Addition of MeS & MnO_x to the GTT Oxide Database

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ABSTRACT

The oxide system CaO-MgO-Al_2O_3-CrOx-MnO_x-FeO_x-SiO_2-MeS (Me=Ca, Fe, Mg, Mn)-(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 on phase equilibria and thermodynamic properties.

The sulphides CaS, FeS, MgS and MnS are essential components for high refractory index materials but are present in radioactive and toxic wastes. Manganese oxides such as MnO and Mn_2O_3 are important for ferrous process metallurgy.

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.

The liquid phase of the binary systems containing MeS, MnO and Mn_2O_3 is described in the same way in order to provide a handle for the use in ternary assessments and later in quaternary systems.

Particular attention was given to the phases Oldhamite (CaS), Niningerite (MgS) and Troilite-HT (FeS), which exhibit very wide mutual solubility. In the thermodynamic assessments of all binary systems containing MeS as well as the ternary Al_2O_3-CaO-CaS, CaO-SiO_2-CaS, CaS-FeS-MgS systems these three solid solution phases were incorporated using available experimental information.

MnO and Mn_2O_3 have been integrated into the reduced core system CaO-MgO-Al_2O_3-FeO-Fe_2O_3-SiO_2. So far thermodynamic descriptions of all binary and some ternary systems could be realised taking into account the available experimental data.

The stoichiometric phases $MnSiO_3$ (Rhodonite), Mn_7SiO_{12} (Braunite) were incorporated using the thermodynamic data of Hf, Sf and Cp from the literature. The wide solubility ranges of Protopyroxene (Mg,Mn) SiO_3 and Rhodonite (Mn,Mg) SiO_3 are critically evaluated according to the experimentally determined phase boundaries.

Manganese is introduced into the thermodynamic description of Olivine (Ca^{+2},Fe^{+2},Mg^{+2},Mn^{+2})1(Ca^{+2},Fe^{+2},Mg^{+2},Mn^{+2})1(Si^{+4})1(O^{-2})4 in order to describe the entire solubility in MgO-MnO-SiO2 system.