SUCCESS STORY

K1-MET SusMet4Planet Competence Center of Sustainable Digitalized Metallurgy for a Climate Neutral and Resource Efficient Planet

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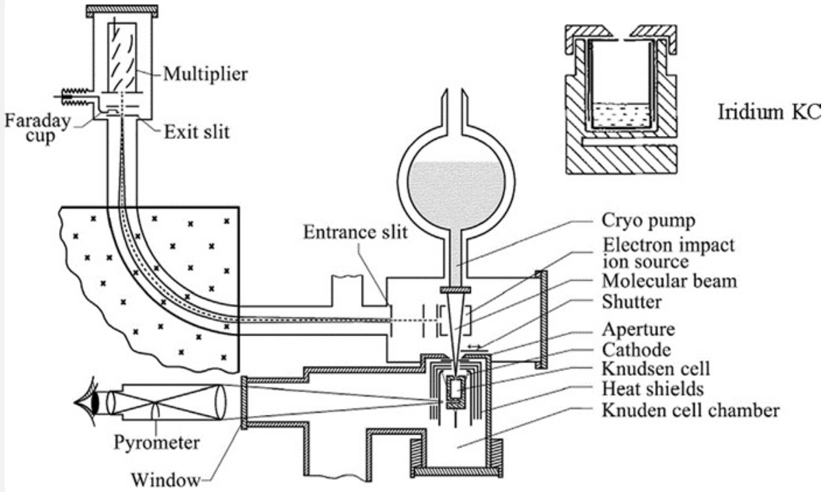

Schematic setup of a Knudsen-Effusion-Mass Spectrometer (KEMS)
[D. Kobertz, M. Müller and A. Molak, Vaporization and caloric studies on lead titanate. Calphad 46 (2014), pp. 62–79. doi:10.1016/j.calphad.2014.02.001]

DETERMINATION OF DIFFUSION AND ACTIVITY COEFFICIENTS IN SLAG

DETERMINATION OF PHYSICO-CHEMICAL PROPERTIES OF SLAGS TO INCREASE THE EFFICIENCY OF HOT METAL AND STEEL PRODUCTION.

Metallurgy is a key enabler for circular economy, because metals have a high recycling potential. In addition to the development of new technologies, the sustainable production of metals also requires accompanied digital systems. Digital twins exemplarily are the basis for the control and optimization of circular economy systems. Linking metallurgical processes enables them to determine material and energy consumption as well as the environmental impact of a circular system. Analysis and simulation tools for metallurgical aggregates are essential for the development of these digital twins. In such tools, thermodynamic and kinetic simulations of metallurgical processes are integrated. The development of this type of tool requires knowledge of thermodynamic data. The diffusion coefficient and the activity of dissolved species in slags are two crucial variables for modeling. In most models, diffusion coefficients are required to describe dissolution processes, and knowledge of activities of the respective species is necessary for the calculation of thermodynamic equilibria.

To investigate the dissolution behavior of CaO and MgO in different slags and to determine the diffusion coefficient, the rotating cylinder method was used. A calculation model was developed to determine the diffusion coefficients from the dissolution experiments, which takes both the diffusive and the convective part of the mass transport into account. The mass transfer from the face and lateral surface of the rotating cylindrical samples is described using dimensionless parameters. Other necessary slag properties (viscosity, density, and saturation concentration) are calculated using different models and FactSage™. The diffusion coefficients of CaO and MgO in different types of slag were determined using the developed experimental setup and calculation model. The results show that the dissolution rate of the oxides increases with increasing temperature. This can be explained by the decrease in slag viscosity and the increasing saturation concentration of the slag with increasing temperature.

Knudsen effusion mass spectrometry (KEMS) was used to determine the activity of CaO and MgO in slags. In this method, the sample is loaded into a heated Knudsen cell and kept at constant temperature until equilibrium between the solid or liquid sample and the vapor phase is reached. A small quantity of the vapor phase exits through an orifice in the lid of the cell. The resulting molecular beam is directed into a mass spectrometer. The measured ion intensities of the respective species are used to calculate the vapor pressures. This enables the determination of the activity of the species in the sample. Because the activity of a species corresponds to the ratio of its partial pressure in a mixture to that in the pure substance. The activities of the respective oxide could be determined from the determined partial pressures of CaO and MgO above the investigated slags and the pure substances.

Impacts and effects

The experimental determined values for the diffusion coefficients and activities of CaO and MgO in slags can be implemented in process models and would allow a more realistic modeling. This could increase the efficiency of metallurgical processes, which in turn enables energy and production time savings, which in turn contributes to the conservation of resources and leads to a reduction in costs.

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