Microstructural model for the time-dependent thermo-mechanical analysis of cast irons

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In this paper, a multiscale modelling approach is followed for the modelling of time and temperature dependent behaviour of compacted graphite cast iron (CGI) material. Cast irons are often used in heavy duty machinery parts subjected to elevated temperatures for prolonged periods of time. This, in combination with its complex heterogeneous microstructure, plays the crucial role in determining the life time of the material. In this work a 2D microstructural model of CGI is developed. The geometry is based on the micrographs of the material. The pearlitic matrix is modelled with the temperature dependent elasto-visco-plastic model calibrated on the pearlitic steel experiments. The graphite particles are modelled as anisotropic elastic. The results of the simulations of tensile and stress relaxation tests at different temperatures between 20\degree C and 500\degree C show that the macroscopic mechanical behaviour of the material deteriorates rapidly above 350\degree C. At the microstructural scale, the anisotropic graphite particles act as stress concentrators promoting the formation of strain percolation paths, that become more critical at higher temperatures.

1 Introduction

Nowadays, several industrial applications rely on components operating at high temperatures over long periods of time. These applications, require materials which can endure the demanding mechanical conditions as well as the often extreme thermal and environmental loads. Cast iron is a typical example of such a material, which has a good compromise between its mechanical and thermal properties. Therefore, it is extensively used for high temperature thermo-mechanical applications. The most prominent examples hereof can be found in the automotive industry, e.g. in cylinder heads and blocks, exhaust manifolds and disk breaks.

The good combination of mechanical and thermal properties of cast iron ensues from its microstructure, composed of graphite inclusions embedded in a ferrite/pearlite matrix. The morphology of the graphite inclusions plays a fundamental role in defining the material properties \cite{1,2} and is frequently used to identify the different cast irons as: Nodular or Spheroidal Graphite Iron (SGI); Compacted or Vermicular Graphite Iron (CGI) and Flake or Lamellar...
Graphite Iron (FGI). In particular, in CGI and FGI the graphite particles form a 3D interconnected network that, combined with graphite’s high thermal conductivity, yields thermal properties superior to those of steels. Nevertheless, the presence of the graphite inclusions proves to be detrimental for the mechanical properties, because they introduce stress concentration sites promoting damage initiation during the early stages of the material’s lifetime [3–9].

At elevated temperatures, the response of the material becomes more sensitive to temperature and time. This is reflected in thermal softening and higher creep or stress relaxations rates [2, 10–21]. Combined with cast iron’s highly heterogeneous microstructure, this may significantly limit the thermo-mechanical life performance of the material by accelerating damage initiation and propagation. Therefore, it is imperative to understand the elevated temperature behaviour of cast iron at different length and time scales in order to provide accurate lifetime predictions of the material and design engineering components accordingly.

In recent years, a few phenomenological models for thermo-mechanical analyses of cast irons have been developed [22–26]. The main limiting requirement of these models is that they rely on a large amount of experimental data. They do not directly account for the influence of microstructural features on the material thermo-mechanical response (i.e. morphology and anisotropy of the graphite inclusions, matrix time and temperature dependent thermo-mechanical behaviour, interaction between the phases and interface behaviour).

In a different approach, microstructural modelling has been used in the past to study the mechanical response of cast irons: SGI [3, 27–33], CGI [34–38] and FGI [39]. In addition to the graphite morphology, typical for each cast iron type, other microstructural information has been included in these models:

- graphite anisotropy, to evaluate its influence on the local and global mechanical and thermo-mechanical response of FGI and CGI [38, 39],
- matrix time-dependent response for high strain rate applications (e.g. machining) [31–33, 36, 37, 40],
- graphite/matrix interface [39, 40] and damage [36, 37, 40].

In spite of the vast amount of work done, hardly any attention was given to the combined effect of time and temperature on the microstructural mechanical response of cast iron. Therefore, a microstructural model for the elevated temperature mechanical analyses of cast irons is here proposed. The model is aimed at transient conditions such as the ones present in engines during their operating life in a temperature range between 20 °C and 500 °C. The point of departure for the present analyses is the cast iron microstructural models presented in [39] and [38], where the temperature dependent thermal and mechanical properties of the graphite and matrix are included, as well as the morphology and anisotropy of the graphite inclusions. In this work, the time and temperature dependent behaviour of the pearlitic matrix is added by means of the thermo-viscoplastic model described in [41]. The developed microstructural model is dedicated here to CGI but can be adapted to FGI or SGI in a straightforward manner by introducing the appropriate morphology of the graphite inclusions.

The goal of this paper is to provide insight into the time-dependent response of CGI for temperatures up to 500 °C. The role played by the microstructure and temperature on the behaviour of the material at both the macro and micro scales is investigated. In order to assess the validity of the model parameters identified on a pearlitic steel for the pearlitic matrix,
micro-indentation tests have been performed. The results from the elevated temperature analyses indicate that the sensitivity of the material to temperature rapidly increases for temperatures above 400 °C. The higher temperature sensitivity is driven by the thermal recovery in the pearlitic matrix. The combination of time, temperature and microstructural heterogeneity leads to higher local plastic deformation and earlier damage initiation at the microstructural level.

This paper is organized as follows. In the next section the CGI microstructural model is introduced. The constitutive behaviour of graphite is discussed in Section 2.1. In Section 2.2, the micro-indentation tests on C75 pearlitic steel and the CGI pearlite matrix are presented together with the pearlite model parameters. The thermo-viscoplastic model for the pearlitic matrix is described in Section 2.3. Then, in Section 3, the elevated temperature analyses on CGI are discussed starting with the tensile tests in Section 3.1, followed by the numerical stress relaxation tests in Section 3.2. The main conclusions are summarized in Section 4.

2 CGI microstructural model

The cast iron investigated in this paper is CGI with a carbon content between 3.5 and 3.8 wt% and a graphite volume fraction between 10 and 12% [42]. The matrix is composed of pearlite (95%) and ferrite (5%). In CGI, the graphite particles predominantly reveal a vermicular morphology, even though nodular particles are always present [43]. Due to the complex and highly heterogeneous 3D morphology of the vermicular graphite particles, it is challenging and computationally demanding to incorporate all relevant microstructural features present in CGI in a descriptive model.

Here, as in [38] a Finite Element Method (FEM) based computational homogenization approach [44] is used to create a microstructural model for CGI. The Representative Volume Element (RVE) geometry is extracted from a 2D scanning electron microscope (SEM) micrograph. A 2D finite element mesh of this image is obtained by converting each pixel into a finite element. The different phases (matrix or graphite) are identified based on the pixel grey scale level. The main advantage of this method is that the 2D shape of the graphite particles is captured with the experimental resolution. One drawback of this 2D model is that it disregards the inherent 3D nature of the CGI microstructure. Nevertheless, these simplifications make it possible to incorporate microstructural details in the microstructure for a RVE size that would be computationally intractable in 3D, especially in the non-linear regime considered here. The CGI microstructure and the corresponding FEM model are shown in Figure 1. The size of the RVE is defined such that it includes a sufficient number of graphite particles with a graphite area fraction of 10.2% (typical for CGI), whereas the size is not too large to compromise the computations.

2.1 Graphite

In graphite, anisotropy dominates both the mechanical and thermal properties. This anisotropy is related to graphite’s layered structure with strong covalent bonds within the basal planes and weak van der Waals bonds between them, which makes graphite a transversely isotropic material (Figure 1.c) [2,5,45–49].

In previous work [38,39], the pronounced effect of graphite’s anisotropy on the local and global response of cast iron has been studied in detail, both numerically and experimentally.
Graphite’s anisotropy within cast irons is related to the crystalline structure of the graphite particle which in turn is defined by the particle principal growth mechanism [2, 45, 46, 48, 49]. The latter also controls the morphology of the particle. In nodular particles, the principal growth direction is the “c” crystallographic direction, which leads to a “onion” type crystalline structure. On the other hand, lamellar particles grow primarily in the “a” crystallographic direction leading to a crystalline structure in which the graphite platelets are mostly oriented parallel to the “a” direction [2, 45–47].

In CGI, the predominantly vermicular graphite particles have a growth mechanism that alternates between the “a” and “c” directions. This leads to particles in which some parts resemble the graphite crystalline structure of nodular graphite, while in other parts it resembles the crystalline structure of lamellar graphite [2, 45, 46, 49]. The nodular structure generally occurs close to the nucleus of the particle, whereas the lamellar type structure generally appears in the elongated “worm” shaped branches of the particle. In these parts, a more clearly oriented structure is present with stacked layers of graphite platelets running parallel to the graphite growth direction. It can therefore be reasonably assumed that the graphite in the elongated “worm” like branches of vermicular particles, behaves as transversely anisotropic, with its principal direction (i.e. “a” direction) oriented parallel to the particle growth direction (Figure 1.c). The corresponding elastic constants for graphite are given in Table 1. The remaining particles, will be assumed isotropic. The elastic constants for isotropic graphite are taken by averaging of the in-plane and out-of-plane properties of graphite, i.e. $E_{11} = E_{22} = 528$ GPa and $\nu_{12} = \nu_{23} = \nu_{31} = 0.0875$.

<table>
<thead>
<tr>
<th>Table 1</th>
<th>Graphite elastic constants: in-plane (directions 1 &amp; 2) and out-of-plane (direction 3) Young’s moduli, Poisson’s ratios and shear moduli [50].</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{11}$ = $E_{22}$ [GPa]</td>
<td>$E_{33}$ [GPa]</td>
</tr>
<tr>
<td>1020.4</td>
<td>36.364</td>
</tr>
</tbody>
</table>

2.2 Matrix

For the pearlite matrix, the thermo-viscoplastic model presented in [41] is used to describe the time-dependent behaviour of CGI. Because of the complexity of performing an independent model parameter identification process for pearlite within CGI, the material parameters as identified in [41] from elevated temperature tests (tensile and creep tests) on C75 pearlitic...
Steel (0.708 wt% percent of carbon) will be used here. To assess whether the pearlitic steel used for the model parameter identification is a valid substitute for the pearlite present in CGI, room temperature micro-indentation tests were performed on both materials. The results from the tests are shown in Table 2, indicating that there is an adequate agreement between both materials in terms of the Young’s modulus and the hardness.

<table>
<thead>
<tr>
<th>Material properties obtained by micro-indentation tests on pearlite in CGI and C75 pearlitic steel</th>
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<tbody>
<tr>
<td></td>
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<tr>
<td>Young’s modulus [GPa]</td>
</tr>
<tr>
<td>Hardness [GPa]</td>
</tr>
</tbody>
</table>

The pearlite thermo-viscoplastic model makes use of twelve material parameters: two elastic constants, $E$ and $\nu$, the thermal expansion coefficient $\alpha$, and nine parameters describing the viscoplasticity. The values of the Young’s modulus for different temperatures used here are given in Table 3 [51] and those of the thermal expansion coefficient in Table 4 [52]. Poisson’s ratio is assumed to be temperature independent and equal to 0.29, based on experimental evidence showing its minor temperature sensitivity in the considered temperature range [53, 54].

<table>
<thead>
<tr>
<th>Elastic modulus of steels for different temperatures [51]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$ [°C]</td>
</tr>
<tr>
<td>$E$ [MPa]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Thermal expansion coefficient of pearlitic steel for different temperature ranges [52]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$ [°C]</td>
</tr>
<tr>
<td>$\alpha$ [µm/m °C]</td>
</tr>
</tbody>
</table>

The remaining parameters, except for the melting temperature $T_m$ and activation energy $Q$, were determined from experimental data on C75 pearlitic steel (from monotonic tensile tests at different temperatures and creep tests at 420 °C). Details are given in [41]. The strain rate sensitivity and thermal function parameters are given in Table 5, and those corresponding to the yield stress, hardening and recovery functions are given in Table 6. The significance of the different parameters is discussed in the following subsection.

<table>
<thead>
<tr>
<th>Strain rate sensitivity and thermal function parameters</th>
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<tbody>
<tr>
<td>350</td>
</tr>
</tbody>
</table>

### 2.3 Pearlite thermo-viscoplastic model

The model developed by Pina et al. [41] is used here to account for the time and temperature dependent behaviour of the pearlitic matrix. The model is based on earlier work by Freed and Walker [55]. The viscoplastic strain rate is based on the Zener-Hollomon relation [56, 57], in
Table 6  Yield stress, hardening and recovery parameters.

<table>
<thead>
<tr>
<th>$\delta$</th>
<th>$D_0$ [MPa]</th>
<th>$h_D$ [MPa]</th>
<th>$m$</th>
<th>$\tau_y(T)$ [MPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.075</td>
<td>9.12</td>
<td>3133</td>
<td>0.38</td>
<td>324</td>
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<tr>
<td></td>
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<td>287</td>
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<td></td>
<td>275</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>240</td>
</tr>
</tbody>
</table>

The viscoplastic strain rate is obtained as the product of two functions: an Arrhenius type thermal function, and a function known as the Zener parameter. The thermal function accounts for the sensitivity of the viscoplastic strain rate to temperature, whereas the Zener parameter characterizes the strain rate sensitivity. This provides a simple way to incorporate the influence of temperature on the viscoplastic strain rate. The evolution of the internal variables due to isotropic hardening, as well as dynamic and thermal recovery are also taken into account.

2.3.1 Kinematics

In the present model the kinematics is described in terms of the right Cauchy-Green strain tensor $C = F^T \cdot F$, where $F = (\nabla_0 x)^T$ is the deformation gradient tensor with respect to the reference configuration, and $x$ the position vector in the current deformed configuration.

The material velocity is taken into account by the spatial velocity gradient tensor $L$ and its symmetric and skew-symmetric parts, i.e., the rate-of-deformation tensor $D$ and the spin tensor $\Omega$, respectively:

$$L = \dot{F} \cdot F^{-1} = D + \Omega, \tag{1}$$

where the superimposed dot denotes the material time derivative.

The rate of the right Cauchy-Green deformation tensor is determined by taking the material time derivative of $C$, that is:

$$\dot{C} = F^T \cdot \dot{F} + \dot{F}^T \cdot F = 2F^T \cdot D \cdot F. \tag{2}$$

The thermal and mechanical contributions to the thermo-mechanical deformation process are defined through the multiplicative decomposition of the deformation gradient tensor $F$ into a thermal part $F_{th}$ and a mechanical part $F_M$ [58]:

$$F = F_{th} \cdot F_M. \tag{3}$$

The tensor $F_M$ expresses the mapping from the reference configuration $\Omega_0$ to the intermediate mechanical configuration $\Omega_M$, and $F_{th}$ maps the deformation from $\Omega_M$ to the current configuration $\Omega$. The mechanical part $F_M$ is further decomposed into an elastic and a viscoplastic part via:

$$F_M = F_e \cdot F_{vp}. \tag{4}$$

The plastic flow is taken volume-preserving, i.e. $J_{vp} = \det(F_{vp}) = 1$ [59].
Considering equations (3) and (4), the expression for the spatial velocity gradient tensor \( L \) in terms of its thermal, elastic and viscoplastic parts can be obtained as an additive decomposition:

\[
L = L_e + L_{vp} + L_{th} = (D_e + \Omega_e) + (D_{vp} + \Omega_{vp}) + (D_{th} + \Omega_{th}),
\]

(5)

where \( L_e, L_{vp} \) and \( L_{th} \) are given by:

\[
L_e = F_{th} \cdot \dot{F}_e \cdot F_e^{-1} \cdot F_{th}^{-1}, \quad (6a)
\]

\[
L_{vp} = F_{th} \cdot F_e \cdot \dot{F}_{vp} \cdot F_{vp}^{-1} \cdot F_e^{-1} \cdot F_{th}^{-1}, \quad (6b)
\]

\[
L_{th} = \dot{F}_{th} \cdot F_{th}^{-1}. \quad (6c)
\]

Finally, an expression for the additive split of \( \dot{C} \) in its thermal, elastic and viscoplastic parts can be obtained by introducing equations (3) and (4) into (2). This yields:

\[
\dot{C} = \dot{C}_e + \dot{C}_{vp} + \dot{C}_{th},
\]

(7)

with

\[
\dot{C}_e = F^T \left( F_{th} \cdot \dot{F}_e \cdot F_e^{-1} \cdot F_{th}^{-1} + F_{th}^{-T} \cdot F_e^{-T} \cdot \dot{F}_e \cdot F_{th}^T \right) \cdot F
\]

(8a)

\[
\dot{C}_{vp} = F^T \left( F_{th} \cdot F_e \cdot \dot{F}_{vp} \cdot F_{vp}^{-1} + F_{vp}^{-T} \cdot \dot{F}_e \cdot F_{th}^T \right) \cdot F
\]

(8b)

\[
\dot{C}_{th} = F^T \left( \dot{F}_{th} \cdot F_{th}^{-1} + F_{th}^{-T} \cdot \dot{F}_{th}^T \right) \cdot F = 2F^T \cdot D_{th} \cdot F.
\]

(8c)

where \( D_e, D_{vp} \) and \( D_{th} \) are respectively the elastic, viscoplastic and thermal rate-of-deformation tensors. The constitutive relations for \( D_{vp} \) and \( D_{th} \) will be defined in the following sections.

### 2.3.2 Thermal deformation

The thermal effects are incorporated in the model via the thermal part of the deformation gradient tensor \( F_{th} \), which is assumed to be purely volumetric [58, 60]. For mechanically and thermally isotropic materials \( F_{th} \), can be defined as:

\[
F_{th} = \phi(T)^{1/3} I.
\]

(9)

The scalar function \( \phi(T) \) describes the volumetric deformation induced by a temperature change \( (T - T_0) \) relative to the reference temperature \( T_0 \). The simplest form for \( \phi(T) \) is [58, 60]:

\[
\phi(T) = 1 + \alpha(T - T_0),
\]

(10)

where \( \alpha \) is the volumetric thermal expansion coefficient which, in general, can be temperature dependent.
Furthermore, from equations (6c) and (9) the symmetric and skew symmetric parts of $L_{th}$ can be obtained as:

\[
D_{th} = \frac{1}{2} [L_{th} + L_{th}^T] = \frac{1}{3} \dot{\phi}(T) I = L_{th},
\]

\[
\Omega_{th} = \frac{1}{2} [L_{th} - L_{th}^T] = 0,
\]

(11a)

(11b)

### 2.3.3 Elastic model

In the constitutive framework applied in this paper, the stress-strain relation is given by a small deformation elastic model which relates the rate of the 2nd Piola-Kirchhoff stress tensor $\dot{S}$ to the rate of the elastic right Cauchy-Green strain tensor $\dot{C}_e$. The 2nd Piola-Kirchhoff stress tensor $S$ is defined as:

\[
S = J F^{-1} \cdot \sigma \cdot F^{-T} = F^{-1} \cdot \tau \cdot F^{-T},
\]

where $\sigma$ and $\tau = J \sigma$ are the Cauchy and the Kirchhoff stress tensors, respectively. The conventional constitutive relation between $\dot{S}$ and $\dot{C}_e$ is then expressed as:

\[
\dot{S} = 4 \dot{\varepsilon}_{elas} : \dot{C}_e,
\]

where $4 \dot{\varepsilon}_{elas}$ is the fourth-order elasticity tensor, for an isotropic material given by [61]:

\[
4 \dot{\varepsilon}_{elas} = [\mu - \lambda \ln(J_e)] C_e^{-1} \cdot 4 \dot{\gamma}^R T \cdot C_e^{-1} + \frac{1}{2} \lambda C_e^{-1} \otimes C_e^{-1},
\]

(14)

with $4 \dot{\gamma}^R T$ the right transpose of the fourth-order identity tensor defined as $4 \dot{\gamma}^R T : A = A^T$.

In (14), $\lambda$ and $\mu$ are the elastic Lamé’s constants.

### 2.3.4 Thermo-viscoplastic model

A classical expression is used to describe the viscoplastic flow, given by $D_{vp}$, which assumes that the viscoplastic deformation accumulates in the direction of the deviatoric stress $\tau^d$, whereby its magnitude is determined by the rate of the viscoplastic multiplier $\dot{\gamma}_{vp}$:

\[
D_{vp} = \dot{\gamma}_{vp} N,
\]

(15)

with $N$ the flow direction, defined in terms of the deviatoric part of the Kirchhoff stress tensor as:

\[
N = 3 \frac{\tau^d}{2 \tau_{eq}}, \quad \tau_{eq} = \sqrt{\frac{3}{2} \tau^d : \tau^d}.
\]

(16)

The definition of the plastic flow given by equation (15) is completed by postulating a zero viscoplastic spin [59]:

\[
\dot{\Omega}_{vp} = 0.
\]

(17)

Next, $\dot{\gamma}_{vp}$ is defined by a Zener-Hollomon decomposition [55–57]:

\[
\dot{\gamma}_{vp} = \theta(T) Z(\varphi, D),
\]

(18)
where \( \theta(T) > 0 \) is an Arrhenius type thermal function and \( Z(\varphi, D) > 0 \) is the Zener parameter; with \( D > 0 \) the drag strength, accounting for the isotropic hardening.

Viscoplastic deformation will take place provided that:

\[
\varphi(\tau_{eq}, \tau_y) = \tau_{eq} - \tau_y(T) \geq 0. \tag{19}
\]

where \( \tau_y(T) \) is the yield stress, which here depends on the temperature only, since hardening is already accounted for in (18).

The Zener parameter is defined as [41]:

\[
Z(\varphi, D) = A \sinh^n \left( \frac{\varphi}{D} \right) = A \sinh^n \left( \frac{\tau_{eq} - \tau_y(T)}{D} \right), \tag{20}
\]

where \( A > 0 \) and \( n > 0 \) are temperature independent rate sensitivity parameters.

The expression for \( \theta(T) \) is given by [41]:

\[
\theta(T) = \begin{cases} 
\exp \left[ -\frac{Q}{RT} \right] & \text{if } \; T_i \leq T < T_m, \\
\exp \left[ -\frac{Q}{RT} \left( \ln \left( \frac{T}{T_i} \right) \right) + 1 \right] & \text{if } \; T_c < T \leq T_i, \\
\exp \left[ -\frac{Q}{RT} \left( \ln \left( \frac{T}{T_c} \right) \right) + 1 \right] & \text{if } \; 0 < T \leq T_c.
\end{cases} \tag{21}
\]

where \( Q \) is the activation energy for creep, \( R = 8.314 \text{ J/molK} \) is the universal gas constant, \( T_m \) is the melting temperature and \( T_i = T_m/2 \) and \( T_c = 350^\circ \text{C} \) are the transition temperatures.

Finally, the evolution equation for the drag strength \( D \) is given by [55]:

\[
D = h(D) [\gamma_{ep} - \theta(T)r(D)] = \theta(T) h(D) \left[ Z(\varphi, D) - r(D) \right], \tag{22}
\]

with the initial value \( D = D_0 \) the minimum or annealed drag strength. Equation (22) describes the evolution of the drag strength as the result of the interaction of strain hardening, dynamic recovery via \( h(D) \), and thermal recovery via \( r(D) \). The corresponding expressions for \( h(D) \) and \( r(D) \) are:

\[
h(D) = h_D \left[ \frac{(D - D_0)/\delta C}{\sinh[(D - D_0)/\delta C]} \right]^m = h_D \left[ \frac{\varphi_D}{\sinh[\varphi_D]} \right]^m, \tag{23}
\]

\[
r(D) = A \sinh^n \left[ \frac{(D - D_0)/\delta C}{\varphi_D} \right] = A \sinh^n [\varphi_D], \tag{24}
\]

with

\[
\varphi_D = \frac{(D - D_0)}{\delta C}, \tag{25}
\]

where \( C \) is the power-law breakdown strength, \( h_D \) is the isotropic hardening modulus, \( \delta \) and \( m \) are material parameters related to thermal and dynamic recovery.
2.3.5 Non-linear system of equations for the viscoplastic behaviour

To summarize, the viscoplastic constitutive model is described by the following set of equations:

\[
\dot{S} = \dot{C}_{elas} : \left[ \dot{C} - 2F^T \cdot \theta(T)Z(\varphi, D)N \cdot F - 2F^T \cdot D_{th} \cdot \dot{F} \right], \quad (26a)
\]

\[
\dot{D} = \theta(T)h(D) \left[ Z(\varphi, D) - r(D) \right]. \quad (26b)
\]

where (26a) is obtained by substituting equations (7), (8b), (15) and (8c) in equation (13), with \( D_{th} \) given by (11a), and using expression (18) for \( \dot{\gamma}_{vp} \).

For the numerical solution of boundary value problems involving this constitutive model, a finite element formulation has been developed and implemented.

3 Numerical simulations on CGI RVE

In this section, the CGI RVE is used to investigate effect of time and temperature on the mechanical response of CGI. First, monotonic tensile tests at 20, 350, 400, 450 and 500 °C are performed to assess the influence of temperature. Then, the time-dependency is investigated by means of stress relaxation tests, which are carried out at the same temperatures as used in the tensile tests.

3.1 Elevated temperature uniaxial tensile response

The tensile tests are performed by prescribing a macroscopic strain of 2.5 % to the RVE in the horizontal direction (see Figure 1). The deformation is applied in 50 seconds, i.e. with a strain rate of \(5 \cdot 10^{-4} \text{ s}^{-1}\). The periodic boundary conditions have been prescribed in such a way that the overall stress state remains uniaxial, see Appendix A for the details.

The resulting macroscopic stress-strain response for the different temperatures is presented in Figure 2. From the results shown in Figure 2.a, it is obvious that the mechanical performance degrades with increasing temperature. Figure 2.b, reveals that also the hardening of the material due to plastic deformation decreases with temperature.

The thermal softening observed in Figure 2.a, can also be noticed when comparing the matrix response at 20 °C and 500 °C. The drop in stress hardening with temperature can be traced back to the decrease of drag strength with increasing temperature, following Equation (22), as shown in Figure 3. At higher temperatures, a higher activation energy promotes thermal recovery which counteracts the effect of strain hardening due to plastic deformation. This is illustrated in Figure 4 where the contributions to the drag strength from plastic deformation, \( D_{\gamma vp} = h(D)\Delta t\dot{\gamma}_{vp} \), and thermal recovery, \( D_r = -h(D)\Delta t\theta(T)r(D) \), are separately presented. Figures 4.a and 4.b, reveal that the higher activation energy at 500 °C not only enables thermal recovery but also enhances plastic flow, leading to a higher contribution of \( D_{\gamma vp} \) to the drag strength. Nevertheless, with the pearlite parameters used, the increase in \( D_{\gamma vp} \) at 500 °C is counteracted by the thermal recovery such that the overall drag strength \( D \) is lower than at 20 °C.

The high microstructural heterogeneity of cast irons (graphite morphology and properties of the phases), combined with the temperature-dependency, have an important effect on the distribution of the local microstructural fields. As shown in Figures 5.a and 5.b, high stress and strain concentrations arise at various locations surrounding the graphite particles. The most
Influence of temperature on the uniaxial tensile response of CGI as predicted by RVE simulations: a) homogenized macroscopic stress-strain response; b) stress hardening as a function of temperature.

Critical areas, are those in the vicinity of anisotropic graphite particles whose long axis is oriented at 45° with respect to the loading direction, especially in regions where several particles are clustered together (see Figure 1). The anisotropic graphite particles oriented transversely to the loading direction show little resistance to deformation upon loading. Consequently, high strains are observed within these graphite particles (Figure 6), and in the matrix adjacent to the tip of the particles, which behaves as a notch in the matrix. At this spots, the high strain areas extend far into the matrix leading to the formation of strain percolation paths (Figures 5.c and 5.d). At higher temperatures, this effect is enhanced even further as demonstrated in Figures 5.b and 5.d. At 500 °C, the stress fields are only half the magnitude of those at
\[ D_{\gamma p} = h(D) \Delta t \dot{\gamma}_{\gamma p} \]

Fig. 4  Uniaxial tensile test, contributions to the drag strength \( D \) from plastic deformation (top) and thermal recovery (bottom) at the end of macroscopic loading: left) at 20 °C; right) at 500 °C.

20 °C, yet they entail higher and more extensive plastic strains. Therefore, it can be expected that damage will initiate earlier and propagate faster at higher temperatures.

### 3.2 Stress relaxation

The stress relaxation simulations are carried out at the same temperatures as the uniaxial tensile tests described in the previous section: 20, 350, 400, 450 and 500°C. The boundary conditions are prescribed such that an overall uniaxial stress state is reproduced (see Appendix A). Two load steps are considered: i) pre-load: a macroscopic strain of 1% is prescribed on the RVE in the horizontal direction (see Figure 1) in 20 seconds, i.e. at a strain rate of \( 5 \cdot 10^{-4} \text{s}^{-1} \); ii) stress relaxation: once the prescribed macroscopic strain is reached, the RVE is held in its deformed state for 2 hours allowing the stress to relax.

The results are presented in Figure 7, where the stress relaxation is defined as the drop in stress between the peak stress reached at the end of the pre-load \( \tau_{T=20s} \) and the stress at the
Fig. 5 Uniaxial tensile test, equivalent von Mises stresses (top) and equivalent viscoplastic strain (bottom) in the matrix phase at the end of macroscopic loading: a) and c) at 20 °C; b) and d) at 500 °C.

end of the relaxation period $\tau_{t=2h}$:

$$Sr = \left[ \frac{\tau_{t=2h} - \tau_{t=20s}}{\tau_{t=2h}} \right] \times 100\%.$$  (27)

Figure 7 gives a clear indication of the effect of the temperature on the time-dependent behaviour of CGI. Below 350°C, there is a negligible difference in the relaxation response of the material. From this point onwards, increasing the temperature leads to a sharp increase in the amount of stress relaxation.

The observed behaviour is driven by the elevated temperature response of the pearlitic matrix, captured by the model described in Section 2.3, and calibrated on the experimental data for pearlitic steel [41]. Experiments indicated that pearlitic phases present a low sensitivity to temperature below 350°C, while above this temperature, the resistance of the material to creep deteriorates drastically which explains the response observed in Figure 7.

In general terms, stress relaxation is driven by the time- and temperature-dependent plastic deformation of the material. As discussed in the previous section, the resistance to plastic
deformation is described in the model by the drag strength. At lower temperatures, stresses can exceed the drag strength and enable plastic deformation and hence stress relaxation. At higher temperatures, the stresses are lower; yet, a higher stress relaxation is observed, which can be explained by the thermal recovery. As a consequence of a higher activation energy, thermal recovery becomes more pronounced at higher temperatures. It counteracts the strain hardening effect of the drag strength enabling plastic deformation. Hence, in spite of the lower stresses, a higher stress relaxation takes place at higher temperature.

To illustrate this situation, Figures 8 and 9 show the incremental viscoplastic strain $\Delta \dot{\gamma}_{vp}$ and the contributions to $D$ from the plastic deformation and thermal recovery in the matrix. Figure 8 reveals a marked difference in the matrix incremental viscoplastic strains $\Delta \dot{\gamma}_{vp}$, at the end of stress relaxation at 20°C and 500°C. Moreover, the difference in $\Delta \dot{\gamma}_{vp}$ can be

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**Fig. 6** Uniaxial tensile test, $\varepsilon_{11}$ strain component in the graphite particles: a) at 20°C; b) at 500°C.

**Fig. 7** Stress relaxation of CGI as predicted by RVE simulations: a) stress relaxation percentage vs. time for the different temperatures; b) stress relaxation percentage as a function of temperature.
traced back to the drag strength and thermal recovery. The higher thermal recovery at 500°C (Figure 9) induces a lower drag strength. This results in a higher amount of plastic deformation and hence more stress relaxation.

The combined effect of microstructural heterogeneity and temperature can be also appreciated in Figures 8 and 9. The presence of the graphite particles introduces stress concentrations in their neighbourhood in the microstructure. At 500°C the contribution to the drag strength $D$ from thermal recovery is twice as high as the contribution from plastic deformation. Therefore, over time the drag strength decreases resulting in higher plastic strain rates and the formation of strain percolation paths (Figure 8). It is expected that this triggers damage at the microstructural level.

4 Conclusions

The aim of this paper was to investigate the elevated temperature mechanical behaviour of cast irons. For this purpose, a new microstructural based model for elevated temperature mechanical analyses of CGI has been developed. The model incorporates the time and temperature dependent response of the matrix and the morphology of the graphite inclusions along with the intrinsic mechanical anisotropy of graphite. The behaviour of the pearlitic matrix is modelled through a thermo-viscoplastic model [41] implemented in a finite element framework. To validate the representativeness of the material parameters identified on C75 pearlitic steel for the behaviour of the pearlitic matrix, micro-indentation tests have been performed on the pearlitic matrix of CGI as well as on a C75 pearlitic steel. The results, in terms of Young’s modulus and hardness, revealed an adequate agreement between the two materials.

From the numerical results of the elevated temperature tests on CGI it can be concluded that:

- The effect of temperature on the mechanical response of CGI is dominant for temperatures above 350°C. This is confirmed by the tensile tests as well as the stress relaxation
tests. In the former, a sharp decrease in the hardening rate with temperature has been observed at the macroscopic level. In a similar fashion, a fast increase in the resulting stress relaxation is perceived for temperatures exceeding 350°C.

- For higher temperatures, the amount of thermal recovery overcomes the contribution of plastic deformation to hardening, leading to a reduction of the drag strength. This, directly influences either the hardening or the relaxation of the material at the local and global level.

- At lower temperatures, the effect of thermal recovery is negligible and the only driver for stress relaxation is dynamic recovery.

- At the microstructural level, the highly heterogeneous microstructure of cast irons leads to stress concentrations in the areas surrounding the graphite particles. As the temperature is increased, the combined effect of time, temperature and heterogeneity promotes...
local plastic deformation at the microstructural scale. This may accelerate the damage initiation and evolution, therefore reducing the time to failure of the material.

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A Computational homogenization

Within the framework of the computational homogenization adopted for the microstructural modelling [44], the microstructural displacement fields \( \bar{u}_m(\bar{X}_m) \) of a given point with the position vector \( \bar{X}_m \) in the reference configuration can be described through a macroscopic contribution (resulting from the macroscopic deformation gradient tensor \( \mathbf{F}_M \)) and a microstructural fluctuation field \( \bar{u}_f(\bar{X}_m) \) that represents the local variations with respect to the average macroscopic fields. Expressing the displacement \( \bar{u}_m(\bar{X}_m) \) within the microscopic volume relative to some arbitrarily chosen point \( k \) yields

\[
\bar{u}_m(\bar{X}_m) = \bar{u}^k(\bar{X}_k) + (\mathbf{F}_M - \mathbf{I}) \cdot (\bar{X}_m - \bar{X}^k) + \bar{u}_f(\bar{X}_m),
\]

where the subscripts \( m, M \) and \( f \) refer to the micro and macro scale quantities and the microscopic fluctuation field, respectively.

In computational homogenization framework, the macro-to-micro scale transition is achieved by imposing that the macroscopic deformation gradient tensor should be equal to the volume average of its microscopic counterpart, i.e.:

\[
\mathbf{F}_M = \frac{1}{V_0} \int_{V_0} \mathbf{F}_m \, dV_0,
\]

From the expression of the microscopic displacement field (28), the microscopic deformation gradient tensor can be obtained and introduced in equation (29) leading to the following boundary integral:

\[
\int_{\Gamma_0} \bar{u}_f \otimes \bar{n}_0 \, d\Gamma_0 = 0,
\]

where \( \bar{n}_0 \) is the normal to the RVE boundary \( \Gamma_0 \) in the reference configuration.

This condition can be fulfilled by means of different boundary conditions, such as uniform displacement, uniform traction and periodic boundary conditions. In this work, periodic boundary conditions are used since they yield better approximation to the apparent macroscopic properties [44]. In the case of a 2D RVE, as used in this work (Figure 10), the periodic boundary conditions lead to the following displacement constraint relations [44]:

\[
\bar{u}_m^+ = \bar{u}_m^- + (\mathbf{F}_M - \mathbf{I}) \cdot (\bar{X}_m^+ - \bar{X}_m^-),
\]

where superscript “+” refers to the top and right part of the boundary, while “−” refers to the bottom and left part (see Figure 10).

Furthermore, the macroscopic gradient tensor \( \mathbf{F}_M \) is prescribed through the RVE corner nodes 1, 2 and 4 in the form of displacements as:

\[
\bar{u}_p = (\mathbf{F}_M - \mathbf{I}) \cdot \bar{X}_p, \quad p = 1, 2, 4
\]
where \( \vec{u}_p \) are the prescribed microscopic displacements and \( \vec{X}_p \) are the position vectors of the respective corner nodes.

The micro-to-macro scale transition is based on the Hill-Mandel principle of macro-homogeneity. Based on this principle it can be shown that the relation between the macroscopic and microscopic stresses is expressed as \([44]\):

\[
P_M \frac{1}{V_0} \int_{V_0} P_m \, dV_0 = \frac{1}{V_0} \sum_{p=1,2,4} \vec{f}_p \otimes \vec{X}_p,
\]

\( (33) \)

where \( P \) represents the first Piola-Kirchhoff stress tensor and \( \vec{f}_p \) are the reaction forces at the prescribed corner nodes. To derive the second equation in \((33)\), the equilibrium condition on the RVE has been used, in combination with the divergence theorem and the periodic boundary conditions \((31)\), see \([44]\) for the details.

From \((33)\) it is clear that to obtain a homogenized uniaxial stress state in the horizontal direction, for the RVE illustrated in Figure 10, the following boundary conditions can be applied on the corner nodes:

\[
\vec{u}_1 = \vec{0}, \quad u_2^x = u^*, \quad u_2^y = 0, \quad \vec{f}_4 = \vec{0},
\]

\( (34) \)

with \( u^* \) the prescribed horizontal displacement. All the other nodes on the RVE boundary are linked through the periodic boundary conditions.

References