Sulphide Database: Evaluation of Thermodynamic Data and Phase Equilibria

TATJANA JANTZEN[1], KLAUS HACK[1], ELENA YAZHENSKIKH[2], MICHAEL MÜLLER[2]

[1] *GTT-Technologies, Kaiserstr. 100, Herzogenrath, D-52134, Germany*

[2] *Institute of Energy and Climate Research, Microstructure and Properties of Materials (IEK-2), Forschungszentrum Jülich, Germany*

ABSTRACT

Non-metallic inclusions such as the sulfides are essential components for steel processing products. Iron containing sulfide systems are important for understanding of desulfurization of molten steel and formation of the sulfides during the solidification process. Moreover, the sulfides can also occur in slags and ashes from coal combustion and gasification.

The Ca-Cr-Cu-Fe-Mg-Mn-S system has been thermodynamically assessed using all available experimental data on phase equilibria and thermodynamic properties. The Gibbs energy of the liquid phase has been modelled using a non-ideal associate solution model according to the successful method of Spear and Besmann.

The compositions of the associate species correspond to those of strong short-range ordering and correlate with neutral metal sulfides.

The Iron sulfide phase commonly called Troilite and CrS modifications at high temperature indicate the same crystal structure and Pearson symbol and form a continuous solid solution. This solid solution phase can be described using two-sublattice formula:

$$(\underline{Cr}, \underline{Fe}, Cu, Mg, Mn, Va)S$$

which allows as modelling the wide existence field of this phase in the binary Fe-S and Cr-S systems as the solubility of such elements as Cu, Mg and Mn in the ternary systems.

The three copper sulfides with the formula approximately to Cu_2S exist in different temperature and composition ranges. Particular attention was given to the high-temperature phase Cu_2S-Digenite which is characterized by wide composition range of solubility.

Assuming that iron, manganese and magnesium atoms can be dissolved in Digenite the following three-sublattice model using ions was proposed in present work:

$$(\underline{Cu^{+1}}, Va)(\underline{Cu^{+1}}, Fe^{+2}, Mg^{+2}, Mn^{+2}, Va)(S^{2-}).$$

All calculations and optimizations done in this work are established using the Factsage thermochemical software package. The Sulfide database contains the gas phase, a multi-component liquid phase, solid solutions Pyrrhotite, Oldhamite, Digenite, Cu_2S-MT,Cu_2S-HT, $CuFeS_2$-HT, MnS and several solid stoichiometric compounds including the elements. The Gibbs energies of pure elements and some known sulfides are taken from the SGPS database, the missing compounds are modelled using compound energy formalism.