MATHEMATICAL MODEL OF PHASE COMPOSITION DIAGRAM OF CaO - SiO₂ - Fe₂O₃ - B₂O₃ SYSTEM

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INTRODUCTION

The CaO - SiO₂ - Fe₂O₃ system is an important component of multicomponent systems, and for a number of productions has also an independent value. It is included, for example, into the six-component CaO - SiO₂ - Al₂O₃ - MgO - FeO - Fe₂O₃ system which describes the processes of production of cement clinker, ceramics, refractory materials, smelting of cast iron, steel, ferroalloys and other production. As independent it describes, for example, the processes of production of pellets by the annealing method from ferriferous quartzite. For this reason this system is a subject of continuous studies.

METHODS OF STUDYING

The method which is based on the thermodynamic assessment of the possibility of the secondary compounds coexistence, as well as the principles of topological geometry of diagrams [1, 2] is applied for the development of the phase composition diagram.

In the graphic representation the CaO - SiO₂ - Fe₂O₃ - B₂O₃ system represents a tetra-hedron made of private systems (Table 1).

Table 1 List and number of private systems

<table>
<thead>
<tr>
<th>Number of components</th>
<th>Systems</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CaO:SiO₂:Fe₂O₃:B₂O₃</td>
</tr>
<tr>
<td>2</td>
<td>CaO-SiO₂:CaO-Fe₂O₃:CaO-B₂O₃; SiO₂-Fe₂O₃:SiO₂-B₂O₃:Fe₂O₃:B₂O₃</td>
</tr>
<tr>
<td>3</td>
<td>CaO-SiO₂:Fe₂O₃:CaO-SiO₂:B₂O₃; CaO-Fe₂O₃:B₂O₃:SiO₂-Fe₂O₃:B₂O₃</td>
</tr>
<tr>
<td>4</td>
<td>CaO-SiO₂:Fe₂O₃:B₂O₃</td>
</tr>
</tbody>
</table>

The data of the carried out studies were planned to be used first of all for high-temperature processes. Therefore for the development of a diagram from the reference media there were selected stable (congruently melting) compounds. They were applied on the triangle of compositions. By triangulation in each three-component system there was determined the number of elementary triangles of the coexisting phases.

In this work there was defined the purpose of studying the regularities of phase forming when entering boric anhydride (B₂O₃) in the CaO - SiO₂ - Fe₂O₃ system. It has a strong effect of lowering viscosity, refractorness, surface tension of the silicate systems, to construct the phase composition diagram and to develop its mathematical model.

RESULTS OF THE STUDIES AND THEIR DISCUSSION

CaO – SiO₂ – Fe₂O₃ system.

It is made of three binary systems: C - S, C - F and S - F [1]. In the first one there are formed four calcium...
silicates: $\text{C}_2\text{S}$, $\text{C}_3\text{S}$, $\text{CS}$ and $\text{C}_3\text{S}_2$, the first and last of which melt with decomposition and therefore they are not accepted for the development of the diagram. In the second one (C - F) there are three ferrites of calcium: two-calcic $\text{C}_2\text{F}$ one - calcic $\text{CF}$ and semi - calcic $\text{CF}_2$. $\text{CF}_2$ is stable. In the third binary system (S - F) there are no chemical compounds [1]. Triple compounds are absent in the system. Triangulation of $\text{C} - \text{S} - \text{F}$ system executed with the use of methods [1, 2] finds in it 4 triangles of the coexisting phases (Figure 1): 1. $\text{C} - \text{C}_3\text{S} - \text{C}_2\text{F}$; 2. $\text{C}_3\text{S} - \text{C}_2\text{F} - \text{F}$; 3. $\text{C}_3\text{S} - \text{F} - \text{CS}$; 4. $\text{F} - \text{CS} - \text{S}$.

**CaO – SiO$_2$ – B$_2$O$_3$ system.**

This system was considered in work [3]. From the list of presented there phases there are excluded $\text{C}_3\text{B}_3$ and $\text{CBS}_2$, which are formed only by the method of hydrothermal synthesis. By data [4] in this system there are two triple compounds: $\text{C}_6\text{BS}$ and $\text{C}_6\text{BS}_2$. But they melt with decomposition and therefore they cannot be used for the development of the diagram.

The compounds which are available in the binary C - S system were listed above, in the $\text{S} - \text{B}$ system chemical compounds are absent, and in the $\text{C} - \text{B}$ system there was established the existence of four calcium borates: $\text{C}_6\text{B}$, $\text{C}_6\text{B}$, $\text{CB}$ and $\text{CB}_2$, from which diborate ($\text{CB}_2$) melts with decomposition [5]. So, for the development of the diagram there were selected 5 binary phases ($\text{C}_6\text{S}$, $\text{CS}$, $\text{C}_6\text{B}$, $\text{CB}$, $\text{CB}$). Triangulation gives the diagram (Figure 1) in which we allocate 6 elementary triangles of the coexisting phases: 1. $\text{C} - \text{C}_3\text{B} - \text{C}_3\text{S}$; 2. $\text{C}_3\text{B} - \text{C}_3\text{S} - \text{F}$; 3. $\text{C}_3\text{S} - \text{F} - \text{CS}$; 4. $\text{C}_3\text{B} - \text{CB} - \text{CS}$; 5. $\text{C}_3\text{B} - \text{CS} - \text{S}$; 6. $\text{CB} - \text{S} - \text{B}$.

**CaO – Fe$_2$O$_3$ – B$_2$O$_3$ system.**

In literature there are no phase composition diagrams of the CaO - Fe$_2$O$_3$ - B$_2$O$_3$ system. Therefore triangulation is carried out by the data of its binary systems. C - F and C - B systems were considered above. In the $\text{B}_2\text{O}_3$ - Fe$_2$O$_3$ system according to data [6] there is the only thing the option of coexistence with $\text{C}_3\text{B}_3$. It should be noted that the executed splitting does not contradict the rule of coexistence of congruent compounds with congruent and isomorphic [1, 7]. Thus, in this system triangulation reveals 7 elementary triangles of coexisting phases: 1. $\text{C} - \text{C}_6\text{B} - \text{C}_6\text{S}$; 2. $\text{C}_6\text{B} - \text{C}_6\text{S} - \text{F}$; 3. $\text{C}_6\text{S} - \text{F} - \text{CB}$; 4. $\text{C}_6\text{B} - \text{F} - \text{CB}$; 5. $\text{C}_6\text{S} - \text{F} - \text{CB}$; 6. $\text{CB} - \text{F} - \text{FB}$; 7. $\text{CB} - \text{FB}$ - B (Figure 1).

**SiO$_2$ – Fe$_2$O$_3$ – B$_2$O$_3$ system.**

The phase composition diagram of the S – F - B system is also constructed for the first time. In binary $\text{SiO}_2$ - Fe$_2$O$_3$ and $\text{SiO}_2$ - B$_2$O$_3$ systems chemical compounds are absent [1, 5], and in Fe$_2$O$_3$ - B$_2$O$_3$ system there are two already mentioned compounds FB and FB$_2$. Therefore it is broken into three elementary triangles of the coexisting phases 11. $\text{S} - \text{F} - \text{FB}$; 2. $\text{S} - \text{FB} - \text{FB}$; 3. $\text{S} - \text{FB}_2 - \text{B}$ (Figure 1).

**CaO – SiO$_2$ – Fe$_2$O$_3$ – B$_2$O$_3$ system.**

The existence of the phase composition diagrams of private three - component systems permitted to make splitting into elementary tetrahedrons the four-component CaO - SiO$_2$ - Fe$_2$O$_3$ - B$_2$O$_3$ system. In addition to the used above ones there was also used the method of “closing” triangles on the tetrahedron by comparison of their compositions [1, 7], which allowed to beat the CaO - SiO$_2$ - Fe$_2$O$_3$ - B$_2$O$_3$ system 9 elementary tetrahedrons of coexisting phases: 1. $\text{CB} - \text{B} - \text{FB} - \text{S}$; 2. $\text{CB} - \text{FB} - \text{S} - \text{FB}$; 3. $\text{CB} - \text{S} - \text{FB} - \text{F}$; 4. $\text{CB} - \text{S} - \text{F} - \text{CS}$; 5. $\text{CB} - \text{CS} - \text{F} - \text{CB}$; 6. $\text{CB} - \text{CS} - \text{S} - \text{FB}$; 7. $\text{CB} - \text{CS} - \text{F} - \text{CS}$; 8. $\text{CB} - \text{CS} - \text{F} - \text{CS}$; 9. $\text{CB} - \text{CS} - \text{F} - \text{CS}$. In Figure there is shown the obtained tetrahedron and its scanning by the edges which can be used for determination of the phase composition.

But searching for the phase composition by geometrical creations in the tetrahedron is complicated, and in five-, six- and more component systems is impossible. The single way is the development of a mathematical model. In this paper, we proposed a method used mathematical description of phase diagrams of the composition, based on the balance of the distribution of the initial phases of the oxides in the image [8]. The mathematical model is created for each (seven) elementary tetrahedron. For example, to obtain such a tetrahedron Node equation: $\text{CB}=2,2523 \cdot \text{C}_0$, $\text{B}= - 1,2523 \cdot \text{C}_0 - 1,3127 \cdot \text{F}_0 + 1 \cdot \text{B}_0$, $\text{FB}_3=2,3127 \cdot \text{F}_0$, $\text{S}=1 \cdot \text{S}_0$, wherein through
C\textsubscript{2}S, F, B\textsubscript{2}O\textsubscript{3}, SiO\textsubscript{2} designated contents of CaO, Fe\textsubscript{2}O\textsubscript{3}, B\textsubscript{2}O\textsubscript{3}, and SiO\textsubscript{2} in the feed in weight percent based on chemical analysis.

In metallurgy importance attached to the formation of an optimal phase composition of agglomerated iron ore (sinter, pellet), giving it a high strength [9,10]. The above model was used as an example for these purposes. In Table 2 there is provided the chemical and phase composition of the sheaf (dead rock) of pellets from ferrous charge for obtaining the product of the required phase composition. It is shown that the addition to the system CaO - SiO\textsubscript{2} - Fe\textsubscript{2}O\textsubscript{3} - B\textsubscript{2}O\textsubscript{3} boric anhydride reduces field dicalcium silicate crystallization and stabilizes the collapse of materials containing it. An example of the positive impact of B\textsubscript{2}O\textsubscript{3} on the properties of iron-ore pellets.

**CONCLUSION**

There is built a diagram of the phase composition of the CaO - SiO\textsubscript{2} - Fe\textsubscript{2}O\textsubscript{3} - B\textsubscript{2}O\textsubscript{3} system and developed its mathematical model. It permits to determine its phase composition by the chemical composition of the material. Using the model it is also possible to define the type and quantity of components of the initial furnace charge for obtaining the product of the required phase composition. It is shown that the addition to the system CaO - SiO\textsubscript{2} - Fe\textsubscript{2}O\textsubscript{3} boric anhydride reduces field dicalcium silicate crystallization and stabilizes the collapse of materials containing it. An example of the positive impact of B\textsubscript{2}O\textsubscript{3} on the properties of iron-ore pellets.

**REFERENCES**

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