Ellingham Diagrams, Stability Diagrams and Binary Phase Diagrams – Speaking Three Different Languages for Thermochemical Properties in FactSage

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ABSTRACT

Thermochemical modelling offers a wide range of possibilities to understand and visualise the existence of stable phases under various process conditions of interest. By making use of the basic thermodynamic properties heat capacity, reaction enthalpies, Gibbs free energies, FactSage proved to be extremely efficient for phase diagram calculations and determining phase stabilities.

However, many different “styles” of visualising thermochemistry data can be found, which often complicates a direct comparison of obtained results with available literature. In common phase diagrams (e.g. the iron-carbon phase diagram), the concentration is plotted on the abscissa and the temperature represents the ordinate.

Beside their frequent use for solid and liquid mixtures, it appears to be very uncommon to see such diagrams for the interaction between a gaseous phase and a solid material.

Research in the field of metal-gas interactions often refers to phase stabilities, displayed in an Ellingham-Richardson style which uses an energy scale instead of (molar) composition. Although identical thermochemical values have been used, the results emphasise totally different parameter ranges of interest.

Beside the frequent use of Ellingham-Richardson diagrams for high temperature applications, especially in steel industry and for tool hardening, this presentation emphasises on the visualisation and translation of thermochemistry data into common diagram styles.

The presentation further draws the listener's attention to the many possibilities of thermochemical modelling in FactSage and helps to narrow the logical gap between different graphical representations of thermochemical data.