Thermodynamic Development on the Al_2O_3-CaO-SiO_2-M_2O (M=K,Na) Systems

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ABSTRACT

The aim of the Virtual High temperature Conversion Processes (VIRTUHCON) project is the theoretical modelling of high temperature conversion processes such as metallurgy and gasification. The thermodynamic properties of molten silicates (slag) are important input quantities for the modelling of phenomena in geoscience and for modelling in process engineering where SiO_2 (silica) is a prime component. Although the alkaline oxides normally appear in minor quantities, they can significantly change the behaviour of the slag properties because of their low melting temperatures thereby considerably lowering the liquidus temperature of the molten oxide mixture. Therefore, it is considered to be worthwhile to obtain the phase diagram and thermochemical information of alkaline oxide containing systems to help scientists in the design or development of new materials and processes.

However, experimental difficulties abound in alkaline bearing systems because SiO_2 is volatile at high temperatures and alkaline oxides are difficult to handle and prone to surface hydrolysis when exposed to air. CALPHAD modelling is therefore considered a suitable choice to provide phase diagram and thermochemical information which cannot be obtained experimentally.

The aims of the present study are a careful review of the available data – phase diagram and thermodynamics – in the system Al_2O_3-CaO-SiO_2-M_2O (M=K, Na) as well as CALPHAD modelling of this system accompanied by strategically planned key experiments. Three compounds, $K_2Ca_2Si_2O_7$, $K_4CaSi_3O_9$ and $K_8CaSi_{10}O_{25}$, were prepared by solid state reactions at 900°C using K_2CO_3, $CaCO_3$ and SiO_2 as educts and their heat capacities using conventional DSC, drop calorimetry and drop solution calorimetry. The ab-initio calculations were conducted on the solid compounds both in binary and ternary systems. These new data was included in the optimization of the ternary phase diagram Al_2O_3-CaO-SiO_2-K_2O. In this contribution, the results of experimental measurements combined with the phase diagram modelling of Al_2O_3-CaO-SiO_2-M_2O (M=K, Na) using the CALPHAD approach systems will be presented.