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Thermodynamic substantiation of compositions of silicon aluminium alloys with increased aluminium content in Fe-Si-Al system

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ABSTRACT

A priority direction of ferrous metallurgy development is to increase in output of the high quality metal and metal products of new assortment. One of the methods to improve a quality of steels is to involve of complex alloys based on aluminum, silicon, manganese, etc. for their output. They are necessary as deoxidizing agents and alloying additives. This paper considers the possibility of the thermodynamic substantiation of the aluminum solubility in the ferrosilicon-aluminum complex alloy (FeSiAl) on the basis of their phase diagrams using the osmotic coefficient of the Bjerrum-Guggenheim. Methodology used is based on the theoretical studies of the phase equilibria using the Bjerrum-Guggenheim concept. It includes a set of computer programs in C# language (C sharp) designed to evaluate a deviation scope of properties of a real system from the ideal one. Criterion for evaluation is an osmotic coefficient of the Bjerrum-Guggenheim. The pattern of change in an osmotic coefficient of the Bjerrum-Guggenheim on the ratio of activity of components in the ideal liquid and solid phases (positive Φi <1 or negative Φi >1) under the boundary forming conditions of crystallization regions of phases related to the melting ferrosilicon-aluminum processes is a direct proof of the possibility to use it as a metal reducing agent. The calculated mathematical dependences of the osmotic coefficient of the Bjerrum-Guggenheim permit us to determine the crystallization temperature of the ferrosilicon-aluminum alloy. The alloying process with rich aluminum content is observed at this temperature. The dependence diagrams of an osmotic coefficient of the Bjerrum-Guggenheim of a crystallizing component on the ratio of its activity in the liquid and solid phases demonstrated that a temperature rise leads to strong negative deviations in silicon properties, and thus to its good mixability in the melt with iron and aluminum. Compositions of silicon-aluminum alloys with high aluminum content in the ferrosilicon-aluminum complex alloy (FeSiAl) were determined on the basis of their phase diagrams using the osmotic coefficient of the Bjerrum-Guggenheim with iron content of 12-37%, aluminum 20-25% and silicon 68-38%. The received theoretical results permit to determine conditions which give the maximum possible aluminum assimilation with the ferrosilicon-aluminum melts supplied from the high-ash coal in the melting process of this metal in the ore-thermal furnaces. Thus it is a direct method to develop the output technology of the complex alloys.

Keywords: phase diagrams, Bjerrum-Guggenheim coefficient, crystallization regions of phases, silicon aluminium alloys, ferrosilicon aluminium, complex alloys.

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Introduction

Today the ferrosilicon-aluminum production with using the high-ash coal raw materials was only organized in Kazakhstan. The aluminum content is regulated by 5 - 15% in Kazakhstan. The basis to develop the technology was a detailed study of a reduction process of silicon and aluminum compounds with using the thermodynamic-diagram analysis of the Fe-Si-Al-C-O system.

The absence of the thermodynamic information for a wide range of composition and temperature makes it impossible to assess the real yield of the reaction products in the melting process of ferrosilicon aluminium. It should be pointed out that for Fe-Si-Al-C system melts the available quite

extensive experimental material on the thermodynamic parameters refers mainly to binary systems of Fe-C, Fe-Si and Si-Al, and also a small number of papers on the triple systems [[1], [2], [3]].

The analysis of the numerous phrase diagrams of various systems determined a common pattern in formation of crystallization regions as a correlation dependence of an osmotic coefficient of the crystallizing component on the ratio of its activity in the liquid and solid phases. The osmotic coefficient of Bjerrum-Guggenheim is able to be as a measure of deviation of the energetic properties of a real system from the ideal one described by Le Chatelier-Shreder equation.

The received data on crystallization regions of phases in the studied systems testify the presence of a regular change in the non-ideality coefficient Φ_i (Bjerrum-Guggenheim coefficient) along a line and crystallization surface of phases and a close connection of this value with the nature of the interparticle interaction of components in the melt and their state.

One of the methods of the technical solutions for melting of the complex alloys, in particular, ferrosilicon aluminium with a high aluminum content of up to 25%, is to conduct the thermodynamic studies of phase equilibria based on the Bjerrum-Guggenheim concept for a triple phase diagram of the Fe-Si-Al system, which will permit to calculate the rational compositions of alloys with the thermodynamic method and to determine areas of existence of an independent phase of aluminium.

Experimental part

The theoretical studies of the behavior of the osmotic coefficient of Bjerrum-Guggenheim of a dissolved substance (e.g. aluminum in iron) depending on the ratios of components in the melt can simultaneously have the positive and negative deviations from ideality. Depending on values of the osmotic coefficient of Bjerrum-Guggenheim in the thermodynamic calculations for various Fe:Al ratios, it will be possible to discuss in which areas of the melt the aluminum is absorbed very well, and in which it can be isolated as an independent phase.

The study of the phase diagrams of iron-based systems was performed according to the well-known classification of phase diagrams [[4], [5], [6], [7]] and taking into account the possibility of the analytical description of all types of their solid-liquid and solid-solid phase equilibrium diagrams based on the nature of the change in the value of the Bjerrum-Guggenheim coefficient near the singular points.

The principle of our procedure is as follows: to take data on temperature and composition from a phase diagram and to find reference data on temperature and enthalpy of melting of a solvent and the dissolved substances for Le Chatelier-Shreder equation. Further our developed program is used: to process the initial data with finding the expressions of the osmotic coefficients of Bjerrum-Guggenheim for the liquid and solid phases, to plot the dependence diagrams of a osmotic coefficient of the crystallizing phases (Φ_i) on ratio of the component activities in the ideal liquid and solid phases and to find a mathematical expression of a correlation dependence. The mathematical expressions for the liquidus and solidus lines as a semi-empirical dependence of the modified equation of Le Chatelier-Shreder were obtained for the ideal system and the detected patterns on the monovariant phase equilibrium lines.

This paper focused on the binary systems of Fe - Al, Fe - Si and Si – Al [[7], [8]] characterized by the presence of the extensive areas of the limited solid ferrite and austenitic solutions and a whole cascade of the intermediate phases that are important for the production of ferrosilicon aluminium.

The binary phase diagrams of iron - aluminum (Fe-Al) and iron - silicon (Fe-Si) are previously described in full with the mathematical expressions from the position of the Bjerrum-Guggenheim concept [9]. Table 1 gives the coefficients of the dependence of the osmotic coefficient $\Phi_i^{'}$ on the ratio of the activity of the liquid and solid phases (exponent of the Le Chatelier-Shreder equation) substituting in equations of (1) or (2), the correlation dependences will be calculated.

$$\Phi_i^{'} = \left(\ln a_i^L / \ln a_i^S\right)/(\ln x_i^L / x_i^S) = A_i + B_i \cdot a_i^L / a_i^S , \quad (1)$$

$$\Phi_i^{''} = A_i + B_i \cdot a_i^L / a_i^S + \frac{C_i}{a_{кр.} - a_i^L / a_i^S} , \quad (2)$$

where $x_i^{L(S)}$ - concentration of a crystallizing component at a given temperature; $a_i^{L(S)}$ - activity of a crystallizing component for an ideal solution calculated by Le Chatelier-Shreder equation; A_i, B_i, C_i - constants determined by the nature of components and interparticle interaction;

$a_{crit.}$.- a value of the ratio of the component activities at T=T_{max} calculated by Le Chatelier-Shreder equation.

Based on these correlation dependences, the equation of crystallization of the first or second component will be calculated, depending on which component the solvent is. The mathematical dependence of the composition on temperature is expressed by equations of (3) or (4).

$$\ln x_i^L = \frac{\Delta H_{m,i}}{R}\left(\frac{1}{T_{m,i}} - \frac{1}{T}\right) \cdot / \Phi_i^{"}, \quad (3)$$

$$\ln x_i^S = \frac{\Delta H_{m,i}}{R}\left(\frac{1}{T_{m,i}} - \frac{1}{T}\right) \cdot \left(\frac{1}{\Phi_i^{"}} - \frac{1}{\Phi_i^{'}}\right), \quad (4)$$

where ⊗$H_{m,1(2)}$ is the enthalpy of melting of the 1st and 2nd components at melting point, J/mol; R is a universal gas constant, 8.3144 J/mol K; $T_{m,1(2)}$ and T - melting point of the 1st and 2nd components and crystallization of melts, K; Φi ' - the Bjerrum-Guggenheim coefficient for the 1st and 2nd components which permits to find a correlation dependence and to calculate a mathematical expression for the ratio of the activities of the i-component in the liquid and solid phases; Φi'' - the Bjerrum-Guggenheim coefficient for the 1st and 2nd components which permits to find a correlation dependence and calculate a mathematical expression for liquidus line of i-component.

These mathematical expressions (3, 4) are the semi-empirical dependencies as a modified Le Chatelier-Shreder equation.

So, referring to Table 1, the crystallization region of α-Fe (Fe-Si system) has two phase transitions, thus it is described by the equation from the melting point of iron 1811 K to the first phase transition:

for crystallization region of α–Fe (5):

$$\Phi_{Fe}^{"} = 1{,}87 - 1{,}47 \cdot a_{Fe}^L / a_{Fe}^S, \quad (5)$$

for region of an ordered phase ofα_2–Fe (6):

$$\Phi_{Fe}^{"} = 0{,}9866 - 0{,}4218 \cdot a_{Fe}^L / a_{Fe}^S, \quad (6)$$

for region of an ordered phase of α_1–Fe (7):

$$\Phi_{Fe}^{"} = 0{,}6349 + 1{,}5733 \cdot a_{Fe}^L / a_{Fe}^S. \quad (7)$$

The crystallization region of α-Fe (Fe-Al system) is calculated by equation (8):

$$\Phi_{Fe}^{"} = 1{,}3606 - 1{,}3319 \cdot a_{Fe}^L / a_{Fe}^S, \quad (8)$$

for region of an ordered phase of α_2–Fe (9):

$$\Phi_{Fe}^{"} = 0{,}5445 - 0{,}3883 \cdot a_{Fe}^L / a_{Fe}^S. \quad (9)$$

The triple system of Fe-Si-Al is the basis of silicon aluminum alloys and the silicon crystallization region in it and the features of thermodynamics of melts in this area are essential for the melting process of ferrosilicon aluminum.

Combining of the calculation results of the osmotic coefficients of Φ_{Si} for different sections of the Si-Fe-Al system (Figure 1) and isotherm Φ_{si} for the different temperatures (Figure 2) permits to identify the characteristics of the behavior of elements in the Fe- Si-Al system. The change in the crystallization beam of the alloys from the Si-Fe to Si-Al system shows (Figure 1) that only near with the Si-Fe system the melts, as noted above, have the component association and a huge negative deviation from ideality (Φ_{si} is much more than one), (Figure 2) [[9], [10], [11]].

In the Si-Al system, the initial additions of Al lead to a significant deviation of the energy characteristics of Si in comparison with values of an osmotic coefficient of the Si-Fe system. But the rate of this deviation with a temperature change is lower, and therefore if the starting is from $a_{Si.}$ = 0.8, the effect of Al will decrease (Figure 1).

The beam with a ratio of 0.19 Fe:0.81 Al (at.) (Figure 1) is characterized by a linear dependence of Φ_{si} caused with a weak development of association of components in the melt. But if the starting is from the ratio of 0.49 Fe:0.51 Al (at.), the bending of Φ_{si} for the beam can be observed.

As the temperature increases, the negative deviation of Si properties from ideality (figure 2) can be intensified and hence its better miscibility with iron and aluminum in the region of Fe : Al = 0.7 : 0.3% (at.), which corresponds to the compositions of ferrosilicon aluminum (FeSiA) alloys with 12-37% Fe and 20-25% Al in recalculation by weight concentrations [9]. The temperature reduction moves the studied area to the Fe-Si binary system. This indicates that at low temperatures Al dissolves better in Fe-Si-rich alloys, and as the temperature

increases, the alloying process with richer aluminum content is facilitated.

The received data on behavior of an osmotic coefficient of Bjerrum-Guggenheim (Φ_{si}) for systems of Si-Al and Si-Fe and also for the two median beams are approximated by the three-term expression (1), provided that the associated complexes are present in the melts (Table 1).

Isotherms of Φ_{si} (Figure 2) for the entire crystallization surface can be easily represented as:

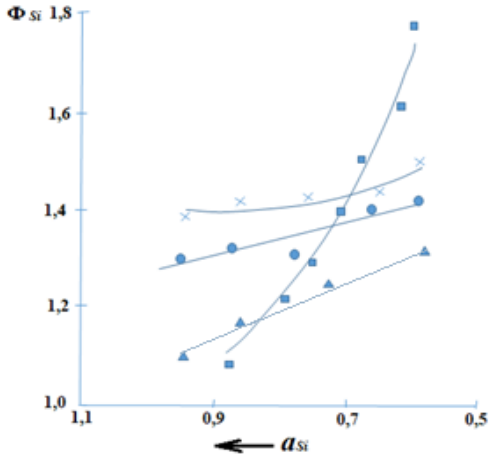
$$\Phi_{gen.Si} = Z_{Fe} \cdot \Phi'_{Si-Fe} + Z_{Al} \cdot \Phi'_{Si-Al} + Z_{Fe}^2 \cdot Z_{Al} \cdot \Phi'_{Fe/Al} + + Z_{Fe} \cdot Z_{Al}^2 \cdot \Phi'_{Al/Fe}, \quad (10)$$

where $Z_{Fe} = x_{Fe}/(x_{Fe} + x_{Al})$, (at.);
$Z_{Al} = x_{Al}/(x_{Fe} + x_{Al})$;

$\Phi'_{Fe/Al}$ - generalized equation of Φ_{si}, determined by the Scheffé's method. By the solving of two linear equations with this value obtained after substitution in the general expression $\Phi_{gen.Si}$, the equation of Φ_{si} for the two beams of 0.491 Fe:0.501 Al and 0.19 Fe:0.81 Al (at.) and Zi values was calculated (Table 1).

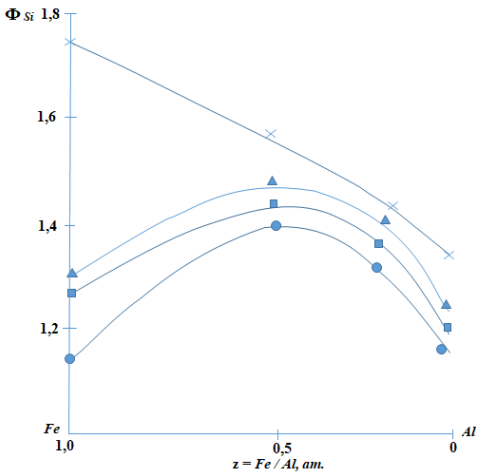
Table 1 - Parameters of crystallization regions of phases in the phase diagram of the binary systems based on iron

System	Phase (Φ' or Φ'')	Coefficients of equation of dependence of (1), (2)			Correlation coefficient	Variance $\pm\otimes_{L,S}$
		A	B	C		
FeSi	δ-Fe(Φ')	13.38	-12.24	-	-0.9978	-
	δ-Fe(Φ'')	1.87	-1.47	-	-0.9995	-
	α_2-Fe(Φ')	24.47	-25.42	-	-0.9907	-
	α_2-Fe(Φ'')	0.99	-0.42	-	-0.9010	-
	α_1-Fe(Φ')	70.07	-81.53	-	0.9905	-
	α_1-Fe(Φ'')	-0.63	1.57	-	-0.9801	-
FeSi-Fe	FeSi(Φ')	1.84	-1.59	-	-0.9920	-
FeSi-Si	FeSi(Φ')	1.55	-1.24	-	-0.9967	-
Si-Fe	Si(Φ')	-0.788	0.3504	-1.358	-	0.0018
Fe-Al ($T^{calc.}_{\alpha\to\alpha_2}$ = 1584K)	α-Fe(Φ')	3.87	-3.17	-	-0.9974	-
	α-Fe(Φ'')	0.399	0.05	-	0.9584	-
	α_2-Fe(Φ')	-1.03	2.50	-	0.9991	-
	α_2-Fe(Φ'')	-0.57	1.17	-	0.9988	-
	ε-phase(Φ')	-118.99	154.37	-	0.9820	-
	ε- phase (Φ'')	-3.27	4.48	-	0.9944	-
	ε- phase (Φ')	-118.99	154.37	-	0.9820	-
	ε- phase (Φ'')	-3.27	4.48	-	0.9944	-
Fe_2Al_5-Fe	Fe_2Al_5(Φ')	5.99	-5.96	-	-0.9998	-
	Fe_2Al_5(Φ'')	3.21	-3.17	-	-0.9988	-
Fe_2Al_5-Al	Fe_2Al_5(Φ')	1.28	-1.27	-	-0.9980	-
	Fe_2Al_5(Φ'')	0.84	-0.83	-	-0.9880	-
Crystal. region $FeAl_3$	Fe_2Al_5(Φ')	0.76	-0.61	-	-0.9998	-
	Fe_2Al_5(Φ'')	0.59	-0.57	-	-0.9978	-
SiAl	Si(Φ')	1.622	-0.58	0.001	-	0.0014
Si-0.491Fe: 0.509Al	Si(Φ')	0.7143	0.3297	-0.352	-	0.0021
Si-0.194Fe: 0.806Al	Si(Φ')	1.2279	-0.0445	-0.029	-	0.0016



■ - Φ_{si}^{Si-Fe}, ▲ - Φ_{si}^{Si-Al}, ● – 0.49Fe:0.51Al, **x** – 0.19Fe:0.81Al

Figure 1 - Change of Φ_{si} along silicon crystallization line in binary systems of Si-Fe and Si-Al



x – 1200^{0}C, ▲ - 1250^{0}C, ■ - 1300^{0}C, ● - 1350^{0}C

Figure 2 - Isotherms of Φ_{si} at different temperatures of Fe: Al = 0.7-0.3% (at.) which corresponds to compositions of Fe-Si-Al alloys with 12-37% Fe and 20-25% Al in recalculation

The obtained results for two binary systems of Si-Fe and Si-Al and two beams with Fe/Al composition ratio at the special temperatures and crystallization region demonstrated a good similarity of the calculated (solid lines) and experimental (points) composition data (Figure 2).

Conclusions

Based on the behavior of the osmotic coefficient of Bjerrum-Guggenheim in the melt of the Fe-Si-Al system using the thermodynamic method, the compositions of silicon-aluminum alloys with increased aluminum content were substantiated. The received mathematical dependences of the osmotic coefficient of Bjerrum-Guggenheim determined the crystallization temperature of the ferrosilicon-aluminium alloy, thus, the process of alloy formation with rich aluminum content was observed. Referring to the character of changes in the osmotic coefficient of Bjerrum-Guggenheim it was determined that the temperature increase leads to the strong negative deviations of silicon properties and thus to its better miscibility in the melt with iron and aluminum for the compositions of Fe: Al = 0.7 - 0.3 %. The optimum ratios of elements in the ferrosilicon aluminum complex alloy with the iron content of 12-37%, aluminum -20-25%, and silicon - 68-38% were defined. This composition characterizes the area of the alloy in which the aluminum melt will fully absorb.

Conflict of interests. On behalf of all authors, the correspondent author declares that there is no conflict of interests.

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Fe-Si-Al жүйесінің алюминий мөлшері жоғары кремний алюминий қорытпаларының құрамын термодинамикалық негіздеу

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ТҮЙІНДЕМЕ

Қара металлургияны дамытудың басым бағыты-жоғары сапалы металл өндірісін және металл бұйымдарының жаңа ассортиментін ұлғайту. Болаттардың сапасын жақсартуға қол жеткізудің бір әдісі - оларды өндіруге алюминий, кремний, марганец және т.б. негізіндегі күрделі қорытпаларды тарту, олар тотықсыздандырғыштар мен легірлеуші қоспалар ретінде қажет. Мақалада алюминийдің күрделі ферросиликоалюминий қорытпасында (FeSiAl) ерігіштігінің термодинамикалық негіздеу мүмкіндігі, олардың күй диаграммалары негізінде Бьеррум-Гуггенгейм осмостық коэффициенті арқылы талқыланады. Қолданылатын әдістеме Бьеррум-Гуггенгейм тұжырымдамасына негізделген фазалық тепе-теңдіктің теориялық зерттеулеріне негізделген және нақты жүйенің қасиеттерінің идеалдан ауытқу дәрежесін бағалауға арналған C# тіліндегі (Csharp) компьютерлік бағдарламалар жиынтығын қамтиды. Бағалау критерийі - Бьеррум-Гуггенгейм осмостық коэффициенті. Кристалдану өрістерінің пайда болуының шекаралық жағдайында идеалды сұйық және қатты фазалардағы компоненттердің белсенділігі (оң Фі <1 немесе теріс Фі >1) қатынасы бойынша Бьеррум-Гуггенгейм осмостық коэффициентінің өзгеру сипаты. ферросиликоалюминийді балқыту процестеріне байланысты фазалар оны металл тотықсыздандырғыш ретінде қолдану мүмкіндігінің тікелей дәлелі болып табылады. Бьеррум-Гуггенгейм осмостық коэффициентінің есептелген математикалық тәуелділіктері ферросиликоалюминий қорытпасының кристалдану температурасын анықтауға мүмкіндік берді, бұл кезде құрамында алюминийі көп қоспалар бар. Кристалданатын компоненттің Бьеррум-Гуггенгейм осмотикалық коэффициентінің оның сұйық және қатты фазалардағы белсенділігінің арақатынасына тәуелділік графиктері температураның жоғарылауы кремнийдің қасиеттерінде күшті теріс ауытқуларға әкелетінін көрсетті, бұл оның жақсы араласуын білдіреді. Темір және алюминиймен балқытады. Күрделі ферросиликоалюминий қорытпасында (FeSiAl) алюминийдің құрамы жоғарылаған кремний-алюминий қорытпаларының құрамы олардың күйлік диаграммалары негізінде темір құрамы 12-37%, алюминий 20-25%, кремний 68-38% бар Бьеррум-Гуггенгейм осмостық коэффициенті арқылы құрылды олардың күй диаграммалары негізінде орнатылған. Алынған теориялық нәтижелер бұл металды кенді-термиялық пештерде балқыту кезінде жоғары күлді көмірден келетін ферросиликоалюминий балқымаларымен алюминийдің максималды мүмкін ассимиляциясын қамтамасыз ететін жағдайларды анықтауға мүмкіндік береді, бұл-өндірістің дамуының тікелей жолы - күрделі қорытпаларды алу технологиясы.

Түйін сөздер: күй диаграммасы, Бьеррум-Гуггенгейм коэффициенті, фазалық кристалдану өрістері, кремний алюминий қорытпалары, ферросиликоалюминий, кешенді қорытпалар.

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Термодинамическое обоснование составов кремнеалюминиевых сплавов с повышенным содержанием алюминия системы Fe-Si-Al

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АННОТАЦИЯ

Приоритетным направлением развития чёрной металлургии является увеличение производства высококачественного металла и металлопродукции нового сортамента. Одним из путей достижения повышения качества сталей является вовлечение для их производства комплексных сплавов на основе алюминия, кремния, марганца и т.д., так необходимых в качестве раскислителей и легирующих добавок. В статье рассмотрена возможность термодинамического обоснования растворимости алюминия в комплексном сплаве ферросиликоалюминии (FeSiAl) на основе их диаграмм состояния через осмотический коэффициент Бьеррума-Гуггенгейма. Применяемая методология основана на теоретических исследованиях фазовых равновесий на основе концепции Бьеррума-Гуггенгейма и включает комплекс компьютерных программ на языке C# (Csharp), предназначенных для оценки степени отклонения свойств реальной системы от идеальной. Критерием оценки является осмотический коэффициент Бьерумма-Гугенгейма. Характер изменения осмотического коэффициента Бьеррума-Гуггенгейма от отношения активности компонентов в идеальной жидкой и твердой фазах (положительный Фі <1 или отрицательный Фі

>1) при граничных условиях формирования полей кристаллизации фаз, относящихся к процессам выплавки ферросиликоалюминия является прямым доказательством возможности применения его в качестве металлического восстановителя. Расчитанные математические зависимости осмотического коэффициента Бъеррума-Гуггенгейма позволили определить температуру кристаллизации сплава ферросиликоалюминия, при которой происходит процесс сплавообразования с более богатым содержанием алюминия. Графики зависимости осмотического коэффициента Бьеррума-Гуггенгейма кристаллизующегося компонента от отношения его активности в жидкой и твердой фазах показали, что рост температуры приводит к сильным отрицательным отклонениям свойств кремния, а значит лучшей смешиваемости его в расплаве с железом и алюминием. Установлены составы кремнеалюминиевых сплавов с повышенным содержанием алюминия в комплексном сплаве ферросиликоалюминий (FeSiAl) на основе их диаграмм состояния через осмотический коэффициент Бьеррума-Гуггенгейма с содержанием железа 12-37 %, алюминия 20-25 %, кремния 68-38 %. Полученные теоретические результаты позволяют определить условия, обеспечивающие максимально возможное усвоение алюминия расплавами ферросиликоалюминия, поступающего из высокозольного угля в процессе плавки этого металла в руднотермических печах, а это прямой путь к разработке технологии получения комплексных сплавов.

Ключевые слова: диаграмма состояния, коэффициент Бьеррума-Гуггенгейма, поля кристаллизации фаз, кремнийалюминиевые сплавы, ферросиликоалюминий, комплексные сплавы.

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