MM 209: Programming Assignment

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1. Roasting

Roasting is the oxidation of metal oxides and sulphur dioxide. Examples include:

$$2Zns + 3O_2 = 2ZnO + 2SO_2$$

$$2PbS + 3O_2 = 2PbO + 2SO_2$$

The roast product (either oxide, sulphate or partial sulphide) would depend on temperature and partial pressure.

2. Phase Rule

Gibbs Phase Rule is expressed by the simple formulation:

$$P + F = C + 2$$

P is the number of phases in the system. A phase is any physically separable material in the system. Phases may either be pure compounds or mixtures such as solid or aqueous solutions--but they must "behave" as a coherent substance with fixed chemical and physical properties.

C is the minimum number of chemical components required to constitute all the phases in the system.

F is the number of degrees of freedom in the system and generally refers to the number of variables that can be independently changed without altering the state of the system.

3. Predominance Area Diagram

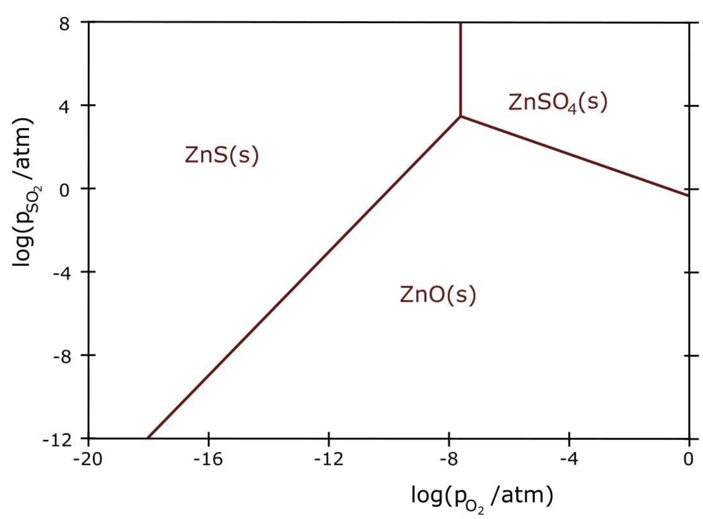

Fig. 1 Predominance Diagram of ZnS-ZnO-$ZnSO_4$ system

The predominance diagram depends on temperature and system. In a two-dimensional diagram, temperature is fixed and we have to consider all the phases which can form in a system.
Along the lines degree of freedom F = 1, which means we would have to vary pO_2 and pSO_2 to obtain phases.
At the point of $ZnS/ZnSO_4/ZnO$ equilibrium, the degree of freedom is zero and this point is called the invariant point.

For our problem, 5 reactions are taking place:

1. $Zn + SO_2 = ZnS + O_2$
2. $ZnS + 2O_2 = ZnSO_4$
3. $ZnO + SO_2 + 0.5O_2 = ZnSO_4$
4. $2ZnS + 3O_2 = 2ZnO + 2SO_2$
5. 2Zn + O2 = 2ZnO

{Temperature is constant}

For **Zn-ZnS** equilibrium (Eq. 1),
$K_1 = pO_2 \div pSO_2$ (since ZnS and Zn are assumed to be pure solids)
$LogK_1 = Log(pO_2 \div pSO_2)$

We see that Zn-ZnS equilibrium is dependent on partial pressures of oxygen and sulphur dioxide

However, for **$ZnSO_4$-ZnS** equilibrium (Eq. 2),
$LogK_2 = -0.5Log(pO_2)$
$ZnSO_4$-ZnS equilibrium depends only on pO_2 and is a vertical line. [Fig. 2]

Similar relations between equilibrium constant and partial pressure can be calculated for each of the above mentioned reactions. Solving all these equations using a programming software would help us estimate the most stable phase at a particular partial pressure of oxygen and sulphur.

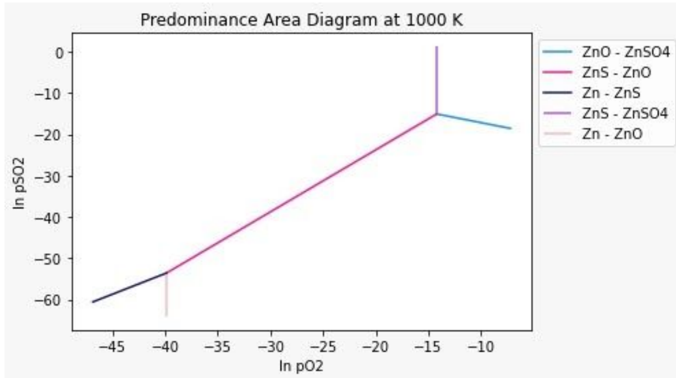

Fig. 2 Predominance diagram at 1000K obtained by us

4. Uses of Predominance Area Diagram

1. PAD shows the stable phase under different conditions/gas pressures
2. PAD predicts possible processing routes
3. One can predict the conditions for formation of a particular phase
4. It is possible thermodynamically to produce metal from sulphide by controlling pO_2

5. References

1. Xie, Fuchun & Yin, Zhou-lan & Tan, Jun & Liu, Chang-qing & Zhang, Ping-min. (2016). Plotting and application of predominance area diagram of Me-S-O system based on topological rules. Journal of Central South University. 23. 1332-1338. 10.1007/s11771-016-3184-z.
2. H S Ray, R Sridhar and K.P Abraham: Extraction of Non Ferrous Metals
3. Introduction to Thermodynamics of Material by David Gaskell
4. Principles of Extractive Metallurgy by Resenquist
5. Standard Thermodynamic Values from here: https://drive.google.com/file/d/1wLhO6Izx6Azg0mCPSuQhnrcqHJ6jMiYz/view?usp=sharing