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MATHEMATICAL MODELING OF THE STRUCTURE OF HIGH-ALLOY STEELS BY THE POTAK – SAGALEVICH DIAGRAM

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Methods and problems of determination of the structure of steels from phase diagrams are considered. Expediency of transition to methods of mathematical modeling is shown. A method of mathematical modeling of the structure of high-alloy steels with the use of the Potak – Sagalevich diagram is suggested.

Key words: steel, structure, computations, modeling, Potak – Sagalevich diagram.

INTRODUCTION

Steels are very important structural materials applied in all spheres of production. To choose the grade of steel most suitable for specific conditions we should know its characteristics, the chemical composition and structure in the first turn, determining the main properties of the metal.

The chemical compositions of available steels are standardized in State Standards (GOST) and Specifications (TU) and can be found in numerous reference editions. At the same time, published data on the structure of the steels are quite limited. This is explainable by the fact that such information is demanded by a limited circle of specialists, welders, metallurgists and heat-treaters in the first turn.

The type of structure of many steels is known. When it is required to have a detailed notion of the structure, the researcher may turn to phase diagrams that give quantitative proportions of the main structural phases (ferrite, martensite, austenite, pearlite) and their combinations depending on the chemical composition.

Several kinds of such diagrams are available, of which the most widely applied one belongs to A. Schaeffler [1]. It is simple for use, has been published in many books, and helps to solve problems of welding and heat treatment. However, it has been shown that this diagram does not give precise data and may even be inapplicable in some cases, for example for steels of the austenitic, martensitic and austenitic-martensitic classes.

In the last decades the Schaeffler diagram has been amended, and new and more perfect phase diagrams have

been suggested. However, they require complex computations and have mainly appeared in the papers of the developers. Therefore, many problems of formation of the final structure of steels remain unsolved. It is obvious that further development of the methods of structural investigation of steels is an important task.

The aim of the present work was to consider the possibilities and methods of computational determination of the structure of steels by mathematical modeling of graphical phase diagrams for an example of the diagram of Potak – Sagalevich.

INITIAL DATA FOR MODELING

The Potak – Sagalevich diagram is estimated by specialists as a considerable contribution into the theoretical and practical science of metals, because it is much more advanced with respect to the Schaeffler diagram. Unfortunately, the former is virtually not used for practical work due to the high complexity and absence of information about it in popular references. For this reason, we present in what follows some data necessary for mathematical modeling.

The appearance of the diagram suggested is given in Fig. 1. It differs from the base diagram of [2] by the absence of points matching the structure of specific steel grades; for further computation, the lines of the diagram are denoted x_i and y_i .

The values of the chromium equivalent Cr_{eq}^f , which allows for the effect (with respect to chromium) of the alloying elements of the steel on formation of δ -ferrite, are laid over the axis of abscissas. The values of the chromium equivalent

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of martensite Cr_{eq}^m , which allows for the effect of all the alloying elements on formation of martensite, are laid over the axis of ordinates.

The values of Cr_{eq}^f and Cr_{eq}^m are computed by the formulas

$$Cr_{eq}^f = Cr - 1.5Ni + 2Si - 0.75Mn - K_f(C + N) + Mo + 4Al + 4Ti + 1.5V + 0.5W + 0.9Nb - 0.6Co - 0.5Cu; \quad (1)$$

$$Cr_{eq}^m = 20 - [Cr + 1.5Ni + 0.7S + 0.75Mn + K_m(C + N) + 0.6Mo + 1.5V + 1.1W + 0.2Co + 0.2Cu + 1.9Ti - 0.1Al], \quad (2)$$

where the names of the elements denote their contents in the steel, and the coefficients K_f and K_m are determined from the curves given in the diagram (Fig. 1).

Formulas (1) and (2) have been supplemented with additional instructions concerning the values of the coefficients at six alloying elements (Ni, Ti, Al, N, C, Nb) depending on the alloying system. The possible effect of other factors on the structure of the metal, such as the state of the metal after melting (cast or deformed), the quenching temperature, the cooling rate, the grain size, the presence of low impurities has also been considered. In this connection, the suggested diagram may be termed a “semi-quantitative” one, because its further amendment is possible.

This has been confirmed by reports of other researchers. Paper [3] should be distinguished as a quite detailed one. It presents the results of creation and application of a mathematical model (which is in fact a novel phase diagram based on the Potak – Sagalevich one) for high-alloy steels. The new data have been obtained by intricate computations. The model has been presented only in the form of mathematical manipulations without graphical representation. A special software has been created for working with this diagram. Exhaustive data on the developed diagram have not been reported, and it is inapplicable for other specialists.

Our analysis of publications on the topic has shown that the available graphic representations of phase diagrams give only a tentative or qualitative assessment of the composition of structural components in steels. Introduction of additional conditions, most of which are not describable quantitatively, may raise the accuracy of the diagrams, but this will complicate substantially the computations and hence makes the diagrams applicable only for research purposes.

METHODS OF STUDY

The problem can only be solved by development and application of relatively simple-to-operate special computer programs. A method for constructing mathematical models of phase diagrams representable in a graphic form has been developed at PNIPU in the 1990s.

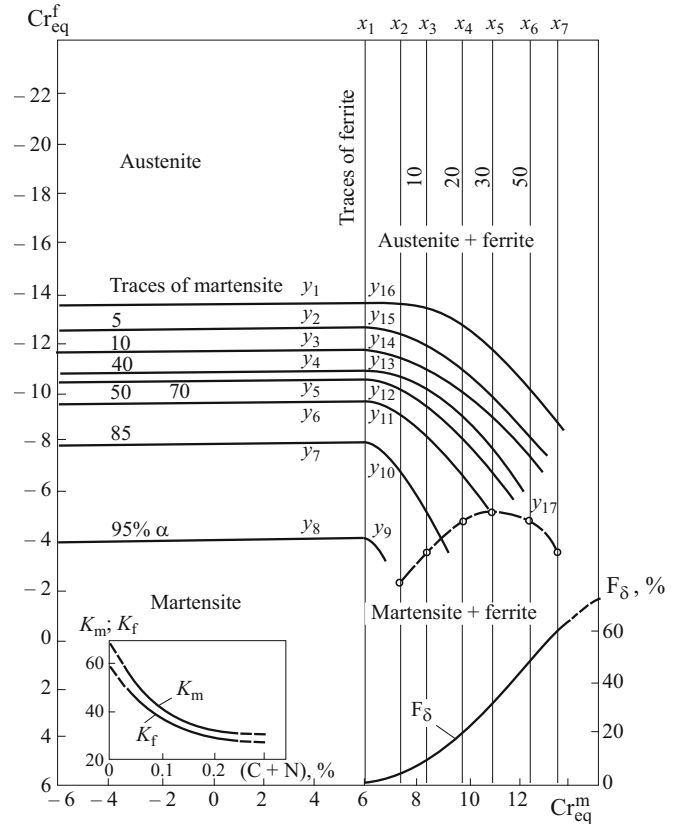


Fig. 1. Phase diagram of Potak – Sagalevich for deformable stainless steels [2].

The studies concerned application of the Schaeffler and Potak – Sagalevich diagrams. Mathematical modeling for the latter diagram turned out to be hard due to the absence of some data. The authors have not explained their choice of the demarcation lines, which should differ for steels of different compositions. In the two-phase and three-phase regions the percentage of the phases is shown only graphically, namely,

- by straight lines $y_1 - y_8$ for the austenite + martensite regions;
- by straight lines $x_1 - x_7$ and curve F_δ in the right-hand bottom part of Fig. 1 for the content of ferrite in the ferrite-containing regions;
- by bent lines $y_9 - y_{16}$ for the content of martensite in the three-phase region A + M + F and the remainder (after subtracting the contents of ferrite and martensite) for the content of austenite.

With allowance for this situation we designed the method of modeling the Potak – Sagalevich diagram in the following stages:

- determination of critical points in the diagram, which can be used for plotting the demarcation lines;
- derivation of the formulas describing each demarcation line and their coding;
- derivation of the formulas for computing the proportions of phases in the two-phase regions of the diagram;

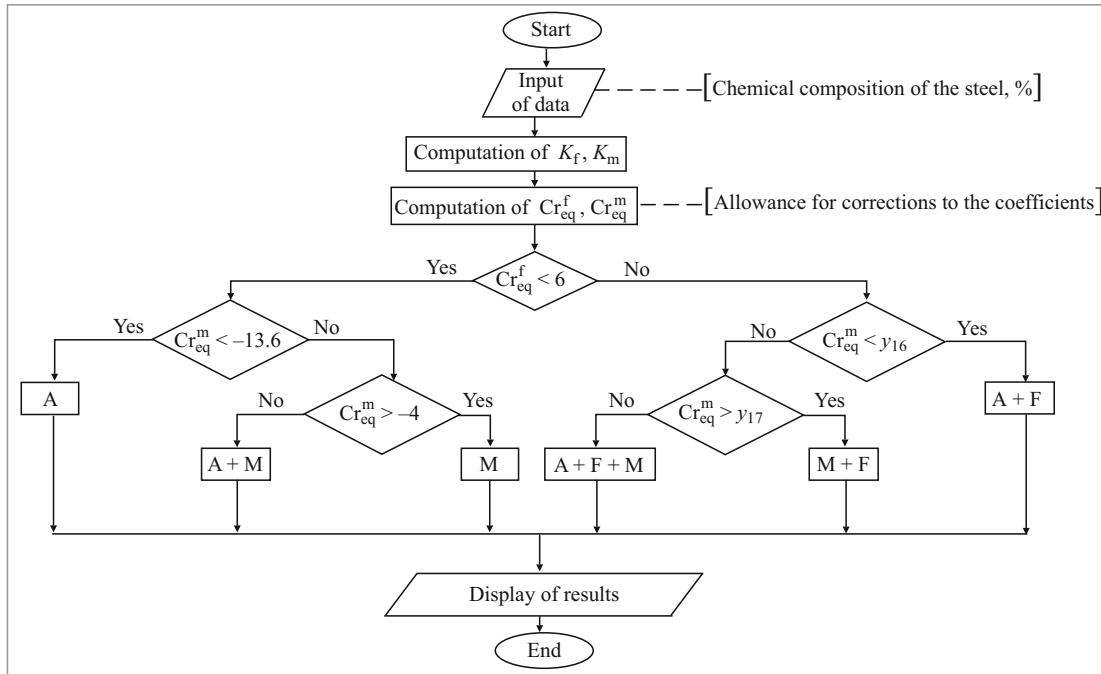


Fig. 2. Block diagram for determining the structure of a steel from the Potak – Sagalevich diagram.

- formulation of the boundary conditions of existence of all the phase regions of the diagram;
- design of a block diagram for determining the structure of the steel from the diagram.

A necessary condition of mathematical modeling is representation of all the available interdependences of the variables in the form of mathematical expressions. For convenience, the lines of the diagram were denoted conventionally as it is shown in Fig. 1. It was not hard to find the location of the straight lines, i.e., vertical lines $x_1 - x_7$ from the corresponding values of the Cr_{eq}^f abscissa and horizontal lines $y_1 - y_8$ from the values of the Cr_{eq}^m ordinate.

Several points were deposited preliminarily on curves $y_9 - y_{16}$ and on the plots of K_m and K_f . Statistical processing of the data gave the corresponding equations (given below). The proportion of phases in the two-phase regions A + F and A + M was determined in a similar manner.

The demarcation line between regions M + F and A + M + F is not determined in the initial Potak – Sagalevich diagram. However, it is possible to find points at intersections of some vertical lines with the curves, which correspond to the same values of the austenite content. They are singled out in Fig. 1. The regularity of their mutual arrangement allows us to assume that they belong to a hypothetical second-order curve given by the dashed line in the figure and denoted y_{17} .

There is no need to present the methodology of the fourth and fifth stages.

COMPUTATIONAL AND MODELING RESULTS

We obtained the following quantitative expressions for all the elements of the mathematical model of the Potak – Sagalevich diagram after conducting the operations and procedures of the method presented above:

(a) demarcation lines of the diagram

Vertical lines	Horizontal lines	Bent lines
$x_1 = 5.0$	$y_1 = -13.6$	$y_9 = 14.3 - 6.93x + 0.647x^2$
$x^2 = 7.4$	$y_2 = -12.6$	$y_{10} = 8.08 - 5.48x + 0.473x^2$
$x_3 = 8.4$	$y_3 = -11.7$	$y_{11} = 7.70 - 6.42x + 0.558x^2$
$x_4 = 9.6$	$y_4 = -10.9$	$y_{12} = -9.03 - 0.83x + 0.096x^2$
$x_5 = 11.0$	$y_5 = -10.5$	$y_{13} = -7.79 - 1.19x + 0.111x^2$
$x_6 = 12.4$	$y_6 = -9.5$	$y_{14} = -8.46 - 1.17x + 0.105x^2$
$x_7 = 13.5$	$y_7 = -7.8$	$y_{15} = -8.57 - 1.35x + 0.113x^2$
	$y_8 = 4.0$	$y_{16} = -7.80 - 1.83x + 0.129x^2$
		$y_{17} = 23.1 - 4.91x + 0.217x^2$

(here x is used for Cr_{eq}^f);

(b) coefficients K in the formulas of the chromium equivalents

$$K_f = 59.57 - 379.68x + 1501.70x^2 - 2083.89x^3; \quad (3)$$

$$K_m = 69.49 - 408.06x + 1297.87x^2 + 1331.10x^3, \quad (4)$$

(here $x = \% C + \% N$);

(c) content of δ -ferrite (F_δ , %) in the ferrite-containing structures

$$F_\delta = 129 - 45Cr_{eq}^f + 4.8Cr_{eq}^{f2} - 0.136Cr_{eq}^{f3}; \quad (5)$$

TABLE 1. Boundary Conditions for Regions of the Diagram

Structure	Boundary conditions
Austenite	$Cr_{eq}^f < 6.0; Cr_{eq}^m < -13.6$
Martensite	$Cr_{eq}^f < 6.0; Cr_{eq}^m > -4.0$
Austenite + ferrite	$Cr_{eq}^f > 6.0; Cr_{eq}^m < y_{16}$
Austenite + martensite	$Cr_{eq}^f < 6.0; -4.0 > Cr_{eq}^m > -13.6$
Martensite + ferrite	$Cr_{eq}^f > 6.0; Cr_{eq}^f > y_{17}$
Austenite + martensite + ferrite	$Cr_{eq}^f > 6.0; y_{17} > Cr_{eq}^m > y_{16}$

(d) content of martensite (M, %) and austenite (A, %) in the A + M region

$$M = 12.9 + Cr_{eq}^m + 3.58Cr_{eq}^{m2} + 3.78Cr_{eq}^{m3}; \quad (6)$$

$$A = 100 - M; \quad (7)$$

(e) content of austenite and ferrite in the A + F region

$$A = 85.4 + 7.21Cr_{eq}^f - 0.8Cr_{eq}^{f2}; \quad (8)$$

$$F = 100 - A. \quad (9)$$

The expressions for the boundary conditions and the chromium equivalents of formation of ferrite and martensite were used to determine the conditions of existence of the structural regions given in the diagram (see Table 1).

The developed mathematical model of the Potak – Sagalevich diagram was used to compose a block diagram for determining the structure of a metal presented in Fig. 2. The diagram gives the principal blocks for determining the kinds of structure. Development of a specific computer program will require a more detailed scheme. For example, to compute the values of chromium equivalents Cr_{eq}^f and Cr_{eq}^m we

should introduce additional corrections to several coefficients, as it has been mentioned above. In addition, a part of the blocks of the diagram should be supplemented by formulas for computing the proportions of phases in the two-phase and three-phase regions. For example, for the A + M block we should indicate that the contents of martensite and austenite are to be computed by formulas (6) and (7), etc. On the whole, such computations are primitive.

CONCLUSIONS

1. To solve some production problems we should possess data on the structure of the steels to be applied. Determination of the structure of the steels from the known phase diagrams is inaccurate and complicate in many cases, and is too laborious for production workers.

2. The suggested mathematical model of the Potak – Sagalevich phase diagram and the method of its application for determining the structure of high-alloy stainless steels make it possible to use computer simulation with the aim to simplify the work and to raise the efficiency and quality of solution of the corresponding production problems.

3. The locations of the interfaces of martensite + ferrite and austenite + martensite + ferrite regions require experimental verification.

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