Mathematical modeling for solidification of multi-component iron-based melt with application of system’s state diagrams

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Abstract. Solidification of carbon steel is to be considered in the Fe-C-O-Si-Mn-Al-S-P system. The mathematical model of this system is created as a set of simpler subsystems and interrelations among them based on experimental data on the phase composition of the solidified metal. An example illustrating the potential of this method is a low-carbon steel ingot’s macrostructure obtained by calculation using the above mentioned method as compared to experimental data.

1. Introduction
Carbon steel is the most commonly used material of modern civilization. This role of carbon steel is prompted by the possibility of changing widely its mechanical and technological properties by means of changing the chemical composition and structure of metal.

All structural features of actual industrial metals (macro- and micro-structure, chemical heterogeneity and contamination with nonmetallic impurities) result from phase transformations occurring during their solidification. The processes of phase transformations can be described based on the state diagrams of multi-component systems. Solidification of carbon steel must be considered in the Fe-C-O-Si-Mn-Al-S-P system incorporating all the components of the actual metal, which have a significant effect on both the solidification process and the properties of the solidified metal.

2. Method
Traditionally state diagrams of multi-component systems are represented as graphic objects of various complexities. Obviously, it is practically impossible to represent the Fe-C-O-Si-Mn-Al-S-P eight-component system as a graphic object or a group of such objects, and, particularly, it is impossible to use them for studying the process of phase transformations occurring during melt solidification. This calls for a new approach to the problem in question.

Such a new approach to describing the multi-component melt solidification consists in that a mathematical description (mathematical model) of the melt solidification is created, rather than a graphic image of the system's state diagram. In such a model it is possible to describe mathematically the phase transformations and analyze their process by numerical methods using a computer. The results of calculations may be presented in conventional forms of representing information on the structure of solidified metal.

Creation of a mathematical model of the multi-component system is greatly simplified through using the decomposition method known from the basic systems theory. This method consists in isolating relatively simple independent components (subsystems) from the complex system, which
function in interrelation with each other. Therefore, the complicated problem of creating a mathematical model for the whole system may be reduced to creating a model for a set of simpler subsystems and interrelations among them.

The decomposition of the Fe-C-O-Si-Mn-Al-S-P system into components should be performed based on experimental data on the phase composition of the solidified metal. Generally, solidified ingots of carbon steel (with the exception of metallic matrix) may contain blowholes consisting predominantly of carbon oxides, iron-manganese oxides and silicates, aluminum oxide and iron and manganese sulfides. For this reason the following subsystems should be identified in the Fe-C-O-Si-Mn-Al-S-P system:

- double Fe-C, Fe-O, Fe-Si, Fe-Mn, Fe-Al, Fe-S, Fe-P subsystems, describing elements' segregation;
- triple Fe-C-O subsystem describing gas emission;
- Fe-Mn-O subsystem describing formation of iron-manganese oxides;
- Fe-Si-Mn-O subsystem describing formation of silicates;
- Fe-Al-O subsystem describing formation creation of aluminum oxide;
- Fe-Mn-S subsystem describing formation of sulfides.

The generalized view of the structure of multi-component systems describing the solidification of carbon steel which contains all the above subsystems and reflects their interrelations, is shown in figure 1. The relations between the subsystems are shown by lines connecting them. The relation shown by vertical lines means that at any stage of solidification the mass of solidified metal in all the double subsystems is the same. The relation shown by horizontal lines means that at any stage of solidification the content of any chemical element in all the subsystems is also the same. Apart from the relations represented by lines, all the subsystems are interrelated by common temperature. These relations are not shown in figure 1.

The limited scope of this report does not allow us to give a detailed mathematical description of the Fe-C-O-Si-Mn-Al-S-P system and all the processes occurring in it during the melt solidification. Therefore we provide only a conceptual description of these issues below.

A mathematical description of the state diagram of any multi-component system can be reduced to a mathematical description of interfaces between the phase states of the system, which is a rather complicated problem. This problem, however, is essentially simplified if we confine ourselves to the mathematical description of the state diagram only for the steel solidification area. In this case the mathematical description of the state diagram can be limited to the equation of the liquidus surface in a multi-dimensional space, the equation of the liquidus surface intersections with interfaces of the system's different phase states, and the solidus surface equation.

With a reasonable degree of accuracy the liquidus surface close to the “iron” corner of the diagram may be considered as a plane in a multi-dimensional space and approximated with a linear polynomial reflecting the effect of the concentration of dissolved elements in liquid iron on the liquidus temperature. In doing so, we can limit ourselves to considering only the effect of those elements whose concentration in carbon steel is sufficiently high.

The equation of the liquidus surface intersections with interfaces of the system's different phase states theoretically may be found by solving the equation system which describes the intersecting surfaces. Essentially, such equations express the functional relation among equilibrium component concentrations at the liquidus temperature. A mathematical description of equilibrium in major subsystems shown in figure 1 and made according to reference data is given in our previously published paper [1].

In the context of the task of calculating solidified metal phase composition it would be convenient, rather than specify the liquidus surface equation explicitly, describe it indirectly by specifying ratios of the elements’ distribution between the solidifying and the liquid metal. Numerical
values of equilibrium distribution ratios for all the elements of the Fe-C-O-Si-Mn-Al-S-P system required for calculations by formula (1), can be found in reference literature.

The mathematical description of metal solidification by means of the multi-component system’s state diagram is based on the equation of the general mass balance and balance equations of separate elements. Such balance equations are supplemented with equations which describe the equilibrium between all the components of the solidifying metal participating in chemical reactions. The mathematical description also includes differential equations describing mass changes of such reactions’ products. The model is described in detail in paper [2].

3. Results
The modeling of melt solidification consists in step-by-step (with the increase of the solidified metal’s mass) calculation of changes in the chemical composition of the liquid and solidifying metal as well as
the mass of non-metallic phases (oxides and sulfides) formed as a result of chemical reactions accompanying the solidification.

When modeling the solidification process of an actual ingot on the basis of the above method, a large amount of information was obtained which it is impossible to present in this paper. An example illustrating the potential of the method under discussion is a steel ingot’s macrostructure obtained by calculation using the above method (0.09% C, 0.36% Mn, 0.0035% O, 0.025% S and 0.012% P) as compared to experimental data (See figure 2).

A reasonably close match between the calculated and experimental results testifies to the possibility of an adequate description of actual metal solidification on the basis of system’s state diagrams.

Figure 2. Macrostructure of a 9-ton ingot according to experimental data (left) and according to calculation (right).

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References
[1] Selivanov V N and Dyuldina E V 2005 Bulletin of the G.I. Nosov State University (Magnitogorsk) No 1 p 17
[2] Selivanov V N and Dyuldina E V 2005 Bulletin of the G.I. Nosov State University (Magnitogorsk) No 3 p 13