MODELING OF PHASE TRANSFORMATION IN DUCTILE CAST IRON

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ABSTRACT

A model of the process and a simulation program were developed to trace the cooling of a nodular graphite iron casting from the beginning of solidification till the ambient temperature. The model uses the previously developed model of solidification (allowing for the nucleation and growth of eutectic grains), the heat transfer and mass diffusion equations for transient conditions pertinent to Fe-C-Si system. The kinetics of graphite and ferrite growth controlled by carbon diffusion was taken into consideration. The possibility of pearlite precipitation was assumed using a relationship of Avrami type, based on the general empirical data.

The developed simulation program enables determination of the kinetics of growth of graphite, austenite, ferrite and possibly also pearlite on the casting cross-section as well as grain density related to boundary conditions of the casting cooling. The computed values of the temperature of a plate casting poured in sand mold, of the volume fraction of graphite, ferrite and pearlite, and of the grain density on the casting cross-section were compared with the experimental results.

Key words: modeling, phase transformation, ductile cast iron,
1. INTRODUCTION

Nodular graphite cast iron has major applications in critical engineering parts due to its excellent properties and castability. The mechanical, physical and utilization properties of this cast iron depend on the content of the solidified graphite and on the individual matrix constituents, and as claimed in [1] they can be anticipated according to the law of additivity. The prediction of local properties of castings is an old dream of foundrymen and casting designers which nowadays is becoming every day more true due to the development of our computational abilities. To predict the mechanical properties of nodular graphite iron it is necessary to simulate the volume fraction of the individual structural constituents present in this cast iron.

Most of the computer modeling programs described in literature are devoted to eutectic transformation [1-6] under the pre-assumed stationary conditions of carbon diffusion in austenite. In [5] a physical model of solidification of the nodular graphite cast iron which quantitatively accounts for the formation of non-eutectic austenite during cooling and solidification of hypereutectic as well as hypoeutectic cast iron has been presented. In investigation [6], process modeling techniques have been applied to describe the multiple phase changes occurring during solidification and subsequent cooling of near-eutectic nodular graphite cast iron, based on the internal state variable approach.

The decomposition of austenite to ferrite plus graphite or to pearlite in nodular graphite cast iron is known to depend on a number of factors which include nodule count, the cooling rate, and alloying additions [7-10].

The problem of modeling the ferritization process in nodular graphite cast iron has been the subject of investigations described in [2-4], [6], [11-13]. In most cases it consists in solving a diffusion equation for stabilized conditions given in [14, 15]. The only exception is [13] which discusses the problem of ferrite growth under transient conditions of diffusion in austenite, but this is done with a non-realistic assumption that the initial graphite dimension equals zero.

The aim of this study was to create a model of structure formation in eutectic nodular graphite cast iron. For modeling of eutectic transformation and the growth of graphite in austenite in a range from the eutectic up to eutectoid transformation and during ferritization, the heat transfer and mass diffusion equations for transient conditions have been used, while pearlitization has been described by a general empirical equation.

2. MATHEMATICAL MODEL OF PROCESS

A model of the kinetics of graphite growth in nodular graphite cast iron solidifying in a foundry mold has been developed. The model allows for the following phenomena:
- solidification of liquid metal with composition of nodular graphite cast iron in a foundry mold from the instant of pouring this mold to ambient temperature,
- graphite nucleation from liquid phase and coupled growth with austenite in the form of eutectic grains,
the growth of graphite nodules in austenite envelope below the temperature of eutectic transformation,

- the formation and growth of ferrite envelope between graphite and austenite below the point of eutectoid equilibrium state,

- graphite growth during eutectoid transformation,

- the possibility of pearlite growth below eutectoid point.

For description of these phenomena the following equations were used:

- heat conduction in cast metal and in mold material,

- nucleation and growth of eutectic grains combined with liquid undercooling,

- increase in volume fraction of the solidified metal using Kolmogorov [16] equation,

- carbon diffusion in, respectively: graphite-austenite and graphite-ferrite-austenite,

- empirical equation interrelating the volume of the precipitated pearlite with undercooling rate.

The boundary conditions of diffusion allow for the silicon effect on carbon solubility at the interfaces of graphite-austenite, graphite-ferrite, and ferrite-austenite as well as for the mass balance on these grains. The effect of the spherical grains mutual contact, i.e. of the real shape of these grains, on the diffusion flux of a constituent was also taken into consideration.

3. SET OF EQUATIONS

The model combines a macro model (heat transfer) with micro model (mass diffusion). The macro temperature field in casting-mold system is:

$$\frac{\partial T}{\partial \tau} = a\nabla^2 T + \frac{q_s}{c_v}$$

where:

- $a$ – thermal diffusivity (for metal or for mold);

- $q_s$ – heat generation rate of phase transformations;

- $c_v$ – specific heat.

The heat generation rate of solidification was solved according to [17,18].

A micro-model of the nodular cast iron graphitization, which takes place in each eutectic grain, was based on the diffusion equation:

$$\frac{\partial C}{\partial \tau} = D \cdot \nabla^2 C,$$

where:

- $C$ – carbon concentration,

- $D$ – carbon diffusion coefficient ($D_a$ - in ferrite, $D_f$ - in austenite),

- $\tau$ – time.

Diffusion field is solved in Elementary Diffusion Field (EDF) [18].

Under real conditions, the grain volume $V_g$ characterized by a spherical symmetry of growth will depend, due to stochastic grain impingement, on grain density $N$ according to Kolmogorov equation:
where \( R \) – radius.

In EDF the surface of diffusion is determined by equation

\[
S_R = \frac{dV_R}{dR} = 4\pi \cdot R^2 \cdot e^{-\frac{N_\alpha}{3} \pi R^3}.
\]

The above set of equations was solved for the austenite and ferrite envelopes with boundary conditions of the individual interfaces present in Fe-C-Si system \([19,10]\):

\[
C_{\gamma/gr} = 0.68 - 0.029 \cdot Si_{\gamma/gr} + \frac{\left( T - 5.5 \cdot (Si_{\gamma/gr} + 1.1)^2 - 731.3 \right) \left( 1.33 - 0.169 \cdot Si_{\gamma/gr} \right)}{415.045 - 9.7 \cdot Si_{\gamma/gr} - 5.5 \cdot Si_{\gamma/gr}^2},
\]

\[
C_{\gamma/\alpha} = 5.203 \cdot 0.00614 \cdot T + 0.1665 \cdot Si_{\gamma/\alpha},
\]

\[
C_{\alpha/\gamma} := 0.1063 \cdot 0.00012 \cdot T + 0.0131 \cdot Si_{\alpha/\gamma},
\]

\[
C_{\alpha/gr} = 2587 \cdot \exp \left( -0.53 \cdot Si_{\alpha/gr} - \frac{12110}{T + 273.15} \right),
\]

and for austenite at the external border of EDF in the solid state \( dC/dr = 0 \).

To determine the linear rate of the front displacement in phase transformation, a carbon mass balance equation at the phase boundary has been used. For the graphite growing in contact with ferrite and austenite, respectively, this equation assumes the following forms:

\[
-D_{\alpha} \frac{dC_{\alpha}}{dr} \bigg|_{r=r_{gr}} = \left( \rho_{gr} - C_{\alpha/gr} \cdot \rho_{\alpha} \right) \frac{dr_{gr}}{d\tau},
\]

\[
-D_{\gamma} \frac{dC_{\gamma}}{dr} \bigg|_{r=r_{gr}} = \left( \rho_{gr} - \rho_{\gamma} \cdot C_{\gamma/gr} \right) \frac{dr_{gr}}{d\tau},
\]

where: \( \rho_{gr}, \rho_{\alpha}, \rho_{\gamma} \) – graphite, ferrite and austenite density, respectively.

To determine the carbon mass balance at the front of austenite transformation in ferrite the following condition has been allowed for:

\[
-D_{\gamma} \frac{dC_{\gamma}}{dr} \bigg|_{r=r_{gr}} + D_{\alpha} \frac{dC_{\alpha}}{dr} \bigg|_{r=r_{gr}} = \left( \rho_{\alpha} \cdot C_{\alpha/\gamma} - \rho_{\gamma} \cdot C_{\gamma/\alpha} \right) \frac{dr_{gr}}{d\tau}.
\]

The possibility of pearlite growth was assumed using general data collected by Laca [20, Fig. 5]. Their use enabled deriving type of Avrami relationship, interrelating the pearlite volume fraction with cooling rate \( T' \):
\[ f_{\text{Pe}} = 1 - \exp\left(-5.2 \cdot 10^{-10} \cdot T^0.15 \cdot \tau_1^2\right), \]  

where: \( \tau_1 \) – time from the beginning of metastable eutectoid transformation.

The above set of equations was solved by difference method with the implicit scheme.

Modeling was performed for thermophysical parameters given in [17] and, additionally for the purpose of the present study, in Table 1. The results of this modeling were confronted with the results obtained on an experimental casting made from the cast iron of composition given in Table 2.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
Latent heat: & - of pearlite evolution \quad 89.7 \text{ J/g} [3] \\
& - of ferrite and graphite evolution \quad 90 \text{ J/g} \\
Activation energy for diffusion of C: & - in ferrite \quad 134 \text{ kJ/mol} [6] \\
& - in austenite \quad 87 \text{ kJ/mol} [6] \\
Initial temperature: & - cast iron \quad 1380 \text{ °C} \\
& - mould \quad 20 \text{ °C} \\
Plate cast thickness & 11 \text{ mm} \\
\hline
\end{tabular}
\caption{Table 1}
\end{table}

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|}
\hline
Content, \% mass. & C & Si & Mn & P & S & Mg \\
\hline
3.44 & 2.41 & 0.12 & 0.04 & 0.009 & 0.041 \\
\hline
\end{tabular}
\caption{Table 2}
\end{table}

4. THE RESULTS OF MODELING

A simulation program was developed and the results of computer simulation were compared with the experimental results obtained for a plate casting of 11-mm thickness made from nodular graphite cast iron.

Figure 1 shows the casting temperature curve obtained by computer modeling and by experiments. The arrests typical of solidification and eutectoid transformation are well visible. In Figure 2 the kinetics of growth of the individual phases, i.e. graphite, pearlite and ferrite, is shown. A very distinct difference in final phase volume fraction on the casting cross-section, especially as regards pearlite and ferrite, is visible. More exact information of the kinetics of graphite growth is given in Figures 3 and 4, including graphite volume and radius, respectively. Three typical periods are distinguished: A - B - solidification, B - C - graphite growth from austenite, C - D - eutectoid transformation. On casting cross-section, the points, which mark the beginning and end of the individual periods, are slightly shifted. A change in the dimension of graphite nodules with ferrite shell is also visible in Figure 4. A decrease in graphite radius at the casting surface is observed.

Figure 5 shows the distribution of volume fractions of the individual phases combined with increasing grain density on casting cross-section. A tendency towards the increasing ferrite volume with respective decrease in pearlite volume at the casting sur-
face is observed, while the volume of graphite remains practically stable. A change in the dimension of graphite nodules is visible in Figure 6. A decrease in graphite radius at the casting surface combined with increasing grain density is observed. The points in Figures 5 and 6 mark the values obtained in an experiment referred to volume fractions of each phase and grain density.

Fig. 1: Cooling curve for plate casting of 11 mm thickness solidifying in sand mold.

Fig. 2: Kinetics of growth of the volume fractions of graphite, ferrite and pearlite in the plate casting. The individual curves are for points 1 (middle) - 10 (surface) on casting cross-section.

Fig. 3: Kinetics of graphite volume fraction growth.

Fig. 4: Kinetics of graphite and ferrite radius growth.
5. SUMMARY

The developed modeling program enables determination of the kinetics of growth of graphite, austenite, ferrite and possibly also pearlite on casting cross-section as well as the grain density combined with boundary conditions of casting cooling from the beginning of solidification till the end of eutectoid transformation.

The computed values of the temperature field, graphite, ferrite and pearlite volume fractions and grain density on casting cross-section reveal satisfactory consistency with experimental results.

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REFERENCES


STRESZCZENIE

Opracowano model procesu i program symulacyjny pokazujący przebieg stygnięcia odlewu z żeliwa sferydłalnego od początku krystalizacji do zakończenia przemian eutektoidalnej. Wykorzystano opracowany wcześniej model krystalizacji, uwzględniający zarodkowanie i wzrost ziaren, przewodzenie ciepła i dyfuzję masy dla warunków nieustalonych wraz z warunkami brzegowymi na granicach grafit-ferryt-austenit, determinowanych układem Fe-C-Si. Uwzględniono kinetykę wzrostu grafitu i ferritu kontrolowaną przez dyfuzję węgla. Przewidziano możliwość wydzielenia się perlitu z wykorzystaniem zależności typu Avramiego, opartej na uogólnionych danych empirycznych.

Opracowany program symulacyjny umożliwia wyznaczenie kinetyki wzrostu grafitu, austenitu, ferritu i ewentualnie perlitu w przekroju odlewu, a także gęstości ziaren w połączeniu z warunkami brzegowymi stygnięcia odlewu. Temperatura w odlewie płyty wykonanej w formie piaskowej, objętości grafitu, ferritu i perlitu oraz gęstość ziaren w przekroju odlewu zostały skonfrontowane z eksperymentem.

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