The kinetic investigations of phase formation processes in the mixture which contains BaO, Al₂O₃, Fe₂O₃ were carried out. The degree of conversion and the activation energy were calculated, the dependence of the reaction rate and the rate constant on reaction temperature was determined.

**Keywords:** activation energy, reaction rate, rate constant.

1. Introduction

The BaO-Al₂O₃-Fe₂O₃ system finds wide application for synthesis of composite materials with target noninflammable, electro-physical and magnetic properties which are used in industry and medicine. Therefore research of possible ways of compounds synthesis in this system and optimization of phase formation parameters in this system are very important. The research of phase formation processes in the BaO-Al₂O₃-Fe₂O₃ system which take place at its synthesis from initial components allows to reveal technological parameters of products synthesis in this system. Therefore kinetic researches of the BaO-Al₂O₃-Fe₂O₃ system are very important and urgent.

At present time kinetic research of the whole BaO-Al₂O₃-Fe₂O₃ system is revealed in the literature in general [1]. But kinetic research of compounds formation in the BaO-Al₂O₃-Fe₂O₃ system has not been found.

The aim of the present paper is carrying out the kinetic research of phase formation processes in the BaO-Al₂O₃-Fe₂O₃ system, optimization of technological parameters of composite materials synthesis with magnetic properties.

2. Experimental

Raw mix produced from primary components such as BaCO₃, Al₂O₃, Fe₂O₃ (analytically pure) is taken in strict stoichiometric relation. Depending on the phase structure of the BaO-Al₂O₃-Fe₂O₃ system synthesis conditions have been set taking into account that final products must be BaO·6Fe₂O₃ and the mixture of BaO·6Fe₂O₃ (50 %) and BaO·Al₂O₃ (50 %). Burning of samples was made in the temperature interval from 1173 to 1673 K with isothermal endurance of 30, 60, 90 and 180 minutes. In the clinkers received by ethyl-glycerate method [2] the content of a free barium oxide was detected. The presence of the free barium oxide in clinkers indicates that synthesis is not finished yet.

Variable factors of the experiment are the temperature and isothermal endurance at definite temperature.

Conversion degree \((G)\) of substances was calculated by following formula:

\[
G = \frac{BaO_{\text{total}} - BaO_{\text{free}}}{BaO_{\text{total}}} \cdot 100\%
\]

The velocity of components interaction of mixes with BaO was calculated according to Ginstling – Brownstein equation:

\[
I = 1 - 2/3G - (1 - G)^{2/3}
\]

where \(I\) - reaction rate, \(G\) - degree of reagents conversion.

Numerical values of the reaction rate constant for each temperature have been obtained from the graph dependence of reaction rate on temperature and endurance time, and equaled to a slope tangent angle of a straight line to an abscises axis.

The rate constant of the reaction calculated according to Boltsman’s law is expressed by the Arrhenius equation:

\[
K = Ae^{-Q/RT}
\]

where \(A\) – pre-exponential factor, \(Q\) – activation energy of a crystal lattice, kJ/mol, \(R\) - universal gas constant which is equal to 8.314 J/mol·K, \(T\) - temperature, K.

Having found the logarithm of this equation, we get

\[
\log K = b - \frac{a}{T}
\]
where \( a = \frac{Q}{2.303R} \), \( b = \lg A \). From here \( Q = a \cdot 4.575 \). From the graph \( \lg K = f(t) \) \( a \) is found which is equal to the slope tangent angle of a straight line to an abscise axis and \( b \) which is equal to segment value cutting off by a straight line on an ordinate axis. For \( \text{BaO-6Fe}_2\text{O}_3 \), \( a = 2.50 \cdot 10^3 \), and for the mixture of \( \text{BaO-6Fe}_2\text{O}_3 \) and \( \text{BaO-Al}_2\text{O}_3 \) \( a = 2.67 \).

3. Results and Discussion

We calculated the activation energy according to the above formulas. Activation energy \( Q \) is 11.44 kJ/mol for \( \text{Ba-6Fe}_2\text{O}_3 \), and 12.20 kJ/mol for the mixture of \( \text{BaO-6Fe}_2\text{O}_3 \) and \( \text{BaO-Al}_2\text{O}_3 \).

Thus the rate constant of the reaction is expressed by the following formulas:

\[
K = 3.16e^{-\frac{11.44}{RT}}
\]

for \( \text{Ba-6Fe}_2\text{O}_3 \), and for the mixture of \( \text{BaO-6Fe}_2\text{O}_3 \) and \( \text{BaO-Al}_2\text{O}_3 \):

\[
K = 2.51e^{-\frac{12.20}{RT}}
\]

Graphic dependence of the conversion degree \( G = f(t) \) and reaction rates \( I = f(t) \) for each temperature and dependence of the decimal logarithm of the rate constant of the reaction \( \lg = f(t) \) are given in Figs. 1-6.

4. Conclusions

Phase formation processes are carried out in investigated system due to the solid-phase reactions. Their velocity is satisfactorily described by Ginstling-Brownstein equation.
Roentgenographic researches confirm the phase formation kinetics in the BaO-Al₂O₃-Fe₂O₃ system.

The carried out researches are important for creation new composite materials with the given magnetic properties. On the basis of kinetic researches composite materials with magnetic properties are obtained which are applied for creation ferromagnetic ceramic materials with high magnetic properties: Curie temperature equals to 560 K and coercive force equals to 250 E.

References