The modeling of crystallization kinetic of Fe-C alloy

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Abstract. The work is aimed on studying the influence of melt state and cooling rate on the solidification processes in model alloys of Fe-C system. The processes, proceeding during the solidification are investigated by a method of the differential thermal analysis. The analysis of the results has shown that the increase of cooling rate results in downturn of liquidus and solidus temperatures and expansion of solidification interval. The formation of equilibrium and microhomogeneous melt promotes the increase of a supercooling degree, downturn of phase transition temperatures, expansion of the interval of eutectic formation. It is established, that the formation of equilibrium melt has favorably affected the formation of casting structure and properties: the large plates of graphite disappears; the linear sizes of flake graphite decrease, its amount increases. On the basis of the results obtained the physical model for Fe-C – alloys solidification, taking into account a melt structural state, is offered.

1. Introduction
By analyzing the kinetic of metal crystallization some authors suppose that microgroups (clusters) existing in liquid metal can be the nucleus of crystallization after melt supercooling below liquidus temperature [1,2]. However this reason has femenological, assumptional character. By X-ray analysis and on the results of physical properties investigations in the melts, a lot of information about parameters of short range order in metallic melts and its changes during heating have been founded [3,4]. There is a lot of physical models of liquid metal structure. To our opinion the quasichemical variant of the microinhomogeneous melt structure model [5] is the most preferable one.

2. Results and discussion
The complex investigations of structure and properties of iron-carbon alloy with 3,2 wt.% C have been carried out. The crystallization process of alloy has been studied.

The temperature dependences of kinematic viscosity of Fe-C alloy in liquid state have been investigated (Figure1). Several temperatures of viscosity abnormal behavior have been found out. The heating above \( t_{\text{an}} \) leads to the anomalous viscosity increasing. The heating above \( t_{\text{c}} \) leads to viscosity hysteresis, that is discrepancy between heating and cooling curves. On the basis of these results it may be anticipated that the melt overheated above the critical temperature has significant transformations in structure and properties in comparison with low-temperature state.

This supposition was checked by the investigation of the short range order parameters in liquid Fe-C alloys by X-rays at different temperatures. The obtained results for temperature dependences of first maximum height and position in structure factor are shown on Figure 2. On the basis of Selykov-Sherer equation [6] and using the results of X-ray analysis, the size of clusters \( r_c \), existing in melt at different temperatures during heating and cooling, has been calculated.

It was anticipated that the temperature dependence of cluster size corresponds to exponential law. In this case the dependences of \( r_c \) could be fitted by:
Heating: $r_{c1} = 31.6e^{-0.0012t}, 10^{-9}$ m.
Cooling: $r_{c2} = 14.5e^{-0.0008t}, 10^{-9}$ m.

The critical nucleus size $R_k$ at different temperatures has been calculated using the results of [7,8] and plotted on Figure 3:

$$R_k = 2\sigma \cdot T_p / (L \cdot \Delta T),$$

where $\sigma$ – interface tension; $T_p$ – melting temperature; $L$ – heat of melting; $\Delta T$ – melt supercooling.

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**Figure 1.** The typical temperature dependence of kinematic viscosity in liquid Fe-C alloys

**Figure 2.** The dependences of position $a(S_1)$ and height $S_1$ of the first maximum of structure factor for liquid Fe-C alloy vs temperature: ● - heating; ○ – cooling.

**Figure 3.** The dependences of critical size of nucleus of crystallization (1) and cluster size (2,3) vs temperature: 2 – metal, heated below the critical temperature; 3 – metal, heated above the critical temperature.
A comparison between sizes of clusters in the melt and nucleus of crystallization shows that they become equal at some melt supercooling (see Figure 3). By analyzing the influence of melt state on cluster size and the crystallization process it was found that melt overheating above the critical temperature leads to formation of its equilibrium homogeneous structure and increase of supercooling. The analysis of dependences plotted at Figure 3 shows that in the case of equilibrium state in Fe-C liquid alloy, the supercooling during crystallization increases for 10-15°C.

To check the results of calculations the experimental investigation of crystallization process in Fe-3.2 wt.% C alloy has been carried out by DTA analysis. During DTA scan specimens have been heated in liquid state with the constant heating rate to \(T_1 = 1400\, ^\circ C\) or \(T_2 = 1600\, ^\circ C\) \((T_1 < t_c < T_2)\), held here for 10 minutes and then solidified with cooling rates from 10 to 80 \(^\circ C\)/min. The liquidus temperatures of investigated specimens \(t_L\) have been determined. For comparison, the equilibrium liquidus temperature in Fe-3.2 wt.% C alloy is 1280°C [8].

On the basis of experimental results the dependences \(t_L = f(V_c)\) have been plotted. They look as:
- Melt, heated up to 1400°C: \(t_L = 1249-0.417 \times V_c, ^\circ C\)
- Melt, heated up to 1600°C: \(t_L = 1237-0.301 \times V_c, ^\circ C\)

The graphical extrapolation of the results to cooling rate \(V_c = 0, ^\circ C\)/min gives the opportunity to determine equilibrium liquidus temperature of liquid metal heated to different temperatures (below and above critical temperature). It has been found that the difference between temperatures is 12°C and determined temperatures are in a good agreement with the calculated ones.

3. Conclusion
1. The clusters existing in the melt could be considered (within the certain limits) as the nucleus of crystallization.
2. The formation of the mirohomogeneous melt leads to increase of its supercooling and decrease of critical nucleus size. The experimental results of the crystallization process investigation by differential thermal analysis prove this assumptions. When the experimental melt supercooling coincides with the calculated one, the sizes of clusters become equal to the critical size of nucleus of crystallization.

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4. References
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