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FEATURES OF THE APPLICATION OF THE HILLERT METHOD IN CALCULATING THE ACTIVITY OF THREE-PHASE SYSTEM COMPONENTS

ОСОБЛИВОСТІ ЗАСТОСУВАННЯ МЕТОДУ ХІЛЛЕРТА ПРИ РОЗРАХУНКУ АКТИВНОСТІ КОМПОНЕНТІВ ТРИФАЗНИХ СИСТЕМ

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Abstract. *The Hillert method for calculating the activity of components along nodes in two-phase regions and isothermal sections of three-phase diagrams has been extended to regions that do not touch the corresponding binary diagrams. This has been made possible by using a modified Hillert equation, in which the replacement of the activity logarithm is a function only of the slope of the conodes for the corresponding nodes. As an example, we show how such calculations can be made using isothermal sections of the Fe-C-X phase diagram, where X is a carbide-forming element and in which several conod triangles are present.*

Key words: *The Hillert equation, the Hillert method, carbide, tie-line, tie-point, tie-line triangles.*

Анотація. *Метод Хіллерта для розрахунку активності компонентів уздовж конод у двофазних областях та ізотермічних розрізах трифазних діаграм поширено на області, які не стикаються з відповідними бінарними діаграмами. Це стало можливим завдяки використанню видозміненого рівняння Хіллерта, в якому заміна логарифму активності є функцією тільки нахилу конод для відповідних вузлів. Як приклад показано, як такі розрахунки можна зробити, використовуючи ізотермічні розрізи діаграми стану Fe-C-X, де X – карбідоутворюючий елемент і в яких присутні кілька конодних трикутників.*

Ключові слова: *Рівняння Хіллерта, метод Хіллерта, карбід, конода, нода, конодний трикутник.*

Introduction.

While using classic Hillert method [1] and its modifications [2] the most significant initial value in computation of activities a_i along the tie-line of two phase region of given isothermal section of three-component (angle h of system h-i-j) diagram of state is the activity a_i^o along the same name tie-line of double system h-i. But it provides for two-phase region being situated closely to diagram h-i. And what if it isn't? In such a case it is necessary to know the activity a_i^o along the least of one tie-line of three component two-phase region $\alpha+\beta$ and then this tie-line is taken as the base one although it is inclined to the axis h-i ($\upsilon_j=0$) and the latter is removed from the region $\alpha+\beta$.

Theoretical research.

The isothermal section is done in Skreinemakers coordinates because it allows applying in the computations a wary simple and sharp Zhukov-Zhiguts equation, in which the coordinates of tie-points or of figurative points of alloys are absent:

$$a_i = a_i^0 \cdot \exp(-\dot{n}), \qquad (1)$$

where a_i^o - component activity along the basic ("zero") tie-line at $X_i=0$ (binary system h-i, when the region $\alpha+\beta$ is contiguous after this tie-line to binary diagram h-i); $\dot{n}$ – tangent of the angle of tie-line inclination of two-phase balance in the system under investigation h-i-j. This allows in its turn for the case shown in figure 1 to make computation a_i along the tie-line $\alpha_I\beta_I$ by equation:

$$\ln a_i^I = \ln a_i^b - \dot{n}_I + \dot{n}_0 \qquad (2)$$

where $\dot{n}_I$ and $\dot{n}_0$ - tangents of angles of tie-line $\alpha_I\beta_I$ and $\alpha_0\beta_0$; a_i^b - known value a_i along basic tie-line $\alpha_0\beta_0$.

Computation for tie-line $\alpha_{II}\beta_{II}$ is being made in the sawed way using the equation:

$$\ln a_i^{II} = \ln a_i^b - \dot{n}_{II} + \dot{n}_0 \qquad (3)$$

where $\dot{n}_{II}$ - inclination of tie-line $\alpha_{II}\beta_{II}$.

It is easy to make sure that the original Hillert equation [3] that contains tie-line coordinates (to say nothing of great approximations needed while it was being deduced [4]) isn't used for such computation as while coming from tie-line $\alpha_0\beta_0$ to tie-line $\alpha_I\beta_I$ and then to tie-line $\alpha_{II}\beta_{II}$ these coordinates change greatly.

In figure 1 as an example the applying of the method investigated is shown to isothermal section (in the region of supercritical temperatures) of systems Fe-C-X (where X – manganese, chromium or their analogs).

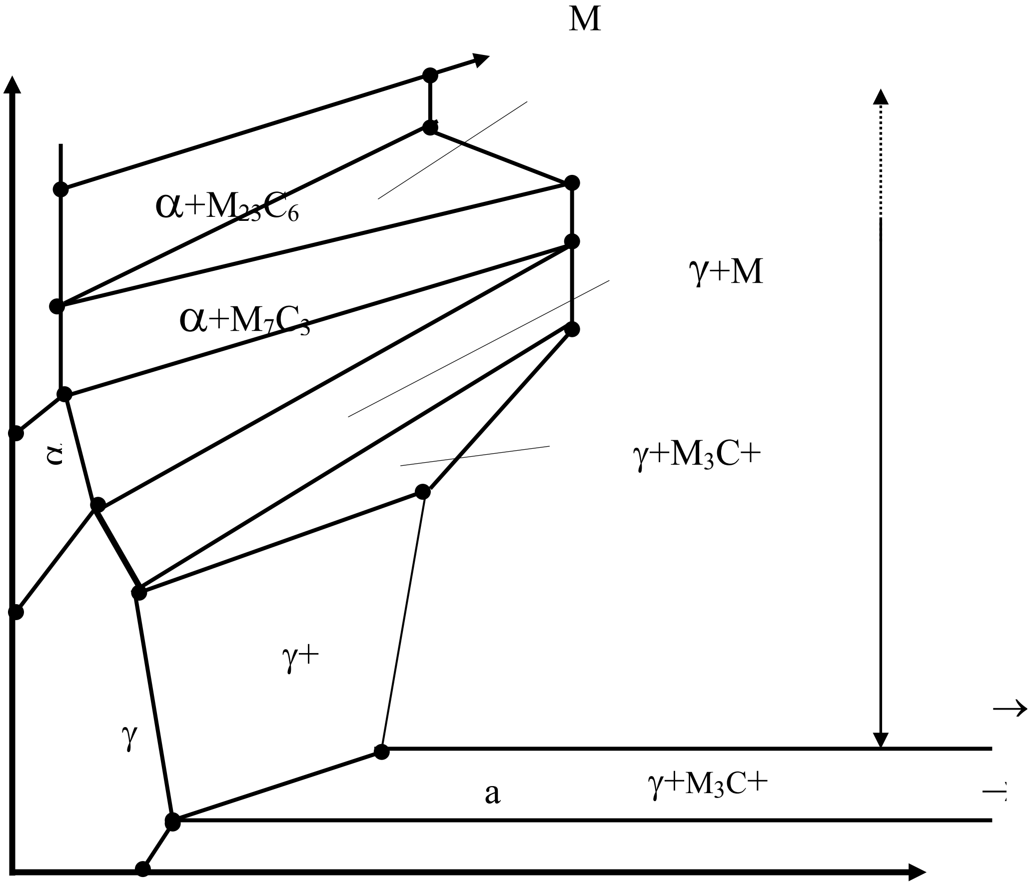

Figure 1 - Schema isothermal section of state diagram of Fe-C-X, alloys in which under a_C>1,0 graphite is formed (under condition that graphite is been selected as a standard state of carbon) and carbide phases M_3C (cementite), M_7C_3, $M_{23}C_6$ and M_3C_2

Original design

In two-phase region $\gamma+C_{\text{гр}}$ (austenite+graphite) the activity of carbon is more than 1.0. In the tie-line triangle $\gamma+M_3C+C_{gr}$ (austenite+alloyed+graphite) the activity of carbon is constant after definition ($a_C=1.0$). These alloys aren't able to graphitize above the given triangle $a_C<1$.

The tie-line $\gamma+M_3C$ of the mentioned triangle serves as base tie-line $\alpha_0\beta_0$ along its $a_C=1.0$. Using of the computations according to equation of type (2) and (3) in the region $\gamma+M_3C$ (here the activity decreases monotonously to the value $a_C<1,0$) to the tie-line $\gamma+M_3C$ of the next tie-line triangle $\gamma+M_3C+M_7C_3$ (activity a_C degreases because $\dot{n}$, and consequently, $\dot{n}-\dot{n}_0$ increase progressively). In the mentioned triangle carbon activity is constant and it allows us to use equations (2) and (3) for computations in tetragon $\gamma+M_7C_3$, where the activity a_C continues to degrease with the increasing of the level of dopingness of alloys.

The triangle $\alpha+\gamma+M_7C_3$, in the inner part of which the carbon activity is constant allows to move the value a_C from the lower right tie-line of triangle to the upper tie-line and to continue computations by the equation of (2) and (3) type in the tetragon $\alpha+M_7C_3$. Prolonging the above mentioned structure for the regions laying above the triangle $\alpha+M_{23}C_6+M_7C_3$, the tetragon $\alpha+M_{23}C_6$ and triangle $\alpha+M_{23}C_6+M_3C_2$ we can lead the computations to the region of highchrome alloys but with large degree of approximation (because the Hillert method, in principal, is perfectly designed only for deluded systems).

Conclusions.

1. The Hillert method is also spread to tie-lines of two-phase regions of triangle simplexes of tree-component diagrams of state Me-C, when these regions are removed from those sides of the mentioned triangles which in two-component under investigation in the computations of its activity.

2. The original Hillert method proved to be unserviceable to solve this problem in contrast to modified method, which uses Screinemakers orthogonal system of coordinates.

3. The reason of this lies in the fact that the modified method doesn't demand the definition and usage in the computations the coordinates of the corresponding tie-point.

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