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Thermodynamic modeling of phase equilibria in the system $Na_2O – CaO – Al_2O_3$

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Abstract

The thermodynamic properties of melts of the $Na_2O – CaO – Al_2O_3$ system are of considerable interest for metallurgy, technology of ceramic materials, optical fibers. State diagrams $CaO – Al_2O_3$, $Na_2O – Al_2O_3$ have been studied by many researchers and do not have the generally accepted version, and the system $Na_2O – CaO$ has not been specifically studied. In the work, thermodynamic modeling of the phase equilibria of the $Na_2O – CaO – Al_2O_3$ system was carried out within the framework of the generalized theory of "regular" ionic solutions. Equations for the activities of the system components are derived. The energy parameters of the model are determined taking into account melting characteristics and experimental data. The state diagrams of binary systems are constructed using the calculated values of the Gibbs energies for the formation of sodium and calcium aluminates from the corresponding oxides. Using the regression equations of the temperature dependences of the energy parameters of binary melts of the $Na_2O – CaO – Al_2O_3$ system, the molar mixing functions of the liquid solution растворa G_m^M, H_m^M, S_m^M and the excess thermodynamic functions G^E, H^E, S^E were calculated at 1500-1800 °C. Lime-alumina melts are stable at all temperatures, experiencing negative deviations from ideality. The Gibbs excess energy G^E is negative and in absolute value varies from 5 to 90 kJ/mol. With an increase in the concentration of Al_2O_3 in the melt and temperature, a tendency toward disorder is clearly manifested: the entropy of the melt mixing changes its sign from "minus" to "plus". $Na_2O – Al_2O_3$ melts are formed with an exothermic effect and ordering, and are also stable. They experience strong negative deviations (for G^E) from ideality. However, the situation changes at 55 mol. % Al_2O_3 and 1700-1800 °C melts of the system are unstable.

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