded. Given these microstructural features, ductile iron can be analyzed as a heterogeneous material with an array of matrix-inclusion.[1]

The properties of ductile iron are controlled mainly by the type of matrix, the presence of defects into it, and the size, shape and distribution of graphite nodules. Therefore, it is very important to investigate the relationship between microstructure features and mechanical properties in order to obtain parts with specified mechanical properties.

One of the approaches to the study of the relationship between the microstructure and the mechanical properties is based on phenomenological models which depend on experimental data. Guo *et al.*[2] studied the relationship between the characteristics of matrix and graphite and different mechanical properties of the SGI, and proposed expressions to determine Brinell hardness, yield strength and ultimate stress based on the microstructural characteristics analyzed.

Wenzhen and Baicheng[3] predicted the mechanical properties of microstructures by means of a solidification model, employing experimental expressions developed by Lundback *et al.* [4]

Another approach employs multiscale modeling and on the micromechanics of a continuum. Pundale *et al.*[5] investigated the influence of volume fraction of graphite and of shape, size and distribution of nodules on the effective Young modulus. They analyzed cells, in which the graphite nodules are assumed to be voids, with two models: a plane stress model and an axisymmetric model. Collini and Nicolleto[6] proposed a unit cell model to predict constitutive law

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and failure of a nodular cast iron. They considered a unit cell with a mixed matrix of ferrite and pearlite; this allowed analyzing the influence of the volume fraction of these micro-constituents on the mechanical properties.

Collini[7] implemented different micromechanical computational models, using the finite element method to determine the elastic-plastic behavior of the material and to identify failure initiation mechanisms. He compared the results obtained by different models and performed validation with experimental results.

According to the literature review, there are no studies in which multi-particle three-dimensional cells with mixed matrix have been analyzed for determining effective properties using micromechanical analysis. For this reason and because of the limitations of two-dimensional models, a comparison between 2D and 3D models becomes important. However, meaningful 2D-3D comparisons can only be made by preserving some similar features between both models. As will be shown next, the procedure commonly used to obtain multiparticulate plane cells is from micrographs. So in order to obtain comparable models, the procedure presented here to obtain a plane model attempts to reproduce the same procedure used to obtain a micrograph.

The micromechanical requires an appropriate representation of the material through what is called a representative volume element (RVE). Obtaining the RVE can be done using two main methodologies[1], one of them uses "synthetic" microstructures generated by computer algorithms. A second methodology is based on micrographs obtained experimentally, using acquisition and image processing to produce digital images and with these the micro-geometries. This second approach has the disadvantage of only allowing the generation of planar geometry and thus only a two-dimensional analysis of the problem.

The appropriate choice of RVE is an essential ingredient, from which the effective properties of the material shall be determined using the principles and laws of micromechanics and the multiscale theories. A RVE must (a) be statistically representative of the macroscopic response analyzed, and (b) have a dimension greater than the minimum size of the heterogeneity that characterizes the microstructure of the material. A RVE can be considered as the minimum volume of material whose performance is equivalent to the macroscopic behavior of the material. To define the size of the RVE, two important issues must be considered: the desired accuracy and the computational cost to solve the model; both of them increase with increasing volume.

Drugan and Willis[8] and Drugan[9] concluded that RVE should have a size equal to or greater than twice the diameter of the spheres to get a 5% error in the modulus of elasticity, being able to reduce this error to less than 1% when the size is increased to 4.5 times the diameter.

To define the RVE it is possible to adopt a geometric or a physical criterion[1,10]. According to the geometric criterion, the RVE must be statistically representative of the microstructure of the material, thus being independent of the physical property to be studied. The physical criterion defines the RVE based on the requirement that, for a given physical behavior, their overall response is not dependent on the applied boundary conditions.

The main objective of this work is to obtain Young's modulus and yield strength of a nodular cast iron using homogenization techniques. To achieve this goal, multiparticulate cell models, in two and three dimensions, are used. Nodules are considered as voids which are embedded in a matrix with different percentages of ferrite. The size and the volumetric density of graphite nodules are the result of the computer simulation of a solidification process, specifically of a block Y (1in).

Experimental Procedure

The assessment of the effective mechanical properties of ductile iron using a micromechanics approach with a synthetic representation of the microstructure of the material is presented in this paper. For the generation of a representative material geometry at microscale level, density and size distribution of graphite nodules and the volume fraction of each microconstituent are taken as data.

In order to provide information related to the volumetric nature of the spheres of graphite, a computer simulation for the solidification of a block-type Y (1in) test is carried out. The model considers thermal and metallurgical problems of solidification of ductile iron, making the coupling between both by the latent heat method. The thermal problem is macroscopically treated, solving the heat equation in the complete domain (part and mold) by the finite element method. The microstructural model used for solidification, due to Boeri[11], simulates the stable equiaxed solidification of a nodular cast iron, of eutectic composition, according to the plurinodular theory. The nucleation of graphite nodules is considered as a continuous process, so that in each time step of the numerical resolution and while certain conditions are satisfied, the nucleation of a set of nodes occurs. Each set is called a family of nodules. In the model used, all nodes belonging to the same family are assumed to have the same radius. Thus, at the end of the simulation, each family will possess a density and a size of nodules that characterizing it, as shown in Fig. 1. The implementation of the solidification model was performed in the general purpose finite element program ABAQUS.[12]

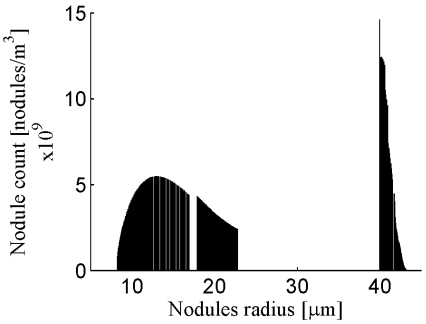

Fig. 1: Simulated nodule size distribution

On the other hand, to define the constitution of the matrix, several cases with different percentages of pearlite and ferrite are considered in order to explore the influence of different matrix compositions on the mechanical properties analyzed.

Using as input data the size and density of nodules of each family and the total volume fraction of graphite resulting from the simulation, and after setting the fractions of ferrite and pearlite in the matrix, the multi-particle cells are generated: (a) a three-dimensional cubic and (b) a two-dimensional square shape. The latter is the result of performing a section of the three-dimensional cell with a plane parallel to one face of the cell and at a random distance from that face.

The two-dimensional model is analyzed as a plane stress problem. From the above, it follows that all cells are formed of a matrix composed of ferrite and pearlite, and nodules of different sizes embedded into it. A perfect elastic-plastic behavior of the matrix elements is assumed. The equality of the Young's modulus to ferrite and pearlite is assumed, accordingly to [13-17]. The microconstituent properties are shown in Table 1.

The nodules are modeled as voids in order to reduce the number of degrees of freedom of the finite element model, and because they do not constitute a reinforcement of the matrix due to its low Young's modulus.[5,7] In order to define the mixed matrix of ferrite and pearlite, first percentages of each microconstituent are chosen, and then it is assumed that all nodes are surrounded by a spherical shell of ferrite such that its predefined percentage is reached. To determine the thickness of the ferrite layer, it is assumed, for simplicity, that the relationship between the radius of each ferrite layer and its corresponding node is constant and equal to a given value that depends on the ferrite fraction.

Table 1: Properties of microconstituents of the matrix[7]

Constitutent material	E [GPa]	ν	σ_0 [MPa]
Ferrite	209	0.3	427
Pearlite	209	0.3	552

The cell used for homogenization should be large enough to have all the information necessary to describe the behavior of the heterogeneous material.[18] The cell that meets this requirement is a RVE. The macroscopic response obtained with these models shows a strong dependence on the size of the volume element. Thus, it is very important to find an optimal size for the volume element that is large enough to adequately capture the physical behavior of the material studied but simultaneously involving the least possible computational cost.

Using a definition of the RVE by geometrical criterion, the appropriate size is obtained based on the characteristics of the micro-geometry regardless of the physical property. The appropriate size of the RVE is that which possesses geometric features equivalent to the analyzed material. The use of this criterion for choosing the size of the RVE, according to some researchers[1], is suitable for micromechanical models used to estimate the elastic behavior of heterogeneous materials. Drugan and Willis[8] demonstrated that, for isotropic heterogeneous materials comprising a matrix and spherical particles of equal size, with size cells between two and five times the diameter of the particles, representative results of macroscopic elastic stiffness are achieved with errors smaller than 5% and 1%, respectively.

As can be noted, according to these authors, the RVE size is independent of the volume fraction of particles.

According to the physical criterion, the size of the cell is appropriate when an increase of the size does not produce change in the physical property analyzed.

In this paper, to obtain a cell size that can be considered representative of the material, a series of cells with increasing volumes were analyzed up to the percentages of phase (geometric criterion) and mechanical properties (physical criteria) converge to a value;

$$\xi = \frac{|A_{i+1} - A_i|}{A_{i+1}} \cdot 100 \qquad (1)$$

where A_i and A_{i+1} are the analyzed property values for cell size i and for next higher cell size $i+1$. A cell is assumed to be representative, i.e. a RVE, when the error ξ is less than 2%.

Based on the results of the works by Drugan and Willis[8] and Drugan[9], the absolute size of the cell, hereinafter cell size L, is the side length of the square cell for bi-dimensional models and the edge length of the cubic cell for three dimensional models. A relative size of cell is also defined by the ratio between L and the radius of the largest nodes, which are those belonging to the family of nodules which is the first to nucleate.

All three-dimensional equal-sized cells include the same number of nodes of each family and the same volume fraction of voids. However, the methodology for obtaining two-dimensional cells entails that the geometric characteristics are particular to each of them, that is, not unique for each cell size. This is because both the number of voids intersected by the plane and the position for which the plane intersects them, are variable. The variability of the geometrical characteristics of the two-dimensional cell leads to a high dispersion of the results, which does not allow convergence of the results with increasing cell size for any of the two criteria. To reduce scatter in the results the concept of averaged of a sample or ensemble averaging is used.[10] The location of the centers of the nodules in the three-dimensional cell is made with the RSA algorithm, thereby generating different cell geometries in each run. In this way it is possible to generate different three-dimensional cells and from them to obtain M two-dimensional cells, each of these plane cells (called *realization*[10]) is a member of what, taken together, is called sample. The response of each realization in the sample $Q^{(K)}$ is generally different, being able to define an average response of the sample $\langle\langle Q\rangle\rangle$ with the following expression:

$$\langle\langle Q\rangle\rangle = \frac{1}{M}\sum_{K=1}^{M} Q^{(K)} \tag{2}$$

Considering an increasingly larger number of realizations and computing a new ensemble average each time a new realization is added to the set, results in an average response $\langle\langle Q\rangle\rangle^k$ computed from K samples. The successive increase of a sample size gives origin to a sequence of $\langle\langle Q\rangle\rangle^k$. This sequence shows a convergence which will decrease the randomness of the results. Then, to define a characteristic value of response for each two-dimensional cell size, the sample size is increased successively until the marginal value of the property studied is negligible. When this occurs, it is assumed that this average value is a characteristic response of this cell size.

For both bi and tri-dimensional cells, determining the mechanical behavior is performed using the asymptotic method of homogenization[19] by solving the displacement field within the cell, produced by subjecting the cell to a set of prescribed macroscopic deformations, by the finite element method. These deformations are imposed by prescribing appropriate displacements to the degrees of freedom of a set of control nodes NC.[20,21]

For the computation of the effective mechanical properties analyzed in this work, it is necessary to obtain the solution of a single boundary value problem. For this, the cell is subjected to a set of prescribed macroscopic strains, in accordance to the indicated in the strain tensor of expression (3), imposed as displacements to the control nodes NC.

$$\varepsilon_{11}^0 = \begin{bmatrix} \varepsilon_{ij}^0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{3}$$

The use of this methodology leads to a homogenization called external[21], in which the stress tensor is calculated as the rate between the reactions in the control node and the cell volume. The homogenization process is performed for each increment of deformation to obtain the stress-strain curves and, from them, the Young's modulus E and the yield stress σ^0.

The model is implemented in ABAQUS using a script developed in Python that generates the different components of the finite element model. The developed program allows: generate cells with periodic geometries, assign the constitutive properties of materials, ensure the periodicity of the finite element mesh (see next section), impose periodic conditions to the opposite faces of the cell and apply the macroscopic strains to the degrees of freedom of the control nodes. For the post-process a specially developed script that reads the results and executes the homogenization is used.

Multiparticulate Cells

For the three-dimensional cell, the graphite nodules are represented by spherical voids having different radii that are obtained from the numerical simulation of the solidification. In each cell, a certain amount of nodules of each family is included. Such amount of nodules is determined by taking in account the volumetric density of nodules of the family and the total volume of the cell:

$$N = \Omega_C N_{vol} \tag{4}$$

where N is the number of nodules pertaining to a family included in the cell, N_{vol} is the volumetric density of nodules obtained from the solidification simulation and Ω_C is the volume of the cell. The value obtained by expression (4) is rounded, because the number of nodes should be a natural number.

For a given volume fraction of ferrite, the radius of the envelope of ferrite is determined by considering the volumetric density and the size of nodules of each group as:

$$\zeta = \sqrt[3]{\frac{f_f}{f_{gr}} + 1} \tag{5}$$

where ζ is the ratio between the radius of the outer sphere of ferrite (r_f) and the radius of the graphite nodule (r_g), f_f is the volumetric fraction of ferrite and f_{gr} is the volumetric fraction of graphite; see Fig. 2.

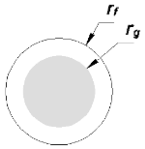

Fig.2: Scheme of the nodule surrounded by the envelope of ferrite.

The three-dimensional multiparticle cell is generated by the Random Sequential Addition method, RSA. This method generates the coordinates of the centers of the spheres in a sequential and random mode. The condition that the nodules should not interpenetrate and must be completely contained within the cell without intersection with the edges of it (see Fig. 3.c) is imposed. This condition is relaxed for the ferrite spheres in such a way that a free contact between them and between a sphere and the faces of the cell is allowed. The only condition is that regions generated among spheres and cell faces have not a reduced volume because this situation makes it difficult to obtain an appropriate finite element mesh.

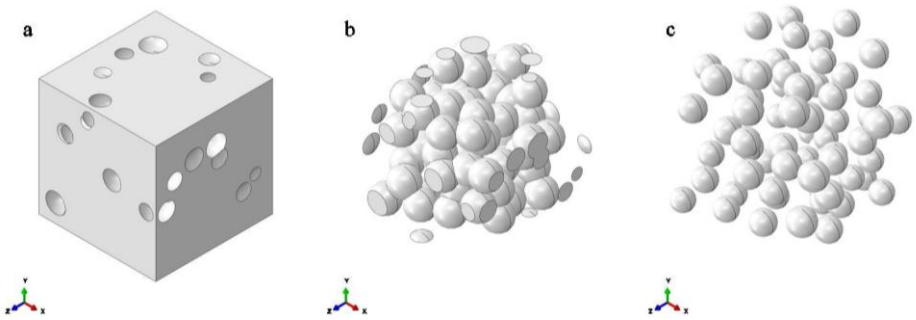

Fig. 3: Parts of the RVE: (a) pearlite, (b) ferrite envelopes, (c) nodules (voids in the simulation)

The two-dimensional cell is obtained by sectioning the final three-dimensional cell through a plane parallel to one face located at a random position. For this, once chosen the plane with which the section will be made, nodules and envelopes of ferrite that are cut are identified and then, the radius of the circles that are the intersections between the plane and each of the parts are determined; see Fig. 4.

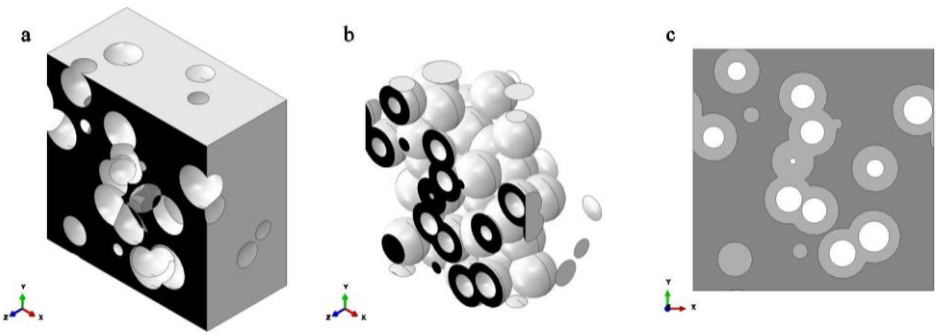

Fig. 4: Scheme of the sectioning to generate two-dimensional model.

To define the macroscopic behavior of the material, the homogenizing asymptotic method is used. It enables the replacement of a heterogeneous medium by an equivalent homogeneous one, allowing obtaining the macroscopic laws using microesctructural information. Some researchers [22, 23] have applied this technique to the modeling material with a not exactly periodic microstructure. Taking this into consideration, the nodular cast iron can be modeled by a periodic repetition of a cell.

This homogenization model requires implementing periodic boundary conditions which require, in turn, that both the geometry of the RVE, Fig. 3 and 4, and the mesh of finite elements be periodic Fig. 5.

The periodicity conditions of the cell is guaranteed if it holds that

$$u_k = \varepsilon_{kl}^0 L + u_k \tag{6}$$

ε_{kl}^0 is the tensor of macroscopic deformation, u_k the displacement of node *k*, and u_k the displacement of its correspondent periodic node. Since u_k is unknown, for numerical implementation of these conditions, some expressions that relate the movement of a pair of points located on opposite sides must be posed. To ensure the periodicity, the boundary conditions to impose on the faces, edges and vertices of the cell are determined by considering the vectors of periodicity of the cell analyzed.[23, 24]

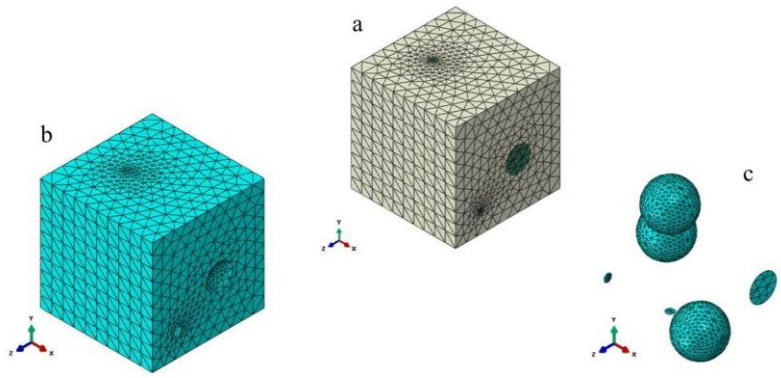

Fig.5: Boundary mesh of parts included on FEM model: (a) assembly of pearlite and ferrite envelope, (b) pearlite and (c) ferrite envelopes.

Results and Discussion

The RVE size determination is performed according to the geometric and physical criteria. Through a series of independent analysis of increasing size cells, first a three-dimensional RVE size is defined according to both criteria and, second, the same is done for the two-dimensional model.

In this work, the geometric analysis focuses exclusively on the convergence of the ferrite volume fraction and the results of a geometric analysis for graphite fraction, reported by Rodríguez *et al.*[25], are used.

Fig. 6 shows the evolution of the ferrite fractions in the cell with increasing relative size thereof; it shows that it is not possible to achieve the convergence to the searched ferrite fraction values in the cell for high fractions of ferrite of matrix. This is because the RSA method used to generate the random distribution of graphite nodules has difficulty in generating distributions with high volume fraction.[10] Because the ferrite is assumed distributed with spherical shells around the graphite, their distribution is coincident with that of the nodules and therefore it is governed by the same distribution method. For this reason in this work we analyze matrices with ferrite fractions of 10, 20 and 30%, values that can be achieved with the method used. The cell sizes finally adopted for each percentage of ferrite are shown in Table 2.

Fig. 7 shows the evolutions of the Young's modulus and the yield strength as functions of relative size of the cell. By this criterion, different sizes of RVE for each percentage of ferrite in the matrix is also obtained, showing that this approach results in larger cell sizes (Table 2) relative to those determined according to the geometric criterion.

In order to defining the size of the two-dimensional RVE, cells with increasing relative size are analyzed. Both for the geometric definition as for physical definition of the RVE size, a dispersion of the results is observed. This is because of the way the cells are generated and that causes a variation in the geometrical characteristics for each cell, as it indicated above.

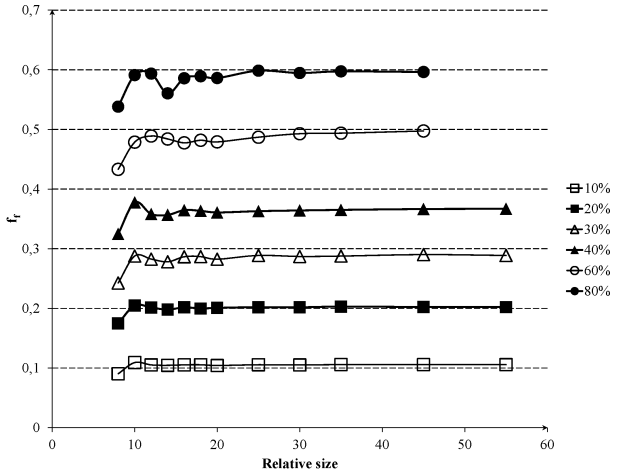

Fig.6: Volume fraction of ferrite in the three-dimensional cells for different percentages of ferrite in the matrix and different relative sizes of the cell.

Table 2: Geometric and physical criteria: RVE relative sizes for different ferrite volume fractions

		f_f [%]		
Model	Criterion	10	20	30
2D	Geometric	18	20	20
	Physical	35	20	22
3D	Geometric	12	12	12
	Physical	15	15	15

In Fig.8 (a) the evolution of the fraction of ferrite for relative size 10 and 20 and 10, 20 and 30% of ferrite in the matrix is observed. Convergence was achieved by increasing the number of realizations in the sample; it can be further noted that the results dispersion decreases with increasing size of the cell used. The characteristic behavior for each cell size is obtained from the average of a set of at least 25 realizations.
In Fig.8 (b) the convergence of the characteristic values by increasing the size of the cell, for the different analyzed percentages of ferrite is observed. The RVE sizes adopted with this criterion, for 2D models, are listed in Table 2.

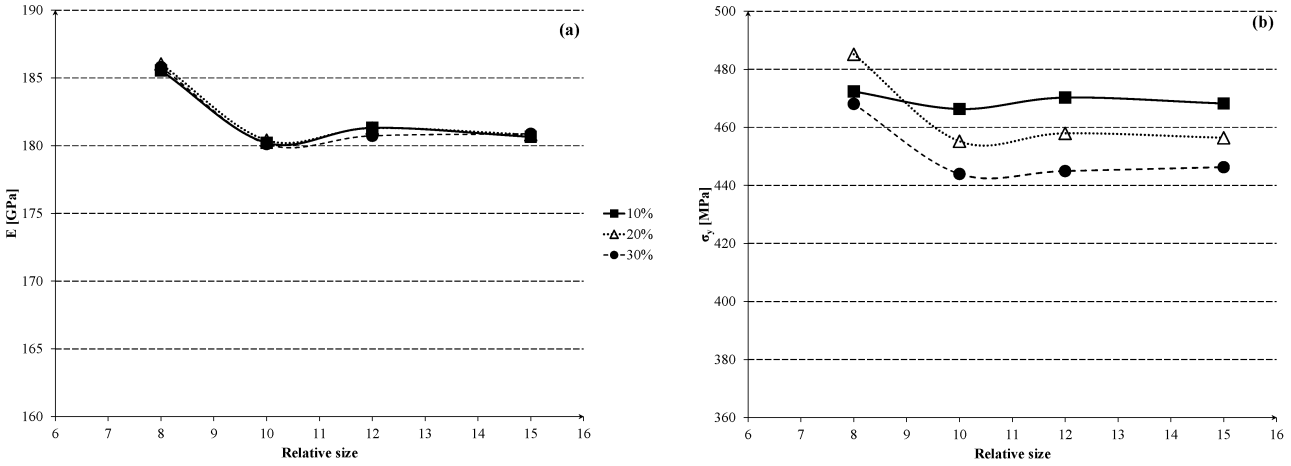

Fig.7: Material properties of three-dimensional RVE with 10, 20 y 30% of ferrite in matrix for each cell size analyzed: (a) Young's modulus E, (b) yield strength σ_y.

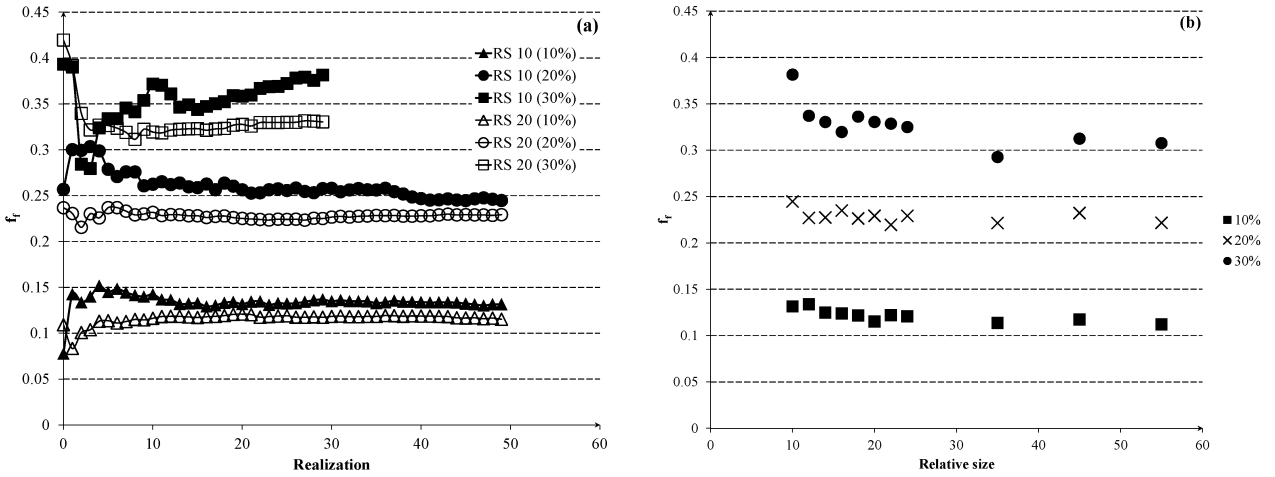

Fig.8: (a) Volume fractions of ferrite for two-dimensional RVE of relative size 10 and 20 with increasing number of realizations, (b) ferrite fraction averaged for each analyzed cell size.

The characteristic results for each two-dimensional cell size, according to the physical criterion, are plotted in Fig. 9. The characteristic values of the properties analyzed show convergence with increasing cell size considered, slower convergence for the values of yield stress is observed. The Young's modulus tends to be equal for all three analyzed ferrite percentages, accordingly to the assumption of equal Young's modulus for ferrite and pearlite. On the contrary, the yield stress decreases with the increase of the fraction of ferrite.

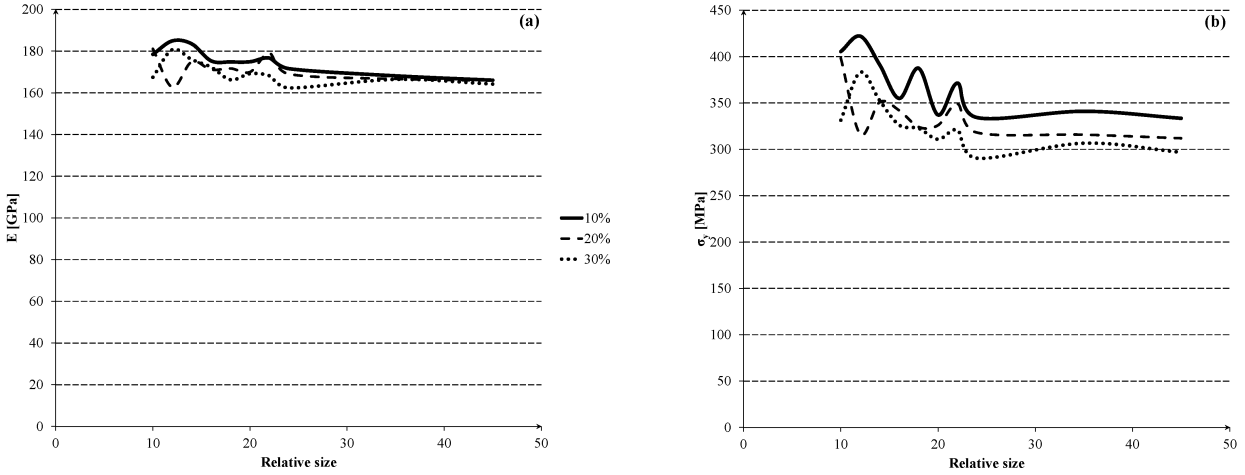

Fig.9: Average material properties of two-dimensional RVE with 10, 20 and 30% of ferrite in matrix for each cell size analyzed: (a) Young modulus averaged, (b) yield strength averaged σ_y.

Given that the physical criterion requires larger cells to achieve convergence, this criterion is used to define the final size of RVE in both models. In Fig. 10 the strain-stress curves for two-dimensional and three-dimensional RVE with 10, 20 and 30% of ferrite in matrix are shown. The 2D model demonstrates greater stiffness [25] as well as a lower yield point. As expected, the increase of volume fraction of graphite causes a reduction of the yield point. No hardening was observed in any of the two models because a perfect elasto-plastic constitutive model was used.

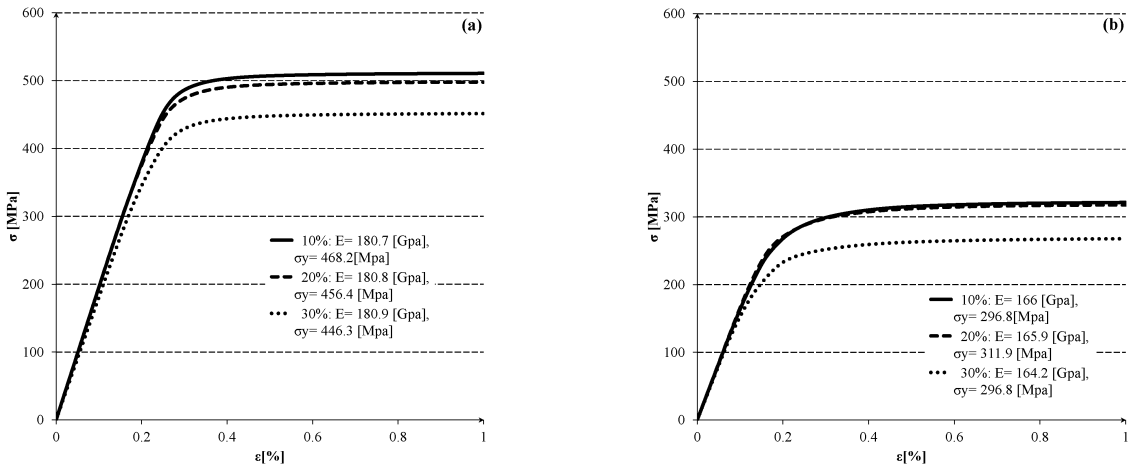

Fig.10: Stress-strain curves for RVE with 10, 20 y 30% de ferrite in matrix: (a) three-dimensional, (b) two-dimensional RVE.

In Fig. 11 the fields of von Mises equivalent stresses calculated for two-dimensional and three-dimensional RVE with ferrite fraction of 20% are shown.

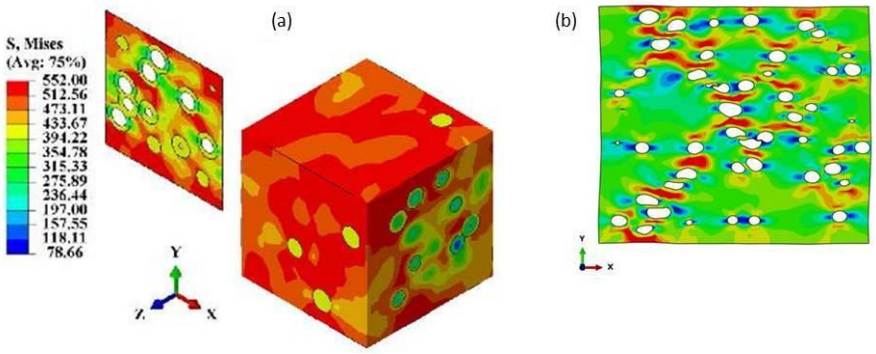

Fig.11: von Mises equivalent stresses for RVE with 20% ferrite fraction in matrix and strain of 0.25% (a) three-dimensional and (b) two-dimensional RVE.

Conclusions

Macroscopic Young's modulus and yield stress for nodular cast irons using the method of asymptotic homogenization for multiparticle models, have been obtained in this work. The generated cells are formed by a mixed matrix with different proportions of ferrite and pearlite and nodules embedded therein. The nodes are represented as voids; the ratio between the radii of the spherical layers of ferrite and the radii of the corresponding nodules is assumed constant.

The RSA method used to obtain the distribution of nodes limits the maximum fraction of ferrite in the matrix that can be achieved.

The different criteria for defining the RVE give different results, being in general the geometric criterion which gives the smaller sizes. With regard to the cells in two or three dimensions, it is noted that lower representative values are obtained for the last. This might be because the three-dimensional models provide a more complete description of the material structure. However, the use of three dimensional models has a much higher computational cost even when compared with that of the two-dimensional RVE of higher relative sizes.

Three-dimensional models have stiffer behavior than two-dimensional models. This is attributed to the assumptions that are made by considering the problem as a plane stress problem. The perfect elastic-plastic constitutive model used for the microconstituents does not allow the macroscopic representation of the strain hardening of the material.

Given the limitations identified in the work, it is considered appropriate to analyze, in future works, other methods to generating cell that would achieve higher ferrite fractions. It is also considered necessary to evaluate other forms of distribution of the ferrite whose characteristics may be, for example, the simulation result of the cooling of the material in the mold.

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