Addition of CaF_2 and P_2O_5 to the Thermodynamic Database for $CaO-MgO-Al_2O_3-CrO_x-FeO_x-SiO_2$ System

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ABSTRACT

The oxide system $CaO-MgO-Al_2O_3-CrOx-FeO_x-SiO_2-(CaF_2,P_2O_5)$ relevant for the development and production of refractory materials as well as for metallurgical slag applications, glass processing and coal combustion has been thermodynamically assessed using all available experimental data.

The Gibbs energy of the liquid phase has been modelled using a non-ideal associate solution model. The compositions of the pure liquid oxide species as well as the associates have been chosen to have two moles of cations per associate thus keeping the successful method of Spear and Besmann [Bes2002].

The liquid phase of the binary systems containing P_2O_5 is described in the same way in order to provide a handle for the use in ternary assessments and later in quaternary systems. Based on the approach by Sara Serena [Ser2011] who used the ionic liquid model $(Ca^{2+})_p(O^{2-}, PO^{3-}, PO_{7/2}^{2-}, PO_4^{3-}, PO_{2.5})_q$ three associates with composition $MeO{\cdot}P_2O_5$, $2MeO{\cdot}P_2O_5$, $3MeO{\cdot}P_2O_5$ have been introduced for the systems $MeO-P_2O_5$ (where metal has the valence Me^{2+}).

For the systems of the type $Me_2O_3-P_2O_5$ one associate species $Me_2O_3{\cdot}P_2O_5$ was included.

In the thermodynamic assessments of the binary systems $Al_2O_3-P_2O_5$, $CaO-P_2O_5$, $Cr_2O_3-P_2O_5$, $FeO-P_2O_5$, $Fe_2O_3-P_2O_5$, $MgO-P_2O_5$ as well as the ternary $FeO-Fe_2O_3-P_2O_5$ system 28 stoichiometric solid phases were incorporated using available experimental information.

CaF_2 has so far been integrated into the reduced core system $CaO-MgO-Al_2O_3-FeO-Fe_2O_3-SiO_2$. This resulted in the thermodynamic description of all binary and 5 ternary systems based on the presently available experimental data.

The stoichiometric phases $3CaO{\cdot}3Al_2O_3{\cdot}CaF_2$, $11CaO{\cdot}7Al_2O_3{\cdot}CaF_2$, $4CaO{\cdot}2SiO_2{\cdot}CaF_2$, $3CaO{\cdot}2SiO_2{\cdot}CaF_2$ (Cuspidine), and $9CaO{\cdot}3SiO_2{\cdot}CaF_2$ were incorporated.

In the $Al_2O_3-CaF_2-CaO$ system special emphasis was given to a self-consistent assessment of the experimentally determined miscibility gap in the liquid phase

Literature

[Bes2002] Besmann, Theodore M.;Spear, Karl E.; J.Am.Cram.Soc. 85[12] (2002) pp2887-2894.

[Ser2011] Serena, Sara; J. Am. Ceram. Soc., 94 [9], (2011), pp. 3094-3103.