THERMODYNAMIC MODELING OF THE MgO – FeO – TiO₂ SYSTEM

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The study of phase diagrams has long been an important tool in the development of science and technology. The most complete information about phase interrelations and the thermodynamic stability of phase combinations is given in the state diagrams in which thermodynamically equilibrium compositions are interconnected with the temperature. With increasing demands of new high technological materials, which are generally complex, it is important that theoretical predictions guide the work of materials scientists.

The MgO – FeO – TiO₂ system is of great interest for the researchers from the standpoint of the possibility of the production of refractory materials which are operated in harsh conditions. However, the unavailability of data on the structure of the above system hampers the development of special materials with prescribed properties. Therefore, this scientific paper delves into the studies of the structure of MgO – FeO – TiO₂ system and solidphase reactions in it.

The MgO – FeO – TiO₂ system was studied in the subsolidus domain at a temperature of 800 – 1900 °C. MgO, FeO, TiO₂ and MgTiO₃, FeTi₂O₅, MgTi₂O₅, FeTiO₃, Fe₂TiO₄, Mg₂TiO₄ are stable compounds in it.

The change in the Gibbs energy of the reactions was calculated to establish the thermodynamic probability of the existence of phases:

 $MgTiO_3 + FeTiO_5 = MgTiO_5 + FeTiO_3$,

 $2 MgTiO_3 + Fe_2TiO_4 = Mg_2TiO_4 + 2 FeTiO_3,$

 $2MgO + Fe_2TiO_4 = Mg_2TiO + 2FeO.$

Based on thermodynamic data, the triangulation of the system, previously unreported, is carried out with regard for all phases stable at this temperature.

As a result of the conducted thermodynamic calculations based on the formed thermodynamic database, the data set the direction of mutual solid-phase reactions in the three-component MgO – FeO – TiO_2 system.