Modelling and simulations of ductile iron solidification-induced variations in mechanical behaviour on component and microstructural level

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Abstract. The mechanical behaviour and performance of a ductile iron component is highly dependent on the local variations in solidification conditions during the casting process. Here we show a framework which combine a previously developed closed chain of simulations for cast components with a micro-scale Finite Element Method (FEM) simulation of the behaviour and performance of the microstructure. A casting process simulation, including modelling of solidification and mechanical material characterization, provides the basis for a macro-scale FEM analysis of the component. A critical region is identified to which the micro-scale FEM simulation of a representative microstructure, generated using X-ray tomography, is applied. The mechanical behaviour of the different microstructural phases are determined using a surrogate model based optimisation routine and experimental data. It is discussed that the approach enables a link between solidification- and microstructure-models and simulations of as well component as microstructural behaviour, and can contribute with new understanding regarding the behaviour and performance of different microstructural phases and morphologies in industrial ductile iron components in service.

1. Introduction

Cast iron is a group of materials which exhibit highly interesting combinations of material properties for applications in e.g. the automotive and transportation areas. The materials are usually classified in three wide groups according to the morphology of the graphite particles found within the material; flake graphite iron (FGI), compacted graphite iron (CGI) or spheroidal graphite iron (SGI). In FGI the graphite particles are found as thin flakes with sharp edges. In CGI the edges are somewhat rounded (vermicular), while in SGI the graphite has formed more or less round graphite nodules. The difference in graphite morphology between these three materials are illustrated in figure 1. The graphite morphology is very important since it controls as well the mechanical as physical material behaviour. In general terms, FGI exhibit low strength but high thermal conductivity, SGI high strength and lower thermal conductivity, while CGI has intermediate strength and conductivity [1]. In this work the SGI material, also known as ductile iron, is studied. The local variations in microstructure formed during solidification are addressed, and the effects of these variations on the mechanical behaviour of a cast SGI component are modelled, both on the macro- and micro-scale.
1.1. Macro-scale behaviour induced by micro-scale variations during solidification

Even for a specific class of cast iron, the graphite on different locations of a cast geometry exhibit local variations in morphology. Measures as roundness, nodularity and nodule count are typically used to further describe the character of the graphite precipitates. Though the precipitates are distributed in a 3D volume, these measures are typically identified from micrographs of a polished flat 2D section of the material.

The graphite morphology is not constant for a specific alloy or component geometry. The graphite morphology is affected by several local parameters which vary throughout the geometry during solidification. One important factor is the local cooling rate, which is highly related to the geometry of the component (e.g. section thickness) and the extraction of heat from the component during solidification. Another important factor is the local chemical composition. Graphite morphology is affected e.g. by the magnesium (Mg) content when the graphite forms, which in turn depends on e.g. the chemical composition of the alloy, the effectiveness of the Mg-treatment, Mg-fading during pouring and solidification and chemical segregation. The graphite morphology thus display local variations throughout the volume of a cast component [2]. Since graphite morphology affects material behaviour, the material behaviour exhibits local variations throughout a cast component.

Not only graphite morphology but also the matrix between the graphite nodules exhibits local variations throughout a component due to local variations in solidification conditions. The matrix typically consists of ferrite, pearlite or combinations of both. In a ferritic-pearlitic matrix, the ferrite is typically formed around the graphite nodules during the solid-state transformation stage of the solidification process. Since ferrite and pearlite have significantly different material behaviour, the local ferrite-pearlite fraction have a great influence on the local material behaviour throughout a component [2]. As for graphite morphology, the area fractions ferrite-pearlite fractions provides information about a 2D cross section, while these microstructural constituents are in fact dispersed through the 3D volume of the casting.

1.2. The closed chain of simulations

The material behaviour throughout a cast iron component thus exhibit significant local variations, which are dependent on complex interactions between component design, casting process parameters and several chemical and physical phenomena, during solidification. To address this problem, two of the current authors have previously presented a simulation strategy called the closed chain of simulations for cast components [3]. The strategy is schematically outlined in figure 2. The strategy is based on numerical solidification models implemented into a casting process simulation, which include the entire casting process including e.g. chemical composition, mould filling and solidification. The casting process simulations are performed using MAGMASOFT™ [4], which is based on the Finite Difference Method (FDM) for solving the governing equations. Local microstructure evolution during solidification and solid-state transformation is predicted using previously developed microstructure formation models, e.g. [5]. Material characterization models which relate
microstructure and mechanical behaviour [6] are applied on the local level, i.e. in every element of the FDM mesh. The predicted material behaviour is then incorporated into a macro-scale Finite Element Method (FEM) simulation of the behaviour of the component in service, using an in-house developed software to generate element specific microstructure-based local material definitions [3]. The simulation strategy has also been applied to cast aluminium components [7]. It has been verified, using Digital Image Correlation (DIC), that by taking these local variations into account, a more accurate prediction of the distribution of stresses and strain is obtained compared to using traditional homogeneous or tabulated material behaviour [8].

The macro-scale simulation is thus able to predict the effect of the local variations in mechanical behaviour onto the global macro-scale stress distribution of the component. It is however unable to predict the effect of the macro-scale stress on micro-scale stress distributions around microstructural features in the loaded region.

Figure 2. Illustration of the closed chain of simulations for cast components [3].

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The current contribution aims to present ongoing work on an extension of the closed chain of simulations. Here the macro-scale FEM simulation results serves as input for a FEM simulation of the micro-scale stress distribution using a representative model of the microstructure. 3D X-ray tomography is applied to generate a representative geometrical model of a real micro-structure, including ferrite, pearlite and graphite nodules. The material properties of each phase is determined using surrogate model based optimization. From the model, as well volume fractions of ferrite, pearlite and graphite as graphite morphology characteristics can be determined in 3D. By predicting the micro-scale distribution of stresses and strains, an increased understanding of the performance of a cast component can be obtained. This will provide important information to aid engineers within mechanical design, solid mechanics and materials science to develop more reliable and robust components.

2. Macro-scale characterization and FEM simulation

In this work, an engine support for a truck was used as a demonstrator. The size of the component is approximately 0.5 m in length, and 0.3 m in height and width. The same geometry and FEM setup has been used in previous work [2, 6, 9], where also the setup of the casting process simulation and the macro-scale FEM simulation is described [9]. In previous work, the Hollomon equation was applied to describe the elasto-plastic material behaviour in the macro-scale simulation as

$$\sigma = K_H \cdot \varepsilon^{n_H}_{pl}$$

(1)
where the strength coefficient $K_H$ and the strain hardening exponent $n_H$ are introduced to relate true stress $\sigma$ and plastic strain $\varepsilon_{pl}$. Following findings in recent work [6], the Ludwigson equation was applied in the current work. The Ludwigson equation provides an extension of the Hollomon equation for small plastic strains and is formulated as

$$\sigma = K_H \cdot \varepsilon_{pl}^{n_H} + e^{(k_L + n_L \cdot \varepsilon_{pl})}$$  \hspace{1cm} (2)

The Ludwigson equation has been found to describe the two-slope plastic behaviour found in SGI [10] with higher accuracy than the Hollomon equation [6]. Material characterization models relating the parameters $K_H$, $n_H$, $k_L$, and $n_L$ to fraction pearlite and nodularity have previously been derived [6], and implemented into the casting process simulation. The local predictions of microstructural features and mechanical behaviour has been shown to be in good agreement with experimental data [2, 6].

Figure 3 shows the stress distribution predicted by the macro-scale FEM simulation at a certain load using three different types of material data: tabulated homogeneous material data and local material data using the Hollomon and the Ludwigson equations. A comparison of the results obtained shows that the implementation of the Ludwigson equation affects the predicted results for stresses and strains already before the tabulated 0.2% offset yield stress of 350 MPa is reached. As also found in previous work [9], the local variations in microstructure causes a redistribution of stresses and strains, an effect which will be even more significant at higher loads. The results show the importance of providing accurate and local material data to the FEM simulation. The difference between using tabulated material data and accurate material modelling using the Ludwigson equation is in this case around 20% difference in predicted stress level. This difference is of utmost importance for the accuracy of predictions of as well static as fatigue performance of the component, which are crucial aspects when designing the component. This highlights the relevance of taking the effect of local microstructure into consideration when analysing the stress distribution in cast components.

**Figure 3:** Predicted von Mises stress in a region of the component subjected to load using (a) homogeneous tabulated material data, and local data using (b) the Hollomon equation and (c) the Ludwigson equation.

Based on the macro-scale FEM simulation, a critical region of the component subjected to high stresses and strains can be identified, and selected for further studies of the response of the microstructure in this region. In the current semi-multiscale approach, the stresses and strains predicted by the microstructure-based macro simulation are used as input for the subsequent micro-scale simulation. For these micro-scale studies, it is important that a relevant and representative stress and strain distribution is used in order to provide relevant results, thus the macro-scale FEM simulation with local Ludwigson data is selected as the basis for the micro-scale FEM analyses.
3. Micro-scale simulation

Studies of microstructures in 3D can be done in various ways. Focused Ion Beam (FIB) is commonly used to generate 3D microstructures, see e.g. [11-12]. Another method which also falls under the same scope is to study the 3D microstructures by deep-etching [13]. However, both of these techniques are rarely used for the purpose of generating FEM-models, but merely for quantitative and/or qualitative analyses. Instead, X-ray tomography (XT) is the prominent method for generating 3D FEM-models of microstructures [14-16].

In the present work, X-ray tomography was used to generate a model of the actual microstructure of the SGI, see figure 4a. From this model, information about the 3D graphite morphology and volume fractions of the different matrix constituents can easily be extracted. Results from these measurements will be further evaluated and presented in upcoming work.

![3D microstructure of the SGI](image)

**Figure 4.** (a) 3D microstructure of the SGI (b-c) Examples of 2D microstructure representations.

If the material curve describing the elasto-plastic behaviour of the separate phases is known, this 3D model can be directly used for FEM simulations of the behaviour and performance of the microstructure in 3D. These curves are however not easily determined. In this work the material curve has been determined using a reversed engineering strategy, where surrogate modelling is used to determine material curve for each individual phase based on experimental tensile testing data.

In order to save computational power and time, the 3D microstructure was sliced to provide 2D cross sections which were used in an optimization algorithm to reverse engineer the material properties for the different phases, see figure 4. The 2D representation, i.e. the representative volume element (RVE), of the microstructure was analysed by applying boundary conditions that originated from critical regions in the macro-scale simulation according to figure 5.

The reversed engineering scheme was based on an assumed material behaviour of the individual metallic phases of the microstructure. In the present study a frequently used relation was used for describing the behaviour of the different phases, namely the Ramberg-Osgood relation

\[ E\varepsilon = \sigma + \alpha \left( \frac{\sigma}{\sigma_Y} \right)^{n-1} \quad (3) \]

where \( \sigma \) is the Cauchy stress, \( \sigma_Y \) the yield stress, \( E \) the Young’s modulus, \( \varepsilon \) the strain and \( \alpha \) and \( n \) are material specific constants. The material behaviour of the graphite is considered to be elastic.
An objective function in the form of a fitness functional to be minimized was then formulated as

$$f_j \left( \sigma_Y, \alpha, n \right) = \sum_{i=1}^{k_i} W_i \| \sigma_{i}^{\text{sim}} - \sigma_{i}^{\text{exp}} \|$$

(4)

Here $\sigma_{i}^{\text{sim}}$ is the simulated average stress of the RVE, and the corresponding stress measured from physical experiments is given by $\sigma_{i}^{\text{exp}}$. The $L_2$-norm is denoted by $\| \ldots \|$ and $W_i$ is a weight factor. The objective function contains three variables per phase, namely $\sigma_Y$, $\alpha$ and $n$. When considering two phases, the objective function will contain six variables by keeping Young’s modulus and Poisson’s ratio fixed. Since the simulations are fairly time consuming it was appropriate to generate a so-called surrogate model. This model was established by generating a set of simulation models by providing combinations of variables. The fitness values for the resulting simulations were used to generate the surrogate model by use of a radial basis function (RBF), see e.g. [17]. The RBF is in the form of

$$f(x) = \sum_{i=1}^{n} \lambda_i A_{ij} + \sum_{i=1}^{n} \beta_i B_{ij}$$

(3)

where the first term is the RBF and the second term is the augmented bias. The minimization of the objective function is done using the Hooke and Jeeves pattern search method. An example of the generated surrogate model for variables $\sigma_Y$ and $n$ is shown in figure 6.
Using the surrogate model, the combination of parameters for each phase that best fits the experimental data was determined. By using this data for the micro-scale FEM simulations, the behaviour and performance of the microstructure subjected to the stresses and strains provided by the macro-scale simulation can be studied. Future work will be aimed at e.g. studying the distribution of stresses and strains in different phases when the microstructure model is subjected to load, and the effect of different graphite morphologies on the components performance. The micro-scale FEM simulation can also be applied to study the initiation and propagation of cracks at cyclic loading and fatigue. The current framework thus enables a link from solidification- and microstructure-modelling to component simulations of as well macro-scale as micro-scale behaviour and performance. By integrating these simulations into the design process for cast components, new possibilities to design cast components with high performance, robustness and quality are enabled.

4. Conclusions
The local solidification conditions in a cast component are critical for the microstructure formation and thus for the mechanical behaviour of a cast iron component. A framework for studying the effect of variations in microstructure due to variations in solidification conditions throughout a cast component has been outlined. The framework is a semi-multiscale approach to predict as well the macro-scale distribution of stresses and strains in the component as well as the response and performance of the microstructure within a critical region. X-ray tomography has been used to generate a representative model of the microstructure in a critical region. Surrogate modelling has been successfully applied to generate the material data needed for the micro-scale FEM simulation based on experimental data. The framework enables new possibilities to include solidification and microstructure modelling into the design process for industrial cast components.

5. Acknowledgements
The work has been performed in the CCSIM2 project within the research profile CompCAST at the School of Engineering, Jönköping University. The Swedish Knowledge Foundation is gratefully acknowledged for financial support of the research profile. The authors would also like to thank Professor Ragnvald Mathiesen and Professor Arne Dahle for providing the X-ray tomography, and Kaveh Amouzgar for assistance with the optimization routine.
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