RECENT EXPERIMENTAL AND MODELLING RESEARCH ON THE THERMODYNAMICS AND PHASE EQUILIBRIA OF MULTI-COMPONENT OXIDE SYSTEMS

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Abstract

Industrial slag systems are complex in terms of their chemical compositions, physico-chemical properties, and the phases and microstructures that can be formed. Each of these characteristic properties can be varied and each are interrelated to each other, presenting the significant challenges to the optimisation of existing processes and the development of new materials. There is a common linking thread between these characteristics and that is the thermodynamics of the systems; this is true for both equilibrium and metastable systems. It is argued that the key to understanding these systems and future developments in the field is access to accurate and robust thermodynamic databases and models of these multi-component, multi-phase systems.

With the advent of improved experimental techniques and powerful computer systems, new experimental data and advanced thermodynamic computer-based models describing the thermochemistry and chemical characteristics of these complex industrial processes are becoming available. These new data and models provide the possibility to predict outcomes of different process operations and to systematically analyse the outcomes of changes to process variables. In doing so this provides a clearer understanding of process chemistry and how this knowledge can be used assist in improvements of the processes.