Prediction of solidification structures in a 9.8 t steel ingot

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Abstract.

The control of the carbon macrosegregation level in steel ingots is important for the structural integrity of the final component. During solidification, the fragmentation of the columnar dendrites is an important source of equiaxed grains, and has a large influence on the macrosegregation and the grain structure. The goal of this study is to show that a numerical model that takes into account fragmentation can describe the formation of the structures and the macrosegregation during solidification of a large steel ingot. The present article describes the multiphase numerical model used in the simulations. The simulation results are compared to experimental data from a 9.8 t ingot cast in A5/6 steel by ArcelorMittal Industeel. The model can then be used to explain the formation of the observed structures. For example, we show that the structural transitions, first from columnar to equiaxed globular and then to equiaxed dendritic at the bottom of the ingot are a consequence of the concurrent transport and growth of the dendrite fragments from the columnar zone. Furthermore, we show that most of the structures are formed very early on during solidification, whereas macrosegregation develops much more gradually.

1. Introduction

During solidification of large steel ingots, the average concentration of alloying elements does not stay homogeneous throughout the ingot. Most alloying elements are more soluble in the liquid than in the solid phase, leading to an enrichment of the liquid as the solidification progresses. This inhomogeneity, called macrosegregation, can lead to variations of local mechanical properties, most notably when the carbon macrosegregation is high. During the forging of the ingot, the macrosegregation is carried through to the final component, which will therefore exhibit inhomogeneous mechanical properties. This is especially important for very large forged components such as pipes and reactor pressure vessels, where the large ingot size can lead to severe macrosegregation. Being able to predict and control macrosegregation is thus crucial for the structural integrity of the components.

The solidification structures (columnar, equiaxed, grain morphology) also influence segregation and mechanical properties. Thus accurately predicting both the macrosegregation and the solidification structures is an important issue for steel ingot producers. The prediction of the structures requires taking into account the fragmentation of the columnar dendrites in the
model [1]. The present study uses the SOLID® multiscale and multiphysics model to predict the structure and macrosegregation of a 1.44 m diameter, 9.8 t steel ingot by taking into account the fragmentation during solidification. The originality of this study lies in prediction and description of the formation of the structures and the macrosegregation, which is not commonly found in literature for such large products.

Fragmentation of the columnar dendrites is an important source of equiaxed grains, especially in castings with no inoculation. Some secondary arms detach and can be swept into the bulk liquid, where they can grow and sediment, leading to a columnar to equiaxed transition. The detachment of secondary arms does not occur because of mechanical breakage [2] but rather due to local dissolution at the root of the secondary arms [3] or remelting of the arms due to temperature increase [4]. During normal coarsening of the columnar structure, secondary arm detachment is quite slow. However, certain situations massively increase fragmentation, such as unconstrained growth of the columnar front [5] or slowdown of the columnar tip velocity [6]. In addition, in steels, the peritectic transformation can also promote the increase in size of the equiaxed region [7].

2. Model used in the SOLID® software
The SOLID® software uses a 2D finite volume method to discretise the set of partial differential equations of a multiphase model (liquid, columnar, equiaxed and interdendritic liquid for both solid phases). The discretised volumetric elements will be referred to as "cells". A cell can contain both columnar and equiaxed solid, in addition to liquid. Cells containing both columnar and equiaxed grains are called mixed cells. Solidification begins with a columnar front starting on the mould walls which can grow and fragment. Fragmentation generates equiaxed grains in the undercooled region ahead of the columnar front. These equiaxed grains are not individually simulated, but are instead represented by average grain size and grain density values in each cell. Fragmentation is implemented using the model developed by Nicolas Leriche in his PhD [8]. Fragmentation uses two parameters: the fragmentation flux density (number of generated grains per surface area of columnar front per second) and the thermal gradient activation threshold. The threshold means that the fragmentation occurs only when the temperature gradient at the columnar front is locally smaller than a given threshold value.

The model calculates the movement of the liquid phases (intergranular and extragranular for both the equiaxed and columnar phases) and of the equiaxed grains. The grains are thus swept up by the liquid flow and grow or remelt depending on local undercooling, and sediment when they reach a large enough size. Grain movement in a cell is blocked when the extragranular liquid fraction is below 0.6. The columnar front in a cell is blocked when the envelope fraction of equiaxed grains in that cell reaches 0.5, leading to a columnar to equiaxed transition (CET). Unlike the columnar structure, equiaxed cells cannot progress from one cell to the next. However, they can generate an equiaxed to columnar transition (ECT), producing new columnar cells. In the model, ECT is set to occur only if there are no equiaxed grains in the surrounding liquid. When ECT starts, a new columnar front is started in the adjacent liquid cells, which can then grow, fragment and can itself be blocked. Further information about the model can be found in [1, 8, 9].

3. Structures and macrosegregation experimentally observed in the 9.8 t ingot
The focus of the present article is a 9.8 t experimental research ingot cast in A5/6 steel by Industeel. It has a diameter of 1.44 m and a height of 0.74 m, which is much smaller than typical commercial Industeel ingots. This ingot was cast specifically for research purposes and was not destined to produce a component. Ingots of this shape (large diameter compared to height) are used to make flat component such as thick plates and disks. The chemical composition of the alloy, given in table 1, was determined by spectroscopy just before casting. The mould is made
Table 1. Chemical composition in wt% of the A5/6 steel used in the 9.8 t ingot.

|   | C   | S   | P   | Si  | Mn  | Ni  | Cr  | Mo  | Cu  | Sn  | Al  | Fe  |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|   | 0.184 | 0.026 | 0.008 | 0.245 | 0.59 | 0.17 | 0.23 | 0.035 | 0.250 | 0.025 | 0.018 | Balance |

Figure 1. Experimentally observed structures of the 9.8 t ingot (Baumann print).

of cast iron and there is no hot top, however the liquid metal is covered by two layers of powder: an exothermal powder with an insulating powder on top. No inoculation was used during the casting. The total solidification time was less than 6 hours. After solidification, the ingot was cut in half along a diameter in order to analyse its macrostructure and segregation. Fig. 1 shows a sulphur print (Baumann method) of the ingot, which detects the sulphur distribution using photo-sensitive paper. This reveals the solidification structures such as dendrites and equiaxed grains. The different macrostructures were then visually identified and manually colour-coded. A columnar region (green) can be seen along the mould walls and the bottom part of the ingot. This bottom columnar layer is covered by an equiaxed structure with fine grains (light blue). In the centre of the ingot is a large columnar zone (orange) with an equiaxed structure of larger dendritic grains (dark blue) on each side. The top of the ingot is mostly columnar, with the centre region being a mix of columnar and equiaxed grains.

Spectroscopy analysis was performed on the open face of the ingot cross-section to measure carbon segregation. Shallow holes of diameter 6 to 8 mm were drilled and the analysis was performed on the resulting chips. The experimental measurements of carbon concentration are presented in fig. 2. Each data point is located by a black dot and its value is given as a percentage variation of the nominal concentration ($\Delta C/C_0$). Contour lines were manually drawn to show carbon macrosegregation. The bottom part of the ingot is negatively segregated, reaching $-15\%$ of the nominal composition. The top centre region, which is the last to solidify, features a large positive segregation, with a maximum of $+331\%$ relative to the nominal composition.

4. Numerical simulation

The solidification of the 9.8 t ingot was simulated using the SOLID® software. The mould geometry is simplified to a cylindrical shape, assuming an axial symmetry. In order to simplify the calculation, a binary Fe–C alloy is used, with 0.184 wt% carbon. The fragmentation parameters were determined by performing a sensitivity analysis on these parameters (not
Figure 2. Experimental measurements of carbon concentration in a cross-section of the 9.8 t ingot, represented as percentage variation of nominal composition ($\Delta C/C_0$). Contour lines were manually drawn according to the values. Only half of the ingot is represented, the centreline is on the left.

Figure 3. Simulation results for the 9.8 t ingot. The structure map is given on the left side, showing the columnar structure (either primary or from ECT) and the grain diameter for the equiaxed structure. On the right side, the carbon composition is given as a percentage of nominal composition.

discussed in this article), and then choosing the values that gave the results closest to the experimental ingot. The chosen fragmentation parameters are: fragmentation flux density of 2000 frag.m$^{-2}$.s$^{-1}$ and activation of fragmentation at a thermal gradient below 100 K.m$^{-1}$. The formation of columnar grains is disabled on the top surface of the ingot, where the liquid metal is in contact with the exothermal powder. Filling was not simulated, the initial state is the mould entirely filled with liquid at a uniform 2$^\circ$C superheat. With a mesh size of 1 cm and a time step of 0.1 s, the total computation time on one CPU core was 40 hours.

The final structure map and carbon segregation pattern at the end of the simulation are given in fig. 3. The same structure colour code was used as in fig. 1: green and orange for columnar, blue for equiaxed. In addition, mixed columnar-equiaxed cells are distinguished by a darker columnar colour (dark green or dark orange). Coarser mesh sizes give similar results,
with a roughly equivalent columnar thickness. Mixed cells contain both columnar and equiaxed
grains, and the equiaxed grains can block the growth of the columnar front if their envelope
fraction reaches 0.5. The equiaxed grains in a blocked mixed cell can then lead to an ECT with
a new columnar front growing in an adjacent cell. This is why along the mould wall and near
the bottom, the columnar changes from primary (green) to ECT (orange) without any visible
equiaxed (blue) cells in between. The simulated macrosegregation is similar to the experimental
results (fig. 2), with a negative segregation at the bottom and a large positive segregation with
the maximum value along the centre axis. The simulated structures also show similarities to
the Baumann print (fig. 1). The top part of the ingot features a large ECT region, which is
similar to the columnar structure observed in fig. 1. Additionally, a transition in equiaxed grain
size can be seen near the middle of the ingot. The lower part of the equiaxed structure is
comprised of grains with a size between 2 and 5 mm in diameter (light blue), but this quickly
gives way to grains which are closer to 10 mm in diameter (dark blue). This transition in grain
size corresponds to the transition from fine equiaxed structure to a larger dendritic structure
with larger grains as observed in the real ingot. However, compared to the experiment, the
negative segregation in the simulation is too close to the bottom of the ingot, and the 10%
to 35% range for the positive segregation does not extend as low. For the macrostructure, two
major differences are immediately apparent: the columnar region along the bottom mould wall
is not as thick as expected, and the large columnar region resulting from ECT (orange) in the
centre of the ingot is absent. Instead, the ECT is limited to a few discrete cells in the central
part of the ingot.

5. Analysis
The simulation shows the entire solidification sequence, explaining when and how the various
structures were formed. The solidification sequence can be divided into the following stages:

- Solidification starts immediately with a columnar front initiating on the mould walls (except
  for the top surface, as this was deliberately prevented). Fragmentation starts after a few
  seconds, generating fragments in the liquid ahead of the columnar front.
- The equiaxed grains produced by fragmentation sediment and start blocking the columnar
  front on the bottom surface. At \( t = 200 \) seconds, the equiaxed structure starts forming at
  the bottom from the accumulation of sedimented grains.
- At \( t = 290 \) s, the equiaxed structure covers the entire bottom of the ingot and has the
  flattened bowl shape seen in fig. 1. The first ECT cells appear on top of this equiaxed
  structure, with the ECT staring in the centre of the “bowl”. This can be seen in fig. 4.a,
  which shows the simulated structure at \( t = 290 \) s, with the columnar front, the sedimented
  equiaxed grains and the ECT starting at the centre. The bowl shape is formed because
  most of the sedimenting grains are coming down from the columnar front growing along the
  mould wall, leading to a higher number of grains on the outer area. The lower grain density
  in the centre is also why the ECT starts there. These structures have a shape similar to
  the experimental results, however the thickness of both the columnar and the equiaxed
  structures is much smaller than expected. In addition, the ECT does not grow into a large
  columnar structure and is instead limited to a few discrete cells. This is because the newly
  formed columnar cells are very quickly blocked by both the continuous flow of sedimenting
  grains, and by their own fragments. A columnar front from an ECT can therefore only
  grow unhindered only in the upper corner of the ingot, where the downward movement of
  the grains prevents them from blocking the columnar front.
- At \( t \approx 1340 \) s, the transition from small equiaxed grains to larger grains starts. Most of
  the columnar front growing along the mould wall has been blocked by equiaxed grains, leaving
  only the top part to fragment. This reduces the equiaxed grain density along the columnar

front, allowing the grains to grow to larger sizes. In addition, this gives the grains more time to grow as they sediment from the top of the ingot to the equiaxed structure at the bottom. These two combined effects lead to an increase in the size of the sedimenting grains and to a rapid increase in the height of the equiaxed region.

- As the equiaxed zone progresses upward, the distance between the upper fragmenting columnar cells and the equiaxed region is reduced, sedimenting grains therefore have less time to grow. The sedimentation of smaller grains slows down the upward progress of the equiaxed region. This slowdown happens at $t \approx 3260$ s, when the top of the equiaxed region is at a distance of 15 cm from the top of the ingot. At that time, less than 20% of the total volume of the ingot is still fully liquid, however there is a large mushy zone formed by the equiaxed structure. The macrosegregation of carbon at $t = 3260$ s is shown in fig. 4.b. At this stage, the macrosegregation is still low: the carbon content in the bulk liquid is $+15\%$ relative to nominal composition.

- For $t > 3260$ s, most of the macrostructures are already in place and there are no major changes. Along the top, the columnar front slowly grows inward from the mould wall, competing with the equiaxed region to fill the remaining liquid volume. This results in the columnar and equiaxed structures that are visible in the top part of the ingot in fig. 3. The end of solidification happens at $t \approx 21800$ s, finishing in the upper region at the centre of the ingot. This stage of the solidification is by far the longest ($18540$ s, $85\%$ of total solidification time), during which the macrosegregation continues to evolve slowly due to liquid flow through the equiaxed mushy zone.

6. Conclusion

The simulation results show that by using only fragmentation as a source of equiaxed grains, it is possible to reasonably predict both the macrosegregation of carbon and the macrostructure of a large steel ingot. The simulation shows that most of the structures are formed early on during solidification, 3260 s in our case, 15\% of the total 21800 s. Conversely, the large positive
segregation forms slowly over a much longer period.

However, the results are not entirely predictive, as the centre ECT columnar region is much smaller in the simulations, and the thickness of the columnar and equiaxed regions below the ECT are much thinner than observed experimentally. The simulation presented here was without filling and using a binary alloy. In order to improve the simulation results, the next step of this study will be to account for the filling stage of the ingot and multiple alloying elements. In addition, further work must be done in order to accurately predict the centre ECT structure.

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