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Distance map based micromechanical analysis of the impact of matrix heterogeneities on the yield stress of nodular cast iron

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Abstract

A method to construct 3D representative volume element (RVE) models of the nodular cast iron microstructure that accounts for the presence of heterogeneities in the matrix is proposed. The main advantage is the possibility to generate a wide spectrum of realistic distributions of the matrix heterogeneities in a simple and fast way. The method takes advantage of the fact that the spatial distribution of some of the matrix heterogeneities is intrinsically connected to the distribution of the graphite nodules, due to the nature of the solidification process. Accordingly, the graphite morphology is reconstructed first via X-ray computed tomography and subsequently used to estimate the distribution of the pearlite and of the Si micro-segregation – considered as case studies – by means of dedicated distance functions. The obtained 3D models are used to show that the spatial variation in the matrix plastic properties associated with the Si micro-segregation is not expected to influence the material yielding behavior significantly. In addition, it is shown that when the matrix pearlite content increases for a fixed overall C concentration, the corresponding decrease in the nodules’ volume fraction can account for as much as 1/3 of the obtained increment in the material macroscopic proof stress.

Keywords

Cast iron; Distance function; X-ray tomography; Heterogeneous microstructure; Representative volume element (RVE)
1. Introduction

Nodular cast iron, also known as ductile iron or spheroidal graphite iron (SGI), is nowadays widely used in key industrial sectors like transport, marine, and energy production, accounting for as much as 25% of the total casting production worldwide ("50th Census of World Casting Production," 2016). The success of this material stems from its unique combination of strength, ductility and toughness, in addition to its excellent castability and lower price compared to standard low-carbon steels (Labrecque and Gagne, 1998).

Due to the high technological importance of SGI, a number of studies have focused on the mechanisms controlling the deformation and fracture at the micro-scale. However, as emphasized in a recent review article, a complete understanding has not been achieved yet (Hütter et al., 2015). The reasons are rooted in the complexity of the material microstructure, composed of graphite nodules embedded in a matrix where multiple phases may coexist depending on chemistry and processing conditions. In this respect, most of the past micromechanical analyses of SGI have considered the material as a two-phase composite where both the matrix and the nodules are regarded as homogeneous, see e.g. (Bonora and Ruggiero, 2005; Buljac et al., 2018; Norman and Calmunger, 2018) and the references therein. Accordingly, constitutive equations relating the mechanical response at the macroscale to the geometrical parameters of the nodules and to the average properties of the matrix have been proposed.

The validity of the homogeneity assumption for the SGI constituents has recently been challenged by experimental observations revealing strong gradients in mechanical properties inside the nodules, which have been related to their complex internal structure (Andriollo et al., 2018a; Bellini et al., 2019). It was also shown that micromechanical models accounting for these gradients can explain the local concentrations of the thermal residual stress detected with X-ray diffraction around the nodules (Andriollo et al., 2018b). Concerning the matrix, it is now widely accepted that the spatial distribution of most of the heterogeneities associated with the casting process, like the micro-segregation, pearlite colonies, porosities, etc. is by all means not uniform (Vazehrad et al., 2015). Therefore, the use of the homogeneity
assumption to characterize the mechanical behavior of the matrix at the microstructural scale appears questionable also.

The need to consider the actual distribution of the matrix heterogeneities in micromechanical analyses of SGI was initially pointed out by Collini and Nicoletto (2005) in relation to the pearlite colonies and was subsequently reasserted by Fernandino et al. (2017) and Xu et al. (2020) in connection with the subdivision of the matrix into first-to-solidify and last-to-solidify regions. However, the development of corresponding microstructural models has been hampered so far by the difficulty of generating realistic 3D representations of the microstructure that include the matrix heterogeneities.

To the authors’ best knowledge, the first micromechanical analyses accounting for the matrix spatial heterogeneity in an explicit way were based on periodic unit cell models and aimed at investigating the tensile response of ferritic-pearlitic SGI (Collini and Nicoletto, 2005; Nicoletto et al., 2006). These models consisted of idealized periodic arrangements of spherical nodules surrounded by ferrite halos and embedded in a continuous pearlite phase. More recently, refined versions have been proposed where the unit cell is replaced by a representative volume element (RVE) containing a random isotropic distribution of spherical nodules (Collini et al., 2019; Rodriguez et al., 2018). A disadvantage of these models is that the generation of an artificial microstructure always requires the introduction of simplifying assumptions, e.g. regarding the shape of the nodules, whose effects may be difficult to estimate. To overcome this limitation, 2D models based on the real microstructure reconstructed from optical micrographs have been proposed and used to study the effect of the matrix subdivision into first-to-solidify and last-to-solidify regions (Fernandino et al., 2017). However, it is worth pointing out that 2D micromechanical simulations of the SGI behavior during tensile loading may differ from the corresponding 3D simulations, due to the inherent three-dimensional nature of the material microstructure (Andriollo et al., 2015). Yet, the accurate determination of quantities like the pearlite spatial distribution or the chemical segregation map over a 3D RVE would require serial sectioning combined with metallographic examinations, which can be quite laborious to perform for standard RVE sizes (Metzger and Seifert, 2015). A breakthrough in this respect is the method proposed by Salomonsson and Olofsson (2017) to construct 3D RVEs from X-ray computed tomography
(CT) data accounting for the pearlite distribution. The former authors used an image analysis technique involving the probability density of intensity to enhance the limited X-ray absorption contrast between the ferrite and the pearlite, so that these two phases could be identified and separated. However, a limitation of the method is the impossibility to capture the distribution of other types of heterogeneities besides the pearlite. Furthermore, the method is not optimal for parametric studies aiming at exploring microstructures with specific mechanical behavior, which is a disadvantage compared to approaches based on artificial microstructures.

In the present work, we construct 3D finite element models of the SGI microstructure by reconstructing the graphite morphology first via X-ray CT and subsequently estimating the distribution of the matrix heterogeneities by means of dedicated distance functions. The key idea is to take advantage of the fact that the spatial distribution of some of the matrix heterogeneities is intrinsically connected to the distribution of the graphite nodules, due to the nature of the solidification process. The main advantage is the possibility to generate, in a simple and fast way, a wide spectrum of realistic distributions of the matrix heterogeneities. The potential of the present approach is demonstrated by means of two case studies that, to the authors’ best knowledge, have never been investigated so far. The first one relates to the fact that the amount of pearlite forming during the eutectoid reaction determines the matrix phase composition, but also the final volume of the nodules. Therefore, it is of interest to assess, for a fixed overall Carbon concentration and different values of the pearlite content, how much of the corresponding variation in the macroscopic yield stress is associated with the change in the matrix phase composition and how much is associated with the change in the nodules’ volume fraction. The second case study concerns the quantification of the impact of the Si micro-segregation on the yielding behavior of ferritic SGI, which is motivated by the fact that common micro-segregation patterns (Freulon et al., 2016) can be expected to produce localized variations of the ferrite yield stress in the order of 50 MPa (Abramowitz and Moll, 1970).
2. Micro-mechanical modelling

As briefly outlined in the introduction, in the present work the 3D finite element models of the SGI microstructure are developed following a two-step procedure. First, a microstructure-conforming mesh corresponding to an RVE where the matrix and the nodules are considered as distinct homogeneous phases is created based on a CT scan. Subsequently, the properties of the mesh elements forming the SGI matrix are assigned based on dedicated distance functions to account for the presence of pearlite and of Si micro-segregation. The details of these steps are given in the next two sub-sections. After that, the constitutive models of the SGI microstructural phases and the homogenization procedure used to calculate the effective response of the RVE models upon tensile loading are presented.

2.1 RVE meshes from X-ray tomography

A SGI specimen already used in a previous work was considered (Zhang et al., 2019). The specimen, with length 10 mm and 1x2 mm² rectangular cross-section, was extracted from a block of near-eutectic SGI grade EN-GJS400-18 with 3.68 wt% C, 2.30 wt% Si, 0.22 wt% Mn and 0.11 wt% Mg. Metallographic examination, described in detail in Zhang et al. (2019), revealed the presence of graphite nodules embedded in a predominantly ferritic matrix, with an overall graphite volume fraction \( \psi_G \) of \( \approx 11.5 \% \) and mean nodule diameter of \( \approx 30 \mu m \).

The specimen was CT scanned with a Zeiss Xradia 520 Versa X-ray microscope, using polychromatic and conical X-ray beams with energies up to 150 keV, which allowed obtaining a voxel size of 1.359 \( \mu m \). From the CT scan, a cubic subvolume of size 300x300x300 \( \mu m^3 \) was extracted and segmented to separate the nodules from the matrix. The nodules contained in the subvolume were subsequently expanded/contracted isotropically about their centroids by an amount determined iteratively in order to obtain three different RVEs – henceforth called RVE9, RVE12 and RVE15 – characterized by values of \( \psi_G \) approximately equal to 9 \%, 12 \% and 15 \%, respectively. These values were selected in order to span the full range of graphite fractions found in the SGIs considered by Collini and Nicoletto (2005), which have nearly constant C concentration (\( \approx 3.7 \) wt\%, similar to that of...
the specimen considered in the present work) and pearlite fraction in the matrix $\psi_p$ varying between 0 % and 100 % – see Figure 1.

The three RVEs were meshed using the meshing toolbox of the software Avizo®. The optimal element size was carefully selected via a mesh sensitivity analysis based on the outcome of the loading simulations – see Section 2.4. An in-house developed code was used to duplicate the nodes along the matrix-nodule interfaces, to allow for the implementation of the cohesive interface behavior described in section 2.3. Eventually, the RVEs were imported into ABAQUS, which was the finite element software used in the present investigation. The corresponding meshes, each consisting of $\approx 500000$ second-order tetrahedral elements, are visualized in Figure 2.

Figure 1: Relationship between graphite fraction and matrix pearlite fraction for a fixed value of the overall Carbon concentration in the SGI microstructure. The data correspond to the SGIs considered by Collini and Nicoletto (2005).
2.2 Spatial distribution of the matrix heterogeneities

2.2.1 Pearlite

The presence of pearlite in the SGI matrix is associated with the eutectoid reaction. During the solid-state cooling of SGI, the transformation of the austenite into ferrite begins as soon as the upper eutectoid equilibrium temperature is reached. This process requires Carbon atoms to diffuse to the graphite nodules, due to the lower solubility of this element in the ferrite compared to the austenite. However, for regions of the matrix located far from the nodules, the Carbon atoms may not have sufficient time to diffuse out of the austenite before the metastable eutectoid temperature is reached. If that happens, pearlite forms instead of ferrite.

To a first approximation, which neglects the segregation-related variation of the stable and metastable eutectoid temperatures, it can then be stated that the probability of a point in the matrix to transform into pearlite increases the larger its distance \(d\) to the closest nodule. This fact can be exploited to estimate the spatial distribution of the pearlite in the matrix, assuming that its volume fraction \(\psi_p\) is known. Indeed, a critical value \(d^*\) is considered, such that the volume \(V(d^*)\) occupied by the set \(\mathcal{F}(d^*)\) of all the matrix points fulfilling the condition \(d > d^*\) corresponds to \(\psi_p\) when normalized by the total matrix volume \(V_{mat}\). Because of the previous statement, simple logical arguments lead to the conclusion that the set \(\mathcal{F}(d^*)\) is the
one with the highest probability of corresponding to the matrix region occupied by the pearlite. This suggests that the pearlite distribution can be estimated based on the distance of the matrix points to the closest nodule.

The concept just presented was utilized in the present work to identify the mesh elements corresponding to the pearlite region of a given RVE. First, a distance map algorithm was run to calculate the distance $d$ of each element centroid to the closest matrix-nodule interface. Based on that, the function $V(d^*)$ was established, which, upon normalization by $V_{mat}$, delivered the pearlite concentration function $\psi_p(d^*)$. The function $\psi_p(d^*)$ was then inverted and used to determine $d^*$ for a prescribed value of $\psi_p$. Finally, the mesh elements forming the pearlite region of the RVE were identified as those fulfilling the condition $d > d^*$. Figure 3 shows the function $\psi_p(d^*)$ computed based on the mesh of RVE12, together with a cross-section showing the estimated distribution of the pearlite in the matrix for a $\psi_p$ value of 50%. It is worth noting that the predicted distribution reproduces well the bull-eye pattern which is typical of mixed pearlitic-ferritic SGI microstructures, confirming that predictions based on the present approach are realistic.

Figure 3: Pearlite fraction in the matrix as a function of the critical distance $d^*$, calculated based on the mesh of RVE12. The inset shows a cross-section of the same RVE that depicts the estimated distribution of the pearlite (green) and of the ferrite (red) for a $\psi_p$ value of 50%.
2.2.2 Si micro-segregation

According to the simplified uni-nodular model (Lesoult et al., 1998), solidification of eutectic SGI can be described in terms of individual solidification units (SU), each consisting of a spherical graphite nodule that grows inside an austenite shell surrounded by liquid metal (see Figure 4). As solidification proceeds, the Si content in the liquid decreases progressively, due to the positive Si partition coefficient $k$ in temperature range of the stable eutectic reaction. This fact, combined with the low diffusivity of Si in the solid phase, leads to a Si concentration $w_{si}$ in the final matrix that is, to a first approximation, a function of the distance $d$ from the surface of the nodule (Lacaze et al., 2016). The specific shape of this function can be estimated based on Scheil’s equation (Lacaze et al., 2016), which can be written as:

$$w_{si}(f_s) = w_{si}^0 (1 - f_s)^{k-1}$$  \hspace{1cm} (1)

where $f_s$ represents the solid fraction and $w_{si}^0$ denotes the Si concentration at the nodule-matrix interface. For the uni-nodular model, the solid fraction can be expressed in terms of $d$ and of the distance $D$ between the nodule surface and the outer boundary of the SU (see Figure 4):

$$f_s = \left(\frac{d}{D}\right)^3$$  \hspace{1cm} (2)

In this expression, the overbars on $d$ and $D$ indicate that both quantities have been normalized with respect to the nodule equivalent radius $r_{eq}$, computed based on the nodule volume $V_n$ as

$$r_{eq} = \frac{3\sqrt{3V_n}}{4\pi}$$  \hspace{1cm} (3)

By inserting Eq. (2) into Eq. (1), the Si concentration as a function of the normalized distance from the nodule surface is obtained:

$$w_{si}(\tilde{d}) = w_{si}^0 \left(1 - \left(\frac{\tilde{d}}{D}\right)^3\right)^{k-1}$$  \hspace{1cm} (4)

In principle, Eq. (4) applies to a single SU. In order to make it applicable to an RVE containing multiple nodules, additional assumptions were introduced in the present work as follows. First, it was assumed that each nodule is associated with a SU and the size of the
latter is proportional to the equivalent radius \( r_{eq} \) of the former. This assumption, which ensures that the overall Carbon concentration is the same in all SUs, implies that \( D \) is also proportional to the SU size. Therefore, the parameter \( \bar{D} \) appearing in Eq. (4) becomes independent of the specific SU, meaning that \( w_{Si} \) depends on the spatial position via \( \bar{d} \) only. This last quantity was defined, for a generic point \( x \) in the matrix, by the equation

\[
\bar{d}(x) = \begin{cases} 
\bar{d}(x) & \text{if } \bar{d}(x) \leq \bar{d}^{cr} \\
\bar{d}^{cr} & \text{if } \bar{d}(x) > \bar{d}^{cr}
\end{cases}
\]

where the distance function \( \bar{d}(x) \) is computed as

\[
\bar{d}(x) = \min \left\{ \frac{d^1(x)}{r^1_{eq}}, \frac{d^2(x)}{r^2_{eq}}, \ldots, \frac{d^n(x)}{r^n_{eq}} \right\}
\]

In this last expression, \( d^i \) and \( r^i_{eq} \) denote the distance to and equivalent radius of the nodule \( i \), respectively, and \( n \) indicates the total number of nodules in the RVE. From a physical standpoint, the meaning of Eq. (6) is that the point \( x \) is associated with the SU that has the lowest solid fraction when the corresponding solidification front reaches \( x \), see Eq. (2).

Concerning the threshold \( \bar{d}^{cr} \) in Eq. (5), it was introduced to account for the inaccuracy of Scheil’s model towards the latest stages of solidification. Its value was defined by the condition

\[
V(\bar{d}^{cr}) = 0.95 \times V_{mat}
\]

where the function \( V(s) \) corresponds to the volume occupied by all the matrix points satisfying the condition \( \bar{d}(x) < s \).

A Python script was developed to prescribe the Si concentration in all the mesh elements forming the matrix of RVE12, under the assumption that no pearlite forms during the eutectoid reaction. The script applies a distance map algorithm repetitively to compute \( \bar{d} \) according to Eq. (6) at the element centroids, after which the Si concentration is estimated using Eqs. (4) and (5). It is worth remarking that, among the three RVEs described in Section 2.1, RVE12 was the only one used to study the impact of the Si micro-segregation.

With respect to the values of the parameters entering Eq. (4), the value of \( k \) was taken from the literature (Kagawa and Okamoto, 1980). Conversely, the values of \( w_{Si}^0 \) and \( \bar{D} \) were set
based on two requirements. The first was to have an average Si concentration in the matrix \( w_{Si}^{avg} \) of 2.2 wt\%. The second consisted in achieving a ratio between maximum and minimum Si concentration \( w_{Si}^{max} / w_{Si}^{min} \) equivalent to the one that can be expected in a real SGI with the same \( w_{Si}^{avg} \). Based on a previous segregation study (Freulon et al., 2016), \( w_{Si}^{max} \) and \( w_{Si}^{min} \) were estimated to be 2.8 wt\% and 0.8 wt\%, respectively. Therefore, the ratio between the two was prescribed to be 3.5. It is worth remarking that the choice of prescribing the ratio \( w_{Si}^{max} / w_{Si}^{min} \) was made because two parameters did not allow imposing distinct conditions on \( w_{Si}^{avg} \), \( w_{Si}^{max} \) and \( w_{Si}^{min} \) simultaneously. To overcome this limitation, a test was conducted where the Scheil-based model, Eq. (4), was replaced with a three-parameter parabolic function of the form

\[
w_{si}(\bar{d}) = w_{si}^0 - p_1 \bar{d} - p_2 \bar{d}^2
\]  

(8)

which, however, has no clear physical basis. The values of the parameters entering the Scheil-based model, Eq. (4), and the parabolic model, Eq. (8), are summarized in Table 1.

<table>
<thead>
<tr>
<th></th>
<th>Scheil-based model, Eq. (4)</th>
<th>Parabolic model, Eq. (8)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k )</td>
<td>( w_{Si}^0 ) [%]</td>
<td>( w_{si}^0 ) [%]</td>
</tr>
<tr>
<td></td>
<td>( \bar{D} )</td>
<td>( p_1 ) [%]</td>
</tr>
<tr>
<td>1.55</td>
<td>2.45</td>
<td>2.80</td>
</tr>
<tr>
<td></td>
<td>2.07</td>
<td>0.296</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.352</td>
</tr>
</tbody>
</table>
2.3 Constituent material models

As mentioned in the introduction, gradients in mechanical properties exist inside the graphite nodules. However, when the SGI is subjected to tensile loading, the nodules tend to separate from the matrix (Iacoviello et al., 2019) and the effect of these gradients on the material response becomes negligible as soon as the macroscopic strain exceeds ≈ 0.1 % (Andriollo et al., 2019). Consequently, in the present investigation the nodules were modelled as homogeneous and isotropic. A linear thermo-elastic constitutive law was chosen, characterized by a Young’s modulus \( E \) of 15 GPa, a Poisson’s ratio \( \nu \) of 0.3 and a thermal expansion coefficient \( \alpha \) of \( 3.8 \times 10^{-6} \text{ ºC}^{-1} \).

The interface between the nodules and the matrix was modelled using the surface-based cohesive formulation available in ABAQUS. The traction-separation law was assumed linear elastic with constant normal stiffness 10 MPa/µm and shear stiffness 5 MPa/µm. As discussed in Andriollo et al. (2019), this assumption was introduced to represent the weak bonding between the nodules and the matrix.

Concerning the matrix, its constitutive behavior was described via an isotropic, rate-independent elastoplastic model with isotropic hardening. The model is based on a von Mises-type yield function:
\[ \Phi = \sqrt{3J_2(\sigma)} - \sigma_y(\varepsilon_{eq}^{pl}) \leq 0 \tag{9} \]

where \( J_2(\sigma) \) is the 2\textsuperscript{nd} deviatoric invariant of the Cauchy stress \( \sigma \) and \( \varepsilon_{eq}^{pl} \) is the equivalent plastic strain. The function \( \sigma_y(\varepsilon_{eq}^{pl}) \) describes the hardening behavior and it is assumed to have the following expression:

\[ \sigma_y = Q_0 + Q_\infty(1 - e^{-b\varepsilon_{eq}^{pl}}) \tag{10} \]

with \( Q_0 \), \( Q_\infty \) and \( b \) as material parameters. The standard additive decomposition of the strain into an elastic, thermal and plastic part is considered, where the elastic strain is related to the Cauchy stress via Hooke’s law. The evolution of the plastic strain \( \varepsilon_p \) is dictated by the flow rule:

\[ \dot{\varepsilon}_p = \lambda \frac{\partial \Phi}{\partial \sigma} = \lambda \frac{3}{2} \frac{s}{\sigma_y} \tag{11} \]

where \( s \) is the deviatoric part of the Cauchy stress, \( \lambda \) is the plastic multiplier and the operator \( (\cdot) \) denotes a rate.

The model just presented was assumed to apply to both the ferrite and the pearlite, although with the two different sets of parameters listed in Table 2. In this respect, the thermo-elastic parameters were taken from the literature, whereas the plastic parameters were calibrated by fitting the tensile curves reported in Figure 5. The parameters of the ferrite were assumed to relate to a Si concentration of 2.2 wt\%, which is the average matrix concentration considered in section 2.2.2. Any deviation \( \Delta w_{Si} \) of the Si concentration from the average was assumed to affect only the values of \( Q_0 \) and \( Q_\infty \), according to the linear expressions

\[ \Delta Q_0 = m_0 \times \Delta w_{Si} \]
\[ \Delta Q_\infty = m_\infty \times \Delta w_{Si} \tag{12} \]

The values of the coefficients \( m_0 \) and \( m_\infty \) were set to 57.9 MPa/wt\% and 76.2 MPa/wt\%, respectively, based on a linear fit of the data reported in Abramowitz and Moll (1970).
Table 2 – Parameters of the elastoplastic model describing the behavior of the SGI matrix.

<table>
<thead>
<tr>
<th></th>
<th>$E$ [GPa]</th>
<th>$\nu$</th>
<th>$\alpha$ [°C$^{-1}$]</th>
<th>$Q_0$ [MPa]</th>
<th>$Q_\infty$ [MPa]</th>
<th>$b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ferrite</td>
<td>205</td>
<td>0.29</td>
<td>$1.35 \times 10^{-5}$</td>
<td>295</td>
<td>543</td>
<td>139</td>
</tr>
<tr>
<td>Pearlite</td>
<td>205</td>
<td>0.29</td>
<td>$1.35 \times 10^{-5}$</td>
<td>365</td>
<td>926</td>
<td>145</td>
</tr>
</tbody>
</table>

Figure 5: Tensile 1st Piola-Kirchhoff stress vs. engineering strain curves corresponding to the ferrite and pearlite phases of SGI. Data taken from Collini (2004).

2.4 Computational homogenization

In order to evaluate the impact of the amount of pearlite and of the Si micro-segregation, each RVE described in section 2.1 was subjected to two loading steps. First, the processing step representing the final part of the solid-state cooling was simulated by prescribing a uniform temperature change from 500 °C to 20 °C. This was done in order to include the residual stress state associated with the mismatch in thermal contraction between the nodules and the matrix into the subsequent simulations (Zhang et al., 2019). Next, tensile loading up to a macroscopic strain of 5 % was applied in order to evaluate the mechanical response of the RVE.
During both loading steps, periodic boundary conditions were imposed on the boundaries of the RVE. That is, considering any two equivalent points \( x \) and \( x + l \) lying on opposite faces of the RVE and separated by the RVE side length \( l \), the following constraints were imposed:

\[
\mathbf{u}(x + d) = \mathbf{u}(x) + \nabla \mathbf{u}_M \cdot l
\]

\[
t(x + d) = -t(x)
\]

(13)

where \( \mathbf{u} \) and \( t \) denote displacement and surface traction and \( \nabla () \) denotes the gradient operator. The vector \( \mathbf{u}_M \) was assumed to represent the displacement of the material at the macroscopic scale, in accordance with the general framework of computational homogenization (Matouš et al., 2017). In order to enforce Eq. (13) on the non-periodic mesh of the RVE, the approach suggested by Nguyen et al. (2012) was followed. In essence, this approach consists in expressing the displacement of the RVE boundary nodes in terms of Lagrange polynomials and then using the coefficients of the latter to enforce periodicity.

During the cooling step, the quantity \( \nabla \mathbf{u}_M \) in Eq. (13) was left unconstrained. Conversely, during the subsequent tensile loading the following constraint was imposed:

\[
\mathbf{e}_x \cdot (\nabla \mathbf{u}_M) \cdot \mathbf{e}_x = \epsilon
\]

(14)

where \( \epsilon \) is the macroscopic uniaxial strain, \( \mathbf{e}_x \) is the unit vector along the Cartesian x-axis and \((\cdot)\) indicates the inner product. For a given value of \( \epsilon \), the corresponding macroscopic uniaxial stress \( \sigma \) was defined as

\[
\sigma = \int_{V_{RVE}} \mathbf{e}_x \cdot \mathbf{\sigma} \cdot \mathbf{e}_x \, dV
\]

(15)

where \( V_{RVE} \) is the volume of the entire RVE.

The RVE effective response, Eq. (15), was used to make a preliminary assessment of the quality of the RVEs considered in the present work. To this end, the RVE12 with \( \psi_p = 50 \% \) and uniform Si concentration was considered. First, tensile loading was simulated along different directions by replacing \( \mathbf{e}_x \) with \( \mathbf{e}_y \) and \( \mathbf{e}_z \) in Eqs. (14) and (15) in order to check the level of isotropy of the RVE, showing almost no differences. Subsequently, the size of the RVE was tested by comparing its response to that of a larger RVE of size 400x400x400 \( \mu m^3 \), again resulting in negligible variations. Based on these results, the size and level of isotropy of the RVEs used in the present investigation were considered appropriate.
Finally, the accuracy of the developed RVEs was assessed by comparing the effective responses of RVE9 with $\psi_p = 75\%$ and of RVE15 with $\psi_p = 25\%$ with the experimental tensile curves reported in (Collini, 2004) for two SGI grades having similar graphite and pearlite fractions. The comparison is shown in Figure 6 and indicates that, despite some discrepancies, the effective response of the two RVE models can be considered realistic, which is deemed sufficient for the present purposes.

![Figure 6: Comparison between the macroscopic tensile curves predicted by two of the present RVE models and the corresponding experimental data by Collini (2004).](image-url)
3. Results and discussion

The procedure introduced in section 2.2.1 to estimate the spatial distribution of the pearlite is a generalization of the previous approaches based on artificial microstructures (Collini et al., 2019; Rodriguez et al., 2018). Conversely, the technique described in section 2.2.2 to estimate the Si micro-segregation over a volume containing multiple nodules is one of a kind in the literature. Consequently, an examination of the predicted segregation pattern and of its implication on the spatial dependence of the matrix properties is deemed necessary before focusing on the impact of the Si micro-segregation and of the pearlite content on the SGI yield stress.

3.1 Si micro-segregation pattern

Figure 7 (a) shows the function \(w_{si}(\tilde{d})\), corresponding to Eqs. (4) and (5), used to estimate the Si concentration in the matrix of RVE12. The function obtained by replacing the Scheil-based model, Eq. (4), with the parabolic model, Eq. (8) is reported in the same figure. It can be seen that, as expected, the parabolic model can reproduce the correct values of \(w^\text{max}_{si}\) and \(w^\text{min}_{si}\) (set to 2.8 wt% and 0.8 wt%, see section 2.2.2) whereas the Scheil-based model underpredicts them. However, for values of \(\tilde{d}\) between 0.8 and \(\tilde{d}^{cr}\), the Si concentration predicted with the Scheil-based model is actually higher than that predicted with the parabolic model. This feature can be explained by the characteristic shape of the original Scheil’s concentration function, Eq. (1), which is known to be relatively flat when the solid fraction is low, i.e. close to the nodules, and very steep towards the latest stages of solidification (Hattel et al., 2005). In Figure 7 (a), it can also be observed that the maximum value of \(\tilde{d}\) is \(\approx 4.7\), which is more than double the value of \(\tilde{d}^{cr}\). Concerning this, it is worth remarking that the regions characterized by values of \(\tilde{d}\) significantly larger than \(\tilde{d}^{cr}\) represent only a small fraction of the matrix volume. This fact is demonstrated by the plot of Figure 7 (b), which shows the Si concentration as a function of \(V(\tilde{d})\) (see Section 2.2.2 for the definition of this quantity). The same plot reveals that the Si concentration predicted with the parabolic model is larger than the average in more than 60 % of the matrix volume. This percentage increases to \(\approx 75 \%\) if the Scheil-based model is considered. Finally, Figure 7 (c) highlights the extent
to which the Si micro-segregation affects the matrix plastic properties. Specifically, the figure shows the value of $R_{p02}$, the proof stress at 0.2 % permanent deformation, as a function of $V(\bar{d})$. It can be seen that, depending on whether the Scheil-based model or the parabolic model is considered, the value of $R_{p02}$ near the nodules is between 15 MPa and 35 MPa larger than that corresponding to $w_{Si}^{avg}$. At the same time, both models predict a drop in $R_{p02}$ ranging from 50 MPa up to almost 100 MPa in the 10 % of the matrix volume that is most distant from the nodules. The consequence of this gradient in plastic properties on the effective response of SGI upon tensile loading will be discussed in the next section.

In order to verify whether the estimated Si micro-segregation pattern is realistic, a comparison is made with the Si concentration measurements of Vazehrad et al. (2015), conducted on an eutectic SGI with the same value of $w_{Si}^{avg}$ used in the present work, i.e. 2.2 wt%. Figure 8 (a) shows the Si map obtained by the former authors over a section of size 400x600 µm². By contrast, Figure 8 (b) shows the Si concentration on a diagonal section of RVE12 estimated with the procedure proposed in Section 2.2.2, assuming that the Scheil-based model applies. Qualitatively, the values of the two Si maps seem to differ significantly near the nodules, where the peak values and gradients seem to be underestimated. While the relatively flat Si concentration profile predicted near the nodules cannot be changed, an attempt to increase its absolute values was made by prescribing $w_{Si}^{max}$ instead of $w_{Si}^{max} / w_{Si}^{min}$ while selecting the parameters of Eq. (4) – see the last paragraph of Section 2.2.2. However, this choice turned out to be incompatible with the constraint on $w_{Si}^{avg}$. It is worth noting that the peak values and the corresponding gradients are captured better if the parabolic model is used, as Figure 8 (c) reveals. Probably, this has to do with the possibility of enforcing $w_{Si}^{max}$, but also with the different curvature of the corresponding function $w_{Si}(\bar{d})$ pointed out in Figure 7 (a). The qualitatively good agreement obtained by using the parabolic model suggests that the present approach could be extended to capture the concentration gradients of the other chemical elements, e.g. Mn, whose segregation patterns are connected to that of Si.
Figure 7: Functions describing the matrix Si concentration and yield stress, according to the Scheil-based model and the parabolic model. (a) Si concentration as a function of the distance $\tilde{d}$. (b) Si concentration as a function of the volume $V(\tilde{d})$. (c) Proof stress as a function of the volume $V(\tilde{d})$. 
Figure 8: Qualitative validation of the method proposed in Section 2.2.2 to estimate the Si micro-segregation in the SGI matrix. (a) Si concentration map determined experimentally by Vazehrad et al. (2015). (b) Contour of the predicted Si concentration on a diagonal section of RVE12, assuming that the Scheil-based model, Eq. (4), applies. (c) Same as (b), but assuming that the parabolic model, Eq. (8), applies. The color code is the same in (a), (b) and (c).

### 3.2 Effect of Si micro-segregation on SGI yield stress

Figure 9 shows the effective tensile response of the RVE12 predicted via the computational homogenization procedure described in Section 2.4. Three cases are considered in the figure: uniform Si concentration in the ferrite matrix, Si micro-segregation estimated with the Scheil-based model, Eqs.(4)-(6), and Si micro-segregation estimated with the parabolic model model, Eqs. (5), (6) and (8). Note that the average Si concentration is the same in all three cases. It is evident that the Si micro-segregation has very little impact on the predicted tensile curves. The figure inset reveals a limited increase of the tensile stress near the macroscopic yield point, which can be explained by the segregation-induced local increase in the matrix yield stress close to the nodules – see Figure 7 (c). Indeed, this delays the onset of microscopic plasticity in the SGI matrix, which is known to begin at the nodules (Fernandino and Boeri, 2019; Kasvayee et al., 2016). However, by comparing Figure 10 (a) to Figure 10 (b), which show the equivalent plastic strain at the microscale when the Si micro-segregation is either neglected or accounted for, the conclusion is that this effect is minimal. Therefore, with respect to the second question raised in the introduction, it can be stated that the spatial variation in the matrix plastic properties associated with the Si micro-segregation is not
expected to influence the SGI yielding behavior significantly. A word of caution is necessary to remark that this conclusion might not hold at larger deformations. Indeed, the Si micro-segregation is expected to cause local embrittlement of the ferrite near the nodules. This effect, which is not accounted for in the present model, might be further enhanced by local peaks in the stress triaxiality (Collini et al., 2019), ultimately leading to a reduction in the macroscopic ductility.

Figure 9: Impact of the estimated Si micro-segregation on the macroscopic stress vs. macroscopic strain effective response of RVE12. The inset shows a magnification of the region near the yield point.
3.3 Effect of pearlite content on SGI yield stress

Figure 11 shows the SGI effective proof stress $R_{p0.2}$ computed for three different values of $\psi_G$ – corresponding to simulations run using RVE9, RVE12 and RVE15 – considering a pearlite fraction in the matrix varying between 0 % and 100 %. It is worth noting that some of the combinations are not realistic. However, one of the advantages of the present approach is that even microstructures that are not obtainable with standard manufacturing processes can be investigated. With respect to Figure 11 (a), it can be observed that $R_{p0.2}$ varies almost linearly with $\psi_G$ for a constant value of $\psi_P$. By contrast, Figure 11 (b) indicates that, for a given value of $\psi_G$, $R_{p0.2}$ tends to increase more rapidly with $\psi_P$ when the value of this last quantity is high. The reason is that, as mentioned previously, yielding of the matrix upon tensile loading starts at the nodules. When the value of $\psi_P$ is low, a small increase of $\psi_P$ means that a small amount of ferrite is replaced by the stronger pearlite in regions far from the nodules, where yielding occurs only at a late stage. Conversely, when the value of $\psi_P$ is high, a small increase of $\psi_P$ means that the ferrite is replaced by the pearlite in regions close to the nodules, where the pearlite is more effective in blocking the formation of the plastic shear bands. The non-linearity associated with this phenomenon might be one of the reasons...
behind the positive curvature of the relationship between proof stress and pearlite fraction that is characteristic of SGI (see the experimental data reported in Figure 12). As already pointed out, it is not possible to change $\psi_G$ and $\psi_P$ independently in a real casting process. The data of Figure 1, which relate to a fixed overall Carbon concentration, show that $\psi_G$ decreases from $\approx 15\%$ down to as little as $\approx 9\%$ if a fully ferritic matrix is replaced by a fully pearlitic one, due to the large amount of Carbon that remains in the matrix by the end of the eutectoid reaction – see the Appendix for a quantitative explanation of this phenomenon. Based on the results presented in Figure 11, this change in $\psi_G$ can be expected to account for as much as $\approx 1/3$ of the overall increase in $R_{p0.2}$. Therefore, with the conversion of the matrix from ferrite to pearlite, only a part of the gain in the SGI strength comes from the additional strength of the pearlite. This fact needs to be taken into consideration when assessing the properties of the pearlite and of the ferrite based on changes in the macroscopic properties of SGI specimens.

Figure 11: Impact of the graphite and pearlite fraction on the effective proof stress of SGI, as predicted by the RVE-based models. (a) Proof stress as a function of $\psi_G$. (b) Proof stress as a function of $\psi_P$. All the values are normalized by the RVE-predicted proof stress at $\psi_G = 11.8 \%$ and $\psi_P = 50 \%$. 
Figure 12: Experimental relationship between the SGI proof stress and the pearlite fraction, measured using either Sn or Cu as pearlite promoter. Data from (Ductile Iron Society, 2013).
4. Conclusions

A method to construct 3D RVE models of the nodular cast iron microstructure that can account for the heterogeneous nature of the matrix was proposed and used to investigate two open issues related to the material micro-mechanical behavior. The method consists of reconstructing the graphite morphology first via X-ray computed tomography and subsequently estimating the spatial distribution of the matrix heterogeneities via dedicated distance functions. The main advantage compared to previous approaches is the possibility to generate a wide spectrum of realistic distributions of the matrix heterogeneities in a simple and fast way, thereby bringing optimized microstructural design of SGI one step closer. With respect to the two case studies considered, the main conclusions can be summarized as follows:

- Qualitatively, the predicted Si micro-segregation pattern resembles that determined experimentally. Better results are obtained when the Si distribution is estimated via the empirical parabolic model instead of via the mechanistic Scheil-based model. This might be a consequence of the assumptions used to extend the equations of the unimodular model to an RVE containing several nodules.

- Based on the predicted Si micro-segregation pattern, a drop in $R_{p02}$ ranging from 50 MPa up to almost 100 MPa can be expected in the 10% of the matrix volume that is most distant from the nodules – assuming that the matrix is fully ferritic. However, this gradient in mechanical properties does not seem to affect significantly the macroscopic yielding behavior of SGI during tensile loading.

- For a fixed overall C concentration, if the matrix pearlite content is increased the corresponding decrease in the nodules’ volume fraction can account for as much as 1/3 of the obtained increment in the material macroscopic proof stress. Therefore, care should be taken when assessing the properties of the pearlite and of the ferrite based on changes in the macroscopic properties of SGI specimens.
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Appendix: Variation of the nodules’ volume during the eutectoid reaction

During the eutectoid reaction the total volume occupied by the nodules increases. The reason is the diffusion of Carbon atoms from the matrix to the nodules due to the lower solubility of this element in the ferrite compared to the austenite. As mentioned in Section 2.2.1, if there is not sufficient time for this diffusion process to occur before the metastable eutectoid temperature is reached, pearlite forms instead of ferrite. As the Carbon content of the pearlite is higher than that of the ferrite, it follows that the higher the amount of pearlite, the lower the increase in the nodules’ volume. This phenomenon can be quantified by considering that the amount of Carbon in the microstructure before and after the eutectoid transformation must be the same. Therefore, assuming that the nodules are entirely made of Carbon, the following equation holds:

\[ V_{n}^{in} \rho_{n}^{in} + V_{\gamma} \rho_{\gamma} w_{C,\gamma} = V_{n}^{fin} \rho_{n}^{fin} + V_{\alpha} \rho_{\alpha} w_{C,\alpha} + V_{p} \rho_{p} w_{C,p} \]  

(A.1)

where the symbols \( V \), \( \rho \) and \( w_{C} \) denote volume, density and Carbon mass fraction, respectively, of a given microstructural constituent, the subscripts \( n \), \( \gamma \), \( \alpha \) and \( p \) denote nodules, austenite, ferrite and pearlite, respectively, and the superscripts \( in \) and \( fin \) denote evaluation of the quantity before and after the eutectoid reaction.

By assuming that \( \rho_{n}^{in} \approx \rho_{n}^{fin} \approx \rho_{n} \), Eq. (A.1) can be rewritten as

\[ \rho_{n}(V_{n}^{fin} - V_{n}^{in}) = V_{\gamma} \rho_{\gamma} w_{C,\gamma} - V_{\alpha} \rho_{\alpha} w_{C,\alpha} - V_{p} \rho_{p} w_{C,p} \]  

(A.2)

A mass balance similar to Eq. (A.1) for Iron provides

\[ V_{\gamma} \rho_{\gamma} w_{Fe,\gamma} = V_{\alpha} \rho_{\alpha} w_{Fe,\alpha} + V_{p} \rho_{p} w_{Fe,p} \]
⇒ \( V_{\alpha} \rho_{\alpha} = \frac{(V_{\gamma} \rho_{\gamma} w_{Fe,\gamma} - V_{p} \rho_{p} w_{Fe,p})}{w_{Fe,\alpha}} \) (A.3)

Insertion of Eq. (A.3) into Eq. (A.2) followed by straightforward algebra provides

\[
(V_{n}^{fin} - V_{n}^{in}) = V_{\gamma} \frac{\rho_{\gamma}}{\rho_{n}} \left( w_{C,\gamma} - \frac{w_{Fe,\gamma} w_{C,\alpha}}{w_{Fe,\alpha}} \right) - V_{p} \frac{\rho_{p}}{\rho_{n}} \left( w_{C,p} - \frac{w_{Fe,p} w_{C,\alpha}}{w_{Fe,\alpha}} \right)
\]

which demonstrates that the larger the volume of the pearlite formed, the smaller the increase of the nodules’ volume during the eutectoid reaction.

References


