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MATHEMATICAL MODEL OF THE PHASE COMPOSITION DIAGRAM OF THE Fe – S - Cu SYSTEM

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The article presents the results of constructing a diagram of the phase composition of the Fe-S-Cu system and its mathematical model. Using the equations obtained in the work, a computer program was created and, using it, an analysis of phase formation in copper ores of various deposits was carried out. It was found that copper ore concentrates from the Berezovsk deposit in Kazakhstan contain Cu_5FeS_4 (20,22 %), CuS (14,21 %) and FeS_2 (65,57 %), and copper ores from the Zyryanovsk deposit contain $CuFeS_2$ (4,03 %), Cu_5FeS_4 (45,29 %) and FeS_2 (50,68 %). Such data allows you to choose the optimal methods for further processing of concentrates, and the mathematical approach itself is more productive than the often used geometric one according to the rule of segments.

Key words: Fe-S-Cu system, diagram, phase, mathematical model, computer program.

INTRODUCTION

Industrial enterprises are aimed at producing products of a certain phase composition: alite ($3CaO·SiO_2$) and belite ($2CaO·SiO_2$) in cement clinker, diopside ($CaO·MgO·2SiO_2$) in stone casting, chromium carbide (Cr_7C_3) in wear-resistant cast iron, corundum (Al_2O_3), mullite ($3Al_2O_3·2SiO_2$) and calcium hexaaluminate ($CaO·6Al_2O_3$) in high-temperature ceramics of spark plugs of internal combustion engines. Only with this approach, i.e. With the targeted formation of the phase composition, it is possible to achieve cost-effectiveness of the process and high quality of the final product. For this reason, special attention is paid to the search for the optimal phase composition of products planned for production.

Typically, the initial selection of the phase composition is made using phase diagrams and physical properties. However, there are certain limitations. It is possible to remove the numerical value of any property from a three-component diagram, but from a four-component diagram it is difficult, but from five, six or more components it is impossible, because in three-dimensional space they cannot be depicted correctly. Note that most of the diagrams available in the literature are three-component, and the production products are multi-component.

The search for the required phase composition can also be carried out using instrumental methods: petrographic, X-ray diffraction (XRD), metallographic. But if it is necessary to study tens and hundreds of blending options to obtain a product of the required properties, instrumental methods will be costly and time-consuming. They cannot be applied at all if the researcher only has the chemical composition of the raw materials intended for extraction. It also note that instrumental methods are applied, as a rule, to solid, frozen materials and their results cannot be attributed to melts due to the possible decomposition of some phases when heated.

It seems that the solution to the problem posed can be facilitated by a mathematical description of phase composition diagrams. The creation of models removes restrictions on the number of components present in the product and the temperature range, bringing the results closer to production conditions. In this work, it is planned to construct a diagram of the phase composition of the Fe-S-Cu system and create its mathematical model.

WAYS OF RESEARCH

The work used the triangulation method [1,2], when the resulting diagram is a set of elementary triangles of

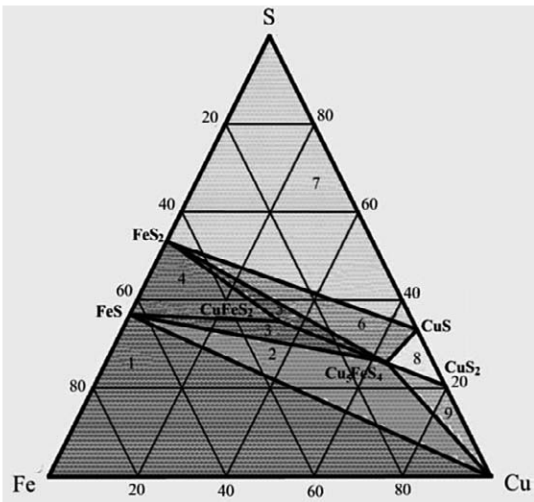

Figure 1 Phase composition diagram of the Fe-S-Cu system

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Table 1 **Summary characteristics of the Fe-S-Cu system**

Number	Triangle	Transformation equations	S / sq. units
1	Cu-Fe-FeS	$Cu = 1 \cdot Cu_0$; $Fe = 1 \cdot Fe_0 – 1,741 \cdot S_0$; $FeS = 2,741 \cdot S_0$.	0, 1579
2	$Cu-Cu_5FeS_4-FeS$	$Cu = 1 \cdot Cu_0 + 1,897 \cdot Fe_0 – 3,303 \cdot S_0$; $Cu_5FeS_4 = – 2,996 \cdot Fe_0 + 5,219 \cdot S_0$; $FeS = 2,099 \cdot Fe_0 – 0,914 \cdot S_0$.	0,0527
3	$CuFeS_2-Cu_5FeS_4-FeS$	$CuFeS_2 = – 4,321 \cdot Cu_0 – 8,198 \cdot Fe_0 + 14,282 \cdot S_0$ $Cu_5FeS_4 = 3,942 \cdot Cu_0 + 4,483 \cdot Fe_0 – 7,810 \cdot S_0$ $FeS = 1,379 \cdot Cu_0 + 4,715 \cdot Fe_0 – 5,472 \cdot S_0$	0,0122
4	$CuFeS_2-Cu_5FeS_4- FeS_2$	$CuFeS_2 = 2,891 \cdot Cu_0 + 16,463 \cdot Fe_0 – 14,338 \cdot S_0$ $Cu_5FeS_4 = – 0,02 \cdot Cu_0 – 9,003 \cdot Fe_0 + 7,841 \cdot S_0$ $FeS_2 = – 1,889 \cdot Cu_0 – 6,460 \cdot Fe_0 + 7,497 \cdot S_0$	0,0089
5	$Cu_5FeS_4-CuS-FeS_2$	$Cu_5FeS_4 = 2,631 \cdot Cu_0 + 5,989 \cdot Fe_0 – 5,216 \cdot S_0$ $CuS = – 1,002 \cdot Cu_0 – 5,705 \cdot Fe_0 + 4,969 \cdot S_0$ $FeS_2 = – 0,629 \cdot Cu_0 + 0,716 \cdot Fe_0 + 1,247 \cdot S_0$	0,0257
6	$S-CuS-FeS_2$	$S = – 0,504 \cdot Cu_0 – 1,148 \cdot Fe_0 + 1 \cdot S_0$ $CuS = 1,504 \cdot Cu_0$ $FeS_2 = 2,148 \cdot Fe_0$	0,1340
7	$Cu_5FeS_4-CuS-Cu_2S$	$Cu_5FeS_4 = 8,984 \cdot Fe_0$ $CuS = – 1,504 \cdot Cu_0 – 5,134 \cdot Fe_0 + 5,964 \cdot S_0$ $Cu_2S = 2,504 \cdot Cu_0 – 2,850 \cdot Fe_0 – 4,964 \cdot S_0$	0,0064
8	$Cu-Cu_5FeS_4-Cu_2S$	$Cu = 1 \cdot Cu_0 + 3,413 \cdot Fe_0 – 3,965 \cdot S_0$ $Cu_5FeS_4 = 8,985 \cdot Fe_0$ $Cu_2S = – 11,398 \cdot Fe_0 + 4,965 \cdot S_0$	0,0097
9	$FeS-FeS_2-CuFeS_2$	$FeS = – 0,00004 \cdot Cu_0 + 3,147 \cdot Fe_0 – 2,741 \cdot S_0$; $FeS_2 = – 1,88762 \cdot Cu_0 – 2,147 \cdot Fe_0 + 3,741 \cdot S_0$; $CuFeS_2 = 2,88766 \cdot Cu_0$.	0,0255

Table 2 **Chemical and phase composition of concentrates**

Kazakhstan concentrates [6]	Element content / %			Phase content / %		
	Cu	Fe	S			
Zhezkazgan	39,5(62,35)	7,95(12,55)	15,9(25,1)	Cu	Cu_5FeS_4	FeS
				3,25	93,35	3,4
Zyryanovsk	25,7(30,43)	25,05(29,66)	33,7(39,91)	$CuFeS_2$	Cu_5FeS_4	FeS_2
				4,03	45,29	50,68
Zhezkentsk	19,65(21,35)	33,4(36,29)	39,0(42,36)	$CuFeS_2$	Cu_5FeS_4	FeS_2
				33,83	4,57	61,6
Berezovsk	17,7(22,24)	26,1(32,78)	35,8(44,98)	Cu_5FeS_4	CuS	FeS_2
				20,22	14,21	65,57

equilibrium coexisting phases. The diagram obtained for the system under study is shown in Figure 1.

It is composed of nine triangles of coexisting phases: 1. Cu-Fe-FeS, 2. $Cu-Cu_5FeS_4-FeS$, 3. $CuFeS_2-Cu_5FeS_4-FeS$, 4. $CuFeS_2-Cu_5FeS_4-FeS_2$, 5. $Cu_5FeS_4-CuS-FeS_2$, 6. $S-CuS-FeS_2$, 7. $Cu_5FeS_4-CuS-Cu_2S$, 8. $Cu-Cu_5FeS_4- Cu_2S$, 9. $FeS-FeS_2-CuFeS_2$.

From the resulting diagram, the phase composition of the concentrate based on its main elements can be determined using the rule of segments [3], plotting its chemical composition on the resulting diagram. To facilitate such calculations, using our own method [4-5], we created a mathematical model of the diagram. Such a model was created for each elementary triangle in the form of equations for the dependence of the phase composition of the concentrate on its chemical composition (Cu0, S0, Fe0). These equations are listed in Table 1.

Using the resulting equations, a computer program was created (Figure 2). After setting the chemical composition of copper ore or concentrate from the console and starting, the computer finds the elementary triangle where the feedstock is located and gives its phase composition in mass percent.

This accelerates the quantitative assessment of the phase composition of various copper raw materials based on their main elements. An example of using the model is shown in Table 2 after recalculating Cu, Fe and S concentrates to 100 % (numbers in parentheses).

A similar analysis using a computer program can be performed for concentrates and other chemical compositions to select the best options for their processing.

Thus, a diagram of the phase composition of the Fe-S-Cu system was constructed and its mathematical model was created. It is suitable for numerical assessment of the phase composition of ores and concentrates with any content of iron, sulfur and copper in order to find optimal methods for their processing.

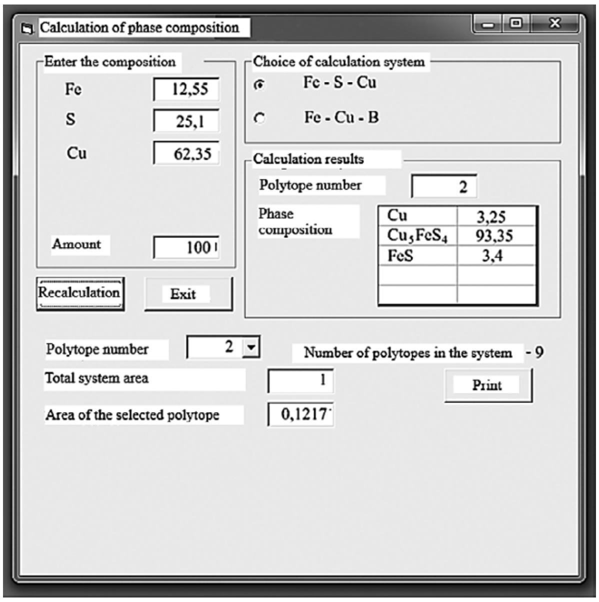

Figure 2 Computer program window

The calculated data obtained satisfactorily coincide with those determined experimentally [6-10]. Let's note some features Zhezkazgan concentrate. It has a low sulfur content. First of all, it goes to the formation of bornite (Cu_5FeS_4) with the enthalpy of formation $H^0_{298,15}$ = -380,3 kJ/mol, zinc sulfides ZnS ($H^0_{298,15}$ = -200,5 kJ/mol) and lead PbS ($H^0_{298,15}$ = -380,3 kJ/mol).

The lowest enthalpy of formation has copper sulfide CuS ($H^0_{298,15}$ = -380,3 kJ/mol) and after the formation of Cu_5FeS_4, ZnS and PbS there is not enough sulfur for its formation and copper remains in free form as Cu (Table 2).

CONCLUSION

The mathematical model of the diagram was developed using our own method, based on the balance of the distribution of the initial elements of the raw materials used among the phases formed under natural or industrial conditions. According to the concept of the method, a mathematical model is created for each elementary triangle of coexisting phases and is represented by equations connecting the phase composition of the raw material or final product with its chemical composition. An important advantage of the presented approach is the possibility of numerical assessment of the phase composition of multicomponent systems, since systems with a dimension of more than four cannot be correctly displayed on a plane. The mathematical model can operate in multidimensional space, and there are no obstacles for it to describe five, six or more component systems inherent in production systems. It is suitable for numerical assessment of the phase composition of ores and concentrates with any content of iron, sulfur and copper in order to find optimal methods for their processing.

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Note: he responsible translator for English language is Nataliya Drag, Karaganda, Kazakhstan