Addition of Titanium oxides to the GTOX oxide database

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The GTOX oxide database containing CaO-MgO-Al_2O_3-CrO_x-FeO_x-MnO_x-ZnO-P_2O_5-SiO_2-(CaF_2, CaS, CrS, FeS, MgS, MnS) relevant for the development and production of refractory materials as well as for metallurgical slag applications, glass processing, coal combustion and gasification has been thermodynamically assessed using all available experimental data. Titanium oxides TiO_2 and Ti_2O_3 have so far been integrated into the reduced core system CaO-MgO-Al_2O_3-FeO-Fe_2O_3-MnO-Mn_2O_3-SiO_2. This resulted in the thermodynamic description of 11 binary and 7 ternary systems based on the presently 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 thermodynamic assessment of the Titanium-Oxygen system given by Waldner and Eriksson [Wal1999] was taken into account, the liquid phase was re-optimized in this work using the non-ideal associate solution model [Bes2002] with the associates Ti_2O_2, Ti_2O_3, Ti_2O_4 resulting from the two-sublattice ionic liquid model used by Waldner and Eriksson. The liquid phase of the binary oxide systems containing TiO_2 and Ti_2O_3 is described with similar sets of associates in order to provide a handle for the use in ternary assessments and later in quaternary systems. For systems of the type Me_2O_3-TiO_2 one associate species $Me_2O_3{\cdot}TiO_2$ was included, while for MeO-TiO_2 systems two associate species, $MeO{\cdot}TiO_2$ and $2MeO{\cdot}TiO_2$, were introduced.

Titanium was also introduced into the thermodynamic description of solid solution phases such as MeO, Cubic Spinel, Titania Spinel, Corundum and Pseudobrookite using available experimental information. In the titanium oxides containing systems particular attention was given to the phase Cubic Spinel which forms the wide completely miscible solid solution Fe_3O_4-$TiFe_2O_4$-$TiMg_2O_4$-$TiMn_2O_4$. The cation Ti^{+4} was introduced on the first sublattice of the present description of the Cubic Spinel phase with additional forty Gibbs energies where the missing values could be estimated using reciprocal equations.

The experimentally determined solubilities of Titanium in MeO and SiO_2-HT are described. Aluminium and magnesium titanates Al_2TiO_5, $MgTi_2O_5$ have the same pseudobrookite structure (general formula Me_3O_5) corresponding to the Al- and Mg-containing endmembers of the Ti_3O_5, $FeTi_2O_5$ (pseudobrookite) and Fe_2TiO_5 (ferropseudobrookite) and are characterized by complete solubility at high temperatures. The phase Pseudobrookite was modelled using the following formula: (Al, Mg, Fe, Ti)(Al, Ti, Fe)(Ti)$(O)_5$ which allows to describe the experimentally determined mutual solubility between Al_2TiO_5, $MgTi_2O_5$, $FeTi_2O_5$, Fe_2TiO_5 and Ti_3O_5. Furthermore, the phase Pseudobrookite exhibits wide solubility with respect to manganese oxide which was also modelled in this work.

[Bes2002] T.M. Besmann, K.E. Spear, J. Am. Ceram. Soc. 85 (2002) 2887-2894.

[Wal1999] P. Waldner, G. Eriksson, Calphad, 23, No.2, (1999) 189-218.