METHOD FOR CALCULATING THE MICROSTRUCTURE & MECHANICAL PROPERTIES OF DUCTILE CAST IRON

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SUMMARY

Ductile Cast Iron (DCI) is now widely accepted as a material for manufacture of thick-walled containers for the storage and transport of spent fuel and intermediate level radioactive waste. Material specifications for DCI in this application (e.g. JIS G 5504, Rehmer et al., 1995) require that both certain mechanical properties and microstructure are achieved throughout the casting. Most important of these requirements include minimum elongation, maximum 20% pearlite in the matrix, and minimum 80% nodularity of the graphite (when measured using the ISO 945 method). These properties all depend upon the cooling conditions during solidification, which vary throughout a casting. This paper will describe a method for calculating the distribution of microstructure and mechanical properties of a thick-walled ferritic DCI casting from a knowledge of the temperature-time history during solidification, as obtained, for example, from a thermal solidification analysis.

INTRODUCTION

In order to be suitable for use in radioactive material transport applications, thick-walled DCI must satisfy requirements on microstructure as well as mechanical properties of the material throughout the casting. Such requirements typically include:

- Minimum tensile properties
- Pearlite content $\leqq$ 20% (Rehmer et al., JIS G 5504)
- Graphite nodularity $\geqq$ 70%* (JIS G 5504)

* 70% when measured in accordance with the JFS method, which is approximately equal to 80% when measured in accordance with the ISO 945 method.

The location on the casting for testing these properties is subject to agreement between the supplier and purchaser. As the microstructure and mechanical properties are functions of the cooling rates during manufacture, these properties will vary throughout the casting. This raises the question of where to measure these properties, i.e. where in the casting are the worst properties to be found.

This paper presents a method for calculating the relevant microstructure and mechanical properties of DCI from cooling rates during casting. These cooling rates can be obtained from a thermal analysis of the casting process. The relevant microstructure properties are nodule count (number of graphite nodules per mm^2), nodularity (percentage of nodules which are spherical in form), ferrite grain size and percentage pearlite. The mechanical properties considered in this paper are yield stress, tensile strength, elongation, static upper shelf toughness J_{IC} and K_{JC}. The method is illustrated for the case of a DCI containing 3.5% carbon, 1.8% silicon and 0.2% manganese.

NODULE COUNT

There are three phenomena to be considered in calculating the nodule count: nucleation, growth and fading. Nucleation is the formation of nuclei of graphite in the molten iron as it starts to solidify, growth is the growth of these particles during the solidification process, and fading is the reduction in the number of nuclei with time due to loss of inoculant etc during solidification.

The rate of nucleation can be obtained from Oldfield's equation (Oldfield, 1966):

$$N = A.\Delta T^2$$

where N = number of nuclei per unit volume

ΔT = degree of undercooling. This is the difference between the eutectic solidification temperature and the actual temperature of the melt.

A = empirical coefficient, determined experimentally.

During solidification the graphite nodule becomes surrounded by austenite, and the rate of growth of the nodule becomes a function of the rate of diffusion of carbon from the melt through the austenite to the growing nodule. This can be obtained from Su's equation (Su et al., 1985):

$$\frac{dR_a}{dt} = \frac{D_c^{\gamma}(C_{al} - C_{ag})R_g}{(R_a - R_g)R_a(C_{la} - C_{al})}$$

where R_a = radius of austenite shell

D_c^{γ} = diffusion coefficient of carbon in austenite

R_g	=	radius of graphite nodule
C_{al}	=	carbon concentration of the austenite at the liquid boundry
C_{ag}	=	carbon concentration of the austenite at the graphite boundry
C_{la}	=	carbon concentration of the liquid at the austenite boundary

The values of C_{al}, C_{ag} and C_{la} can be obtained from the phase diagram of the alloy under consideration.

The nodule count, uncorrected for fading, is obtained by solving the above two equations simultaneously . During solidification the undercooling increases until at a certain point the rate of release of latent heat is greater than the rate of removal of heat, at which point the temperature starts to rise. At this point no further nodules are assumed to form, and the nodule count is obtained from the maximum undercooling calculated. In general to solve this type of problem it is necessary to carry out a coupled thermal-microstructure analysis. However, in the case of DCI used for radioactive materials transport packages , i.e. with thick walls and significant inoculation to increase the nodule count, the undercooling is only a fraction of a degree, and is possible to decouple the two. Figure 1 shows the results of solving these equations for the DCI in question for a range of cooling rates at the solidification temperature.

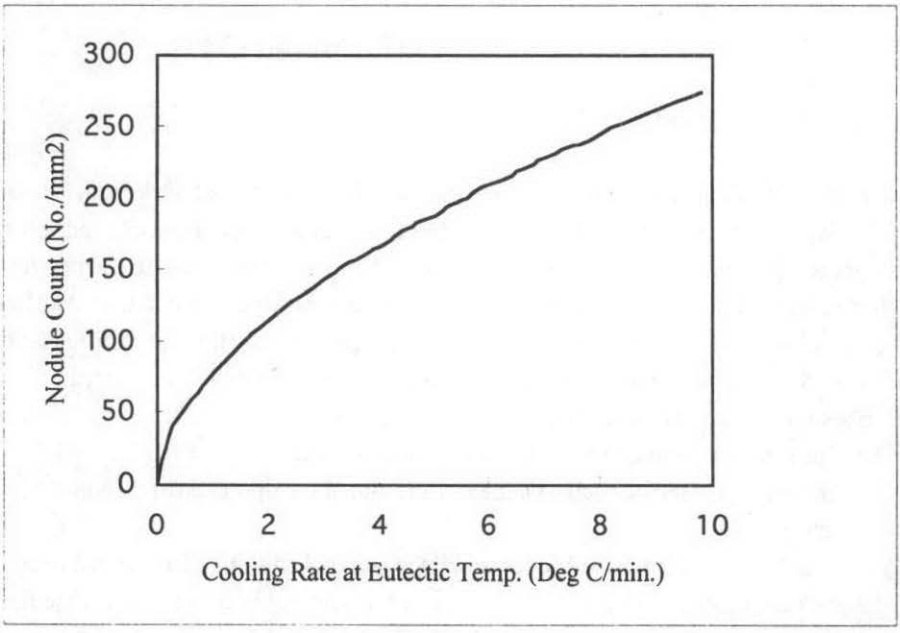

Figure 1 **Relationship between Cooling Rate at Eutectic Temperature and Nodule Count**

Fading is the reduction in the number of locations within the melt which can potentially act as nuclei for the formation of graphite. The extent of this phenomenon depends upon the type of inoculant used, but in general there is an exponential decrease in the nodule count. To correct for this effect the nodule count from Figure 1 should be multiplied by $\exp(-t/t^*)$, where t is the time between inoculation and the start of the solidification reaction, and t^* is a parameter dependant upon the type of inoculant used (Wessen, 1997).

NODULARITY

The percentage nodularity is a function of the eutectic solidification time. There is very little quantitative published research on the relationship between nodularity and solidification time, only one paper has been found (Iwabuchi et al., 1987) from which the following equation was derived.

$$\text{Nodularity (by JFS method)} = 87.5\exp(-0.0539t) \quad (\%)$$

where t = time from start to finish of the eutectic reaction in hours

Nodularity from the JFS method is related to that from the ISO method using the equation (JIS G 5502):

$$\text{ISO 945 Nodularity value} = 4.58 + 1.05(\text{JFS Nodularity Value})$$

PERCENTAGE FERRITE/PEARLITE

The method of calculating the percentage ferrite/pearlite followed that of Wessen (Wessen, 1997). When the temperature falls below the stable eutectoid temperature (around 750-800 ℃, depending upon the composition of the iron) austenite can decompose to ferrite. As the carbon content of ferrite is much smaller than that of austenite the carbon released diffuses to the graphite nodules. The rate of transformation is governed by the rate of diffusion of carbon in ferrite, and the rate of incorporation of carbon into the nodules. Wessen describes this process as a three stage process as follows:

- Formation of a complete ferrite shell around the nodules
- Growth of the ferrite shell governed by the rate of incorporation of carbon into the nodule
- Growth of the ferrite shell governed by the rate of diffusion of carbon in ferrite.

In the work described in this paper problems were encountered in trying to apply the first stage. However this first stage appears to be a refinement, and the essentials of the process can be captured with the second and third stages only. The growth rate of ferrite in stage 2 is given by:

$$\frac{dl^{\alpha}}{dt} = \frac{(C_c^{\alpha\gamma} - C_c^{\alpha gr})}{(C_c^{\gamma\alpha} - C_c^{\alpha\gamma})} \cdot \left(\frac{R_g}{R_\alpha}\right)^2 \cdot \exp\left(\frac{4\pi R_\alpha^3}{3}\right) \mu$$

and the rate of growth in stage 3 is given by:

$$\frac{dl^{\alpha}}{dt} = \frac{(C_c^{\alpha\gamma} - C_c^{\alpha gr})}{(C_c^{\gamma\alpha} - C_c^{\alpha\gamma})} \cdot \frac{R_g D_c^{\alpha}}{l^{\alpha} R_\alpha}$$

where

l^{α}	=	thickness of ferrite shell
R_α	=	Radius of the ferrite shell
R_g	=	Radius of the graphite nodule
D_c^{α}	=	Coefficient of diffusion of carbon in ferrite
μ	=	parameter describing the rate at which carbon atoms can be incorporated on to the graphite surface

$C_c^{\alpha\gamma}$, $C_c^{\alpha gr}$ and $C_c^{\gamma\alpha}$ are derived from the phase diagram for the alloy in question.

When the temperature falls below the metastable eutectoid temperature (about 30℃ below the stable eutectoid temperature, depending upon the composition of the iron in question) then pearlite starts to form from any remaining austenite. The growth rate of pearlite is faster than that of ferrite, and is given by $(dR_p/dt) = k\Delta T^2$, where $k \sim 9.4 \times 10^{-10}$ (Wessen, 1995). In solving these equations it is necessary to take account of segregation of silicon and manganese, and their effect on the eutectoid temperatures.

The results for the iron in question are shown in Figure 2.

FERRITE GRAIN SIZE

No method of calculating ferrite grain size of DCI has been found in the literature. However, from the data in Table 5d of Frenz (Frenz, 1991), it was found that ferrite grain size is approximately equal to (nodule diameter × 1.6). This result was valid for both heat treated and non-heat treated samples. The results of Yanagisawa (Yanagisawa, 1983) are consistent with this for carbon contents between 3 - 4 wt%, but for carbon contents outside this range the relationship is not valid.

MECHANICAL PROPERTIES

There have been many studies of the relationship between microstructure and mechanical properties of DCI. However in most cases only a limited range of microstructural parameters have been studied, so that the range of application of the formulae deduced is rather limited. Formulae containing a greater number of parameters and with a wider

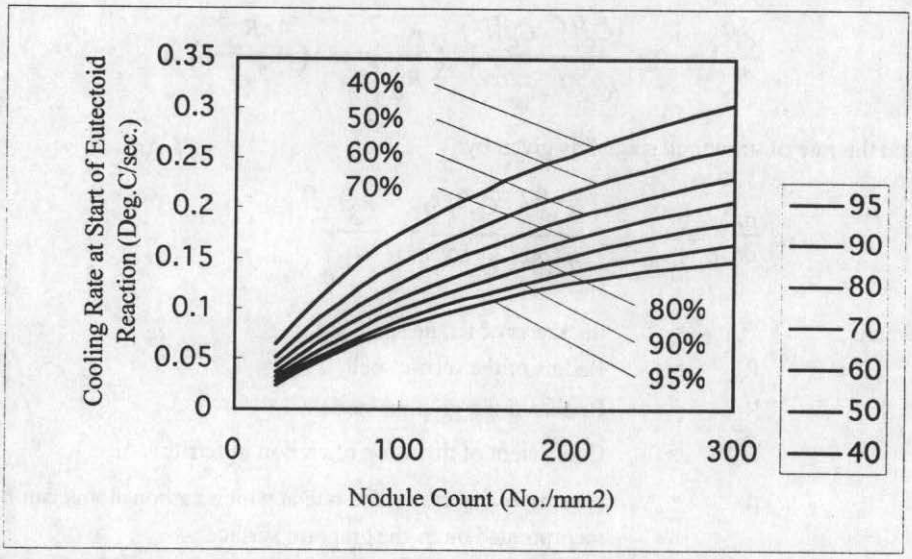

Figure 2 **Variation of Ferrite Percentage with Nodule Count and Cooling Rate at the Start of the Eutectoid Reaction**

range of application have been deduced using the results of a number of separate studies as follows:

$$\text{Yield Stress} = 52 + 63.2\times\%\text{Si} + 0.663\times\%\text{Pearlite} + 21.6(1 - 0.0656\times\%\text{C})(\text{Ferrite Grain Size})^{-0.5} \quad \text{(MPa)}$$

$$\text{UTS} = 147 + 68.1\times\%\text{Si} + 1.77\times\%\text{Pearlite} + 26.7(1 - 0.0656\times\%\text{C})(\text{Ferrite Grain Size})^{-0.5} \quad \text{(MPa)}$$

These formulae were derived by combining formulae from Frenz (Frenz, 1991) and Yanagisawa (Yanagisawa, 1985).

$$\text{Elongation} = 37.85 - 0.093\times\text{CMMH} - 0.032(95 - \text{Nodularity}) \quad (\%)$$

where CMMH = (Ferrite Hardness × %Ferrite + Pearlite Hardness × %Pearlite)/100

Ferrite Hardness = 64 + 44%Si + 9%Mn + 114%P + 10 %Cu + 7%Ni + 22%Mo

Pearlite Hardness = 249 + 26%Si + 12%Mn + 234 %P + 16%Cu + 17.5%Ni + 26%Mo

This formula was obtained by combining formulae from Venugopalan (Venugopalan, 1990) and Okada (Okada, 1969).

$$J_{IC} = 23.6 + 581\times D_A - 0.5(95 - \text{Nodularity}) - 0.06\times\text{Pearlite} - 0.004\times(\text{Nodularity}\times\%\text{Pearlite}) \quad (\text{kJ/m}^2)$$

Where D_A = average nodule diameter

This formula has been obtained by combining formulae provided by Salzbrenner (Salzbrenner, 1989) and Bhandhubanyong (Bhandhubanyong et al., 1985).

The static upper shelf fracture toughness, K_{JC}, can be obtained from $K_{JC} = (EJ_{IC})^{0.5}$.

In all the above mechanical property equations %Pearlite = (100 - %Ferrite), and Nodularity is measured according to the JFS Method.

CONCLUSION

Using the method described above the distribution of microstructure and mechanical properties of DCI can be calculated from the temperature-time histories obtained from a thermal solidification analysis of the casting process. Work is currently in progress on the validation of this methodology.

It should be noted that this method does not take account of the effect of trace elements, some of which can have an important effect on the microstructure and mechanical properties of DCI.

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