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Modeling of phase equilibria of the system Ca, Fe // O, S in the framework of the generalized theory of regular ionic solutions

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Abstract

Sulfur refers to the harmful impurities of cast iron, deteriorating the quality of the metal. Therefore, much attention is paid to the problem of reducing sulfur in the iron, and then in steel. Most of the sulfur is dissolved in the iron as FeS. One method of non-domain removal of sulfur from cast iron is desulfurization. As a reagent in this process, powdered calcined lime CaO is used.

The article presents the results of thermodynamic modeling of the Ca, Fe // O, S system within the framework of the generalized theory of "regular" ionic solutions. The equations for calculating the activity of the components of the system under study are derived. The energy parameters of the model are calculated taking into account the experimental data and melting characteristics of pure oxides and sulfides for the systems CaO – CaS, FeO – FeS, FeS – CaS, FeO – CaO. The values of the energy parameters are in good agreement with the experimental data. Calculated binary state diagrams of the system under study. The diagrams FeO – FeS, CaO – CaS, FeO – CaO, FeS – CaS are calculated over the entire molar fraction from 0 to 1. The Gibbs energy of the exchange reaction FeS + CaO = FeO + CaS is determined on the basis of the following data: thermodynamic parameters characterizing the processes the melting of oxides and sulfides of iron and calcium, the values of the reduced thermodynamic potential Φ_T^o and standard enthalpies of substances $\Delta_f H_{0,i}^o$ at absolute zero. Based on the values of the energy parameters calculated for the doubles and the Gibbs energy of the exchange reaction, a FeS – CaO diagram with a simple eutectic at 90 mol. % FeS and 10 mol. % CaO, melting at 1407 K.

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