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Thermodynamic investigation of the Al_2O_3-M_2O (M=K,Na) systems

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The aim of VIRTUHCON is the theoretical modelling of high temperature conversion processes such as metallurgy and gasification. The thermodynamic properties of molten oxide systems (slag) are represent as important feature for the modelling of such processes. Compared to experimental methods thermodynamic equilibrium modelling is able to provide valuable prediction results within less time at lower costs. In order to perform calculations concerning systems which have a complicated structure and strong interactions between the constituents an adequate thermodynamic model and assessed thermodynamic data are needed. The accuracy of the calculation depends on the reliability of the database and adaptability of the model.

The goal of the present work is to describe the thermodynamic properties of the binary Al_2O_3-M_2O (M is an alkali oxide) which is part of the complex Al_2O_3-CaO-MgO-SiO_2-M_2O system. The CALculation of PHAse Diagram (CALPHAD) method is applied to describe the thermodynamic properties of these two binary systems. First principle calculation (VASP) is applied to get the enthalpies of formation and heat capacities of the intermediate compounds. Based on the information from literatures and ab initio data, the binary systems are assessed. The ionic two-sublattice model was applied to represent the liquid mixture in the Al_2O_3-M_2O systems, and this model can be easily extrapolated to high order system. A set of self-consistent thermodynamic parameters to describe the phases of these systems have been obtained. The calculated phase equilibria from the new optimized database show agreement with the experimental points.