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A 2-D nucleation-growth model of spheroidal graphite
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A B S T R A C T

Analysis of recent experimental investigations, in particular by transmission electron microscopy, suggests spheroidal graphite grows by 2-D nucleation of new graphite layers at the outer surface of the nodules. These layers spread over the surface along the prismatic direction of graphite which is the energetically preferred growth direction of graphite when the apparent growth direction of the nodules is along the basal direction of graphite. 2-D nucleation-growth models first developed for precipitation of pure substances are then adapted to graphite growth from the liquid in spheroidal graphite cast irons. Lateral extension of the new graphite layers is controlled by carbon diffusion in the liquid. This allows describing quantitatively previous experimental results giving strong support to this approach.

1. Introduction

Graphite spheroids in spheroidal graphite cast iron are known to consist of piling up of graphite layers having their $c$ axis oriented parallel to the spheroid radius. To accommodate for the change in orientation in the tangential direction, the spheroids appear to be divided in adjacent sectors which are easily observed by optical microscopy as illustrated in Fig. 1. The change in orientation of the $c$ axis at the boundary between two sectors may amount from 10 to several tens of degrees, while the orientation changes within sectors are more limited [1,2].

It has long been recognized that graphite layers within spheroids are arranged in growth blocks which are elongated along the prismatic $a$ direction of the graphite structure [3]. This would imply that graphite grows along the prismatic (tangential) direction during spheroidal growth even though the overall (apparent) growth direction is the radial one. Two types of models have been suggested in the past to account for this tangential growth: i) those based on screw dislocations [4] or cone-helix growth [5–7]; and ii) those based on the continuous growth of a graphite layer folding around the spheroid [8,9]. In the first type, tangential growth proceeds around screw dislocations or cones emanating from the spheroid’s centre (Fig. 2-a), giving features that would agree with the observation of sectors. However, transmission electron microscopy (TEM) observations have shown that the orientation of the $c$ axis along a sector tilts at random and in either ways [10] which implies that continuous growth around a screw dislocation did not occur. The second type of models (Fig. 2-b) would hardly explain the formation of sectors as already stressed by Gruzleski [9]. However, a slight modification where nucleation of new layers proceeds at the step between two neighbouring sectors which was suggested by Double and Hellawell [11] would (Fig. 2-c).

There has been a renewed interest these last years for investigating the growth mechanism of spheroidal graphite [12–14]. Qing et al. [14] report observation of defects and dislocations in graphite, but do not seem to have observed long range ordered arrangements of these defects that would support the screw dislocation or the cone-helix mechanism. Amini and Abbaschian [12] observed both plate-like and spheroidal growth of graphite in Ni-C samples. They proposed a model for plate-like growth including thickening of the plates by 2-D nucleation and lateral extension of new graphite layers. To explain spheroidal growth, Amini and Abbaschian suggested a roughening transition at the graphite liquid interface which would have no reason for giving sectors as observed. Stefanescu et al. [13] proposed graphite spheroids build-up as so-called tad-pole dendrites. These dendrites emanate from the centre of the spheroids and are made of plate-like growth blocks stack upon each other, though not filling the space as does graphite in spheroids. Considering the model shown in Fig. 2-c and recent TEM

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observations [2,15] suggest to extend to spheroids the 2-D nucleation and growth model developed by Amini and Abbasschian [12] for plate-like growth of graphite from the liquid. Such an approach has been in fact already suggested based on a simple model [16] and is presented here in a much more formal and quantitative way.

2. 2-D nucleation

Let \( n \) be the number of 2-D nuclei per unit area of the graphite/liquid interface. The nucleation rate \( J_a = \dot{n} = dn/\dot{t} \) is given by Ref. [17]:

\[
J_a = \frac{N_A}{V_m} \left( \frac{L \cdot \Delta T}{R \cdot T \cdot T_m} \right)^{1/2} \frac{3 \cdot \beta \cdot D}{2 \cdot a_0} \exp \left( - \frac{\Delta g^*}{R \cdot T} \right)
\]

(1)

where \( N_A \) is Avogadro’s number, \( V_m \) is the molar volume of the liquid, \( L \) is the melting enthalpy and \( T_m \) the melting temperature, \( R \) the gas constant, \( T \) the current temperature and \( \Delta T = T_m - T \) is the undercooling, \( \beta \) corrects for structural factors [18], \( D \) is the diffusion coefficient in the liquid, \( a_0 \) is the atomic radius, \( \Delta g^* \) is the excess energy needed for nucleus formation and \( k_B \) is Boltzmann’s constant. \( \beta \) is expected to take values close to 1 for simple molecules (atoms) and lower than 1 for complex molecules, it will be set to 1 in all the following calculations.

In the above expression, \( L \cdot \Delta T/T_m \) is an estimate of \( \Delta G_m \), the molar free enthalpy change upon melting of the solid. As suggested by Turnbull and Fisher [19], the fact that graphite precipitates here from an alloy and not from a pure melt may be accounted for by multiplying \( J_a \) by the atomic fraction of carbon, \( x_c \). Equation (1) may thus be written:

\[
J_a = x_c \cdot \frac{N_A}{V_m} \left( \frac{\Delta G_m}{R \cdot T} \right)^{1/2} \frac{3 \cdot \beta \cdot D}{2 \cdot a_0} \exp \left( - \frac{\Delta g^*}{R \cdot T} \right)
\]

(2)

Considering nuclei at the surface of a nodule form as discs of radius \( r \) and height \( h \), the corresponding free energy change is given as:

\[
\Delta g = -\pi \cdot r^2 \cdot h \cdot \frac{\Delta G_m}{V_m} + 2 \cdot \pi \cdot r \cdot \sigma_e
\]

(3)

where \( V_m \) is the graphite molar volume and \( \sigma_e \) is the step energy by length.

Differentiating with respect to \( r \) gives the critical value \( r^* \):

\[
r^* = \frac{1}{h} \frac{\sigma_e}{\frac{\Delta G_m}{V_m}}
\]

(4)

and

\[
\Delta g^* = \frac{\pi}{h} \frac{\sigma_e^2}{\frac{\Delta G_m}{V_m}}
\]

(5)

Note that \( h \) cannot be determined by this procedure and is most generally considered as being the height of one single atom layer. According to Cahn et al. [18], the step energy per length \( \sigma_e \) is related to the surface energy \( \sigma \) by:

\[
\sigma_e = \sigma \cdot a \cdot \sqrt{\xi}
\]

(6)

where \( a \) is the height of one single atom layer and \( \xi \) is interface diffuseness which is 1 at most for a sharp interface and can be much smaller in practice [18].

Using the expression for \( \sigma_e \) and setting \( h = a \), one obtains:

\[
r^* = \frac{1}{a} \frac{\sqrt{\xi} \cdot \sigma}{\frac{\Delta G_m}{V_m}}
\]

(7)

\[
\Delta g^* = \frac{\pi \cdot a \cdot \xi \cdot \sigma^2}{\frac{\Delta G_m}{V_m}}
\]

(8)

Calculations have been made with \( x_c = 0.175 \) which is the eutectic composition in the Fe-C system, \( a = a_0 = 3.51 \cdot 10^{-10} \) m (distance between basal planes), \( D = 5 \cdot 10^{-9} \) m\(^2\) s\(^{-1}\) as previously selected [20], \( \sigma = 1 \) J m\(^{-2}\) for the prismatic planes (see the review of available data [21]). \( V_m = 7.5 \cdot 10^{-6} \) m\(^3\) mol\(^{-1}\) and \( V_m = 5.31 \cdot 10^{-6} \) m\(^3\) mol\(^{-1}\), \( T = 1450 \) K, and \( |\Delta G_m| = 13.64 \cdot \Delta T \) J mol\(^{-1}\) [22], where \( \Delta T \) is the undercooling with respect to the graphite liquidus and is defined positive. One obtains:

\[
r^* = 0.4 \cdot \frac{\sqrt{\xi}}{\Delta T} \cdot 10^{-6} \text{m}
\]

(9)

\[
\Delta g^* = 4.3 \cdot 10^{-16} \cdot \xi \cdot \frac{\Delta T}{J}
\]

(10)

\[
J_a = 10^{28} \cdot (\Delta T)^{1/2} \cdot \beta \cdot \exp \left( - \frac{21500 \cdot \xi}{\Delta T} \right) \text{m}^{-2} \cdot \text{s}^{-1}
\]

(11)

Fig. 3 shows \( r^* \) and \( J_a \) versus \( \Delta T \) calculated for \( \beta \) set to 1 and \( \xi \) set to 0.1, 0.5 and 1. A value of \( \xi \) of about 0.1 would seem reasonable as it would give a few hundreds of nuclei per second on the outer
surface of a nodule 10 μm in radius growing at an undercooling of 50 K.

3. Growth kinetics

For describing the effective growth of a faceted crystal along the direction of the facet plane, Cahn et al. [18] and Hillig [17] considered two limits for 2-D nucleation and growth, when either nucleation or spreading of the layers is controlling.

In the first case, it is considered that a new layer nucleates only when the previous layer has spread over the corresponding crystal facet, this is the so-called MNG (mono-layer growth) process [23]. Following Tiller [24], we can ask the question: “What is the radius of disk, $R$, of a crystal facet which has unit probability that a new nucleus will form on top of the disk in the time $\tau$ that it takes to the original disk to grow to its maximal extension?” Assuming a constant ledge velocity, one then has:

$$J_a \left( \frac{\pi \cdot R^2}{4 \cdot \pi} \right) \cdot \tau = 1$$  \hspace{1cm} (12)

For the present case, we shall consider that the crystal facet is the outer surface of a sector. If a nodule of radius $R_G$ has $N_S$ similar sectors, then:

$$\tau = \frac{N_S}{J_a \left( 4 \cdot \pi \cdot R_G^2 \right)}$$  \hspace{1cm} (13)

Within this time interval $\tau$, $N_S$ new nuclei are expected to spread over the surface of the $N_S$ sectors, i.e. on a distance that scales as $L_S = 2 \cdot R_G \cdot \sqrt{N_S}$. Fig. 4 illustrates the change of $\tau$ versus undercooling (with respect to graphite liquidus) for $\xi = 0.1$, $N_S = 100$ and $R_G$ set to 1, 10 and 50 μm. When the nucleation rate becomes reasonable — at an undercooling larger than 50 K as seen above — the corresponding spreading time becomes so small that this model does not seem to be appropriate. This has been emphasized by plotting on the same graph the corresponding spreading velocity, which becomes unphysically high for undercoolings higher than 50 K. This trend is certainly related to the fact that the far field diffusion of carbon is not accounted for by the model which was derived for precipitation in pure melts.

The other alternative is the so-called PNG (poly-layer growth) mechanism [23] that is controlled by the growth rate and not by the nucleation rate. The growth rate $G$ is now given as [17]:

$$G_{PNG} = a \cdot \left( \frac{\pi}{3} \cdot J_a \cdot (V_l)^2 \right)^{1/3}$$  \hspace{1cm} (14)

where $V_l$ is the spreading rate of the ledge and has been here assumed constant. Other exponents and relations could be obtained when using different laws for spreading rate [23].
If there is no constraint, \( V_I \) can be expressed as its value for a straight ledge \( V_{\text{se}} \), which is according to Cahn et al. [18]:

\[
V_{\text{se}} = \frac{D |\Delta G_m|}{h \cdot R \cdot T} \cdot \beta \left( 2 + \xi^{-1/2} \right) \tag{15}
\]

Inserting this latter expression in Equation (14), one obtains for the PNG process with \( h = a \):

\[
G_{\text{PNG}} = \frac{\pi}{2} x_c \cdot \frac{N_a}{v_m} \left( \frac{|\Delta G_m|}{R \cdot T} \right)^{5/6} \cdot \beta \left( 2 + \xi^{-1/2} \right)^{2/3} \cdot \exp \left( -\frac{\Delta g^*}{3 \cdot k_B \cdot T} \right) \tag{16}
\]

With the values already used, \( G_{\text{PNG}} \) becomes:

\[
G_{\text{PNG}} \approx 0.05 \cdot (\Delta T)^{5/6} \cdot \beta \left( 2 + \xi^{-1/2} \right)^{2/3} \cdot \exp \left( \frac{-7200 \cdot \xi}{\Delta T} \right) \text{m} \cdot \text{s}^{-1} \tag{17}
\]

Fig. 5 shows with dotted lines the evolution of \( G_{\text{PNG}} \) according to equation (17) for \( \beta \) set to 1 and \( \xi \), set to 0.1, 0.5 and 1. The horizontal interrupted line corresponds to the experimental thickening rate of graphite plates along their \( e \) direction as estimated by Amini and Abbaschian [12]. This value of 0.1 \( \mu \text{m s}^{-1} \) is obtained for an undercooling of 40 K at \( \xi = 0.1 \) and 200 K at \( \xi = 0.5 \), both values being well within the reported experimental range [12] of undercooling values with respect to graphite liquids.

For the same reason than for the MNG model, the PNG model is expected to predict too high growth rates. There is an alternative cooling scheme made use of a Zener-type formulation which gives [26]:

\[
V_{\text{se}} = \frac{D \cdot \rho_{\text{gra}}}{\kappa} \cdot \frac{x_{C}^{10} - x_{C}^{l}}{x_{C}^{\text{gra}} - x_{C}^{l}} \cdot \frac{1}{\rho} \cdot \left( 1 - \frac{\rho^*}{\rho} \right) \tag{18}
\]

where \( x_{C}^{10} \), \( x_{C}^{l} \) and \( x_{C}^{\text{gra}} \) are the carbon mole fraction in the bulk liquid, at the liquid graphite interface and in graphite respectively. \( \rho^* \) is the critical curvature radius of the plate tip that would cancel the composition difference \( (x_{C}^{10} - x_{C}^{l}) \). \( k \) is a constant of order unity, set to 1 by Amini and Abbaschian but to 2 by Hillert [26].

\[
\rho^* = \frac{2 \cdot \sigma}{|\Delta G_m|/V_m^{\text{gra}}} \tag{19}
\]

Using the usual Zener’s proposal, the plate grows at the maximum possible rate which corresponds to \( \rho = 2 \cdot \rho^* \), so that for \( k \) set to 2:

\[
V_{\text{se}} = \frac{D \cdot \rho_{\text{gra}}}{\kappa} \cdot \frac{v_m^{\text{gra}}}{v_m} \cdot \frac{x_{C}^{10} - x_{C}^{l}}{x_{C}^{\text{gra}} - x_{C}^{l}} \tag{20}
\]

According to the Fe-C phase diagram, \( x_{C}^{10} - x_{C}^{l} \approx \Delta T/11900 \) where \( \Delta T \) is the undercooling with respect to graphite liquidus close to the eutectic composition. With \( x_{C}^{\text{gra}} = 1 \) and \( x_{C}^{l} \) approximated to the eutectic composition, i.e. \( x_{C}^{l} = 0.175 \), and all other values as before, \( V_{\text{se}} \) can be expressed as:

\[
V_{\text{se}} = 6.0 \cdot 10^{-8} \cdot (\Delta T)^2 \text{m} \cdot \text{s}^{-1} \tag{21}
\]

At an undercooling of 50 K, this expression leads to a growth rate of 150 \( \mu \text{m s}^{-1} \) which is two orders of magnitude higher than the steady state value reported by Amini and Abbaschian [12]. In fact, these authors did introduce a value of 5 \( \mu \text{m} \) for \( h^* \) instead of the calculated value of \( \rho^* \), and this explains most of the discrepancy between the two estimates.

Alternatively, the growth rate \( V_{\text{se}} \) of the plate could be calculated using the model developed by Trivedi [27] which relates the Pélet number \( P = \rho \cdot V_{\text{se}} / 2 \cdot D \), to the dimensionless supersaturation, \( \Omega_0 = (x_{C}^{10} - x_{C}^{l})/(x_{C}^{\text{gra}} - x_{C}^{l}) \). With the values given above, \( \Omega_0 = 10^{-4} \cdot \Delta T \) and is small enough for any reasonable undercooling that the approximate solution worked out by Bosze and Trivedi [28] may be used. According to this solution, one has:

\[
\frac{\rho^*}{\rho} = \frac{3}{32} \cdot \Omega_0 \tag{22}
\]

and

\[
P = \frac{9}{16 \cdot \pi} \cdot (\Omega_0)^2 \tag{23}
\]

With further mathematical manipulations, Bosze and Trivedi arrived at:

\[
V_{\text{se}} = \frac{9}{8 \cdot \pi} \frac{D}{\rho} \cdot (\Omega^*)^2 \tag{24}
\]
where \( \Omega_* \) is given as:

\[
\Omega_* = \frac{\Omega_0}{1 - \frac{1}{2 \pi} \left( \frac{\Omega_0}{\Omega_1} \right)^2}
\]  

(25)

Bosze and Trivedi stressed the fact that the solution thus obtained is valid over a quite large range of supersaturation values. Here however, we can restrict ourselves to low supersaturation values for which \( \Omega_* \approx \Omega_0 \). It is then of interest to compare the two above expressions (equations (20) and (24)) of the growth rate by expressing their ratio. Without considering the change in molar volume, this ratio writes:

\[
\frac{V_{\text{Zener}}}{V_{\text{PNG}}} = \frac{8}{9 \pi} \frac{1}{D_t} \left( 1 - \frac{\rho^*}{\rho} \right)
\]  

(26)

This ratio scales as \( (\Omega_0)^{-1} \) indicating the Zener-type model can strongly overestimate the growth rate in the present case and thus that equation (24) is certainly to be preferred. Inserting the expression of \( \rho^* \) in the above final relation of Bosze and Trivedi gives:

\[
V_\infty = \frac{27}{256 \pi} D_t (\Omega_0)^3
\]  

(27)

With the same numerical values as before this writes:

\[
V_\infty \approx 2 \times 10^{-16} (\Delta T)^4 \text{m} \cdot \text{s}^{-1}
\]  

(28)

The overall growth rate \( G \) of a nodule of radius \( R_c \) from the liquid is now calculated according to the PNG model. After insertion of the appropriate values in equation (14), one obtains:

\[
G_{\text{PNG}} = 2.6 \times 10^{-11} (\Delta T)^{17/6} \cdot (\beta)^{1/3} \cdot \exp \left( \frac{7200 \cdot \xi}{\Delta T} \right) \text{m} \cdot \text{s}^{-1}
\]  

(29)

The solid lines in Fig. 5 show the evolution of \( G_{\text{PNG}} \) according to equation (29) for \( \beta \) set to 1 and \( \xi \) set to 0.1, 0.5 and 1 as before. As expected, the predicted values are much lower than those calculated with equation (17) at any undercooling. Interestingly enough, it is seen that the \( G_{\text{PNG}} \) value for \( \xi = 0.1 \) levels out in the range of undercoolings of interest.

4. Application

As a check of the appropriateness of the above approach, it was applied to previously reported results [16]. In these experiments, a sample (8 mm in diameter, 10 mm in height) of cast iron with 3.75 wt.% C and 2.7 wt.% Si was remelted in graphite crucibles by heating up to 1350 \( ^\circ \)C. The cast iron had been spheroidized with a slight over-treatment in magnesium for allowing short remelting. However, to avoid too large magnesium loss which would have hindered spheroidal growth during solidification, the samples were cooled immediately after reaching 1350 \( ^\circ \)C. Two cooling rates were used, 20 \( ^\circ \)C/min (referred as “slow” cooling rate afterwards) or 350 \( ^\circ \)C/min (referred as “high” cooling rate). Before introducing a sample in the crucible, some commercial inoculant amounting to 0.2% of the weight of the sample was located at the bottom of the crucible.

After processing, the samples were sectioned along a vertical axial section and prepared for metallographic observations. Fig. 6 shows an example of the upper surface of one sample cooled at 20 \( ^\circ \)C/min. Large spheroids are seen to have grown and floated while the remaining of the sample consisted in a standard microstructure of a spheroidized cast iron. The large spheroids are expected to have nucleated at the bottom of the sample as soon as the metal started to cool from 1350 \( ^\circ \)C and to have grown freely in the liquid until the bulk of the material solidified as the eutectic temperature was reached. If an eutectic undercooling of 10–20 \( ^\circ \)C is considered, this latter temperature must have been about 1150 \( ^\circ \)C. Accordingly, the time for growth of the graphite precipitates from the liquid was about 34 s and 600 s for fast and slow cooling respectively.

The half-size of the five largest precipitates of the two samples was then measured for comparison with predicted spheroid radius. These measurements are reported in Fig. 7 as rectangles showing the scatter of the data.

At the start of cooling, the liquid is assumed saturated in carbon at a level corresponding to 1350 \( ^\circ \)C. Then, during primary graphite growth, its carbon content \( x_l \) decreases. This must be accounted for in the calculations by tracking the evolution of the undercooling with respect to graphite liquidus. At any time during cooling, the change \( dx_l / dx_l \) is obtained from a carbon balance as:

\[
\text{Fig. 6. Upper part of the metallographic section of a sample cooled at 20 \(^\circ\)C/min.}
\]  

\[
\text{Fig. 7. Time evolution of primary graphite spheroids in a melt cooled at a rate of 20 \(^\circ\)C/min (slow cooling) or 350 \(^\circ\)C/min (fast cooling).}
\]
where $g^\text{gra}$ and $d^\text{gra}$ are the volume fraction of graphite and its derivative. One has:
\begin{equation}
d^\text{gra} = 4 \cdot \pi \cdot N^\text{gra} \cdot (R^\text{C})^2 \cdot dR^\text{C}
\end{equation}
in which $N^\text{gra}$ is the number density of graphite spheroids.

At each step time, the value of $\Delta t$ is thus updated according to the new value of $x^\text{C}$, owing to the very limited number of primary spheroids that were observed at the top of the samples (Fig. 6), low values of $N^\text{gra}$ were considered, namely 0.01, 0.1 and 1 mm$^{-3}$. The calculated evolution with time of the spheroids radius is plotted in Fig. 7. In the case of fast cooling, changing the nodule count within the range considered had no effect and all three curves are superimposed. On the contrary, in the case of slow cooling, increasing the nodule count increases carbon pick up from the liquid and thus leads to a decrease of the final spheroids size. Comparison of the present calculations with experimental measurements shows a fair agreement when $N^\text{gra}$ is between 0.1 and 1 mm$^{-3}$.

5. Conclusion

Reviewing past and recent experimental information on spheroidal graphite growth in cast iron suggests it grows by continuous 2-D nucleation and lateral extension of graphite layers at the outer surface of the nodules. A model corresponding to such a schematic has been derived for graphite precipitation from the liquid using a classical 2-D nucleation law and various laws for lateral extension of the growth steps following previous approximations [29,30]. These models, values for all physical parameters are from literature predictions when compared to experimental observations. In these models, values for all physical parameters are from literature information but interface diffuseness. Future extension of this approach is sought for accounting for the effect of impurities on lateral extension of the growth steps following previous approaches [29,30].

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