High Temperature Corrosion of Multiphase, Multi-component Alloys in Gaseous Atmospheres under Varying partial pressure of Oxygen, Sulphur and Carbon

Thermo-Calc Software

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Abstract

Thermodynamic calculations are useful to predict the stability of phases on the surface of complex alloys in function of alloy composition and the partial pressure of elements in the gas phase that lead to corrosion at high temperatures. Typical examples are Oxidation, Sulfidation, Carburization and Metal Dusting, and many more. Calculations are not limited to iron-based alloys but are also possible for many other alloy classes such as Ni superalloys, Ti-alloys, Al-alloys, Cu-alloys, ...

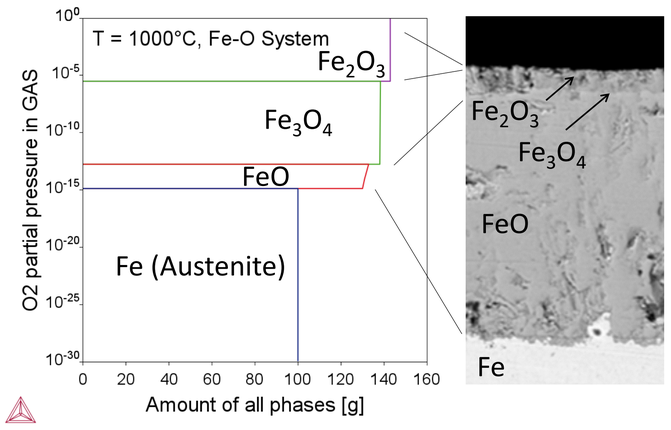
Calulating the kinetics of high temperature corrosion remains a challenge as for this diffusion of charged species through the growing oxide layer must be calculated. Efforts are currently under way inside Thermo-Calc Software AB, to develop a mobility database for oxide materials.

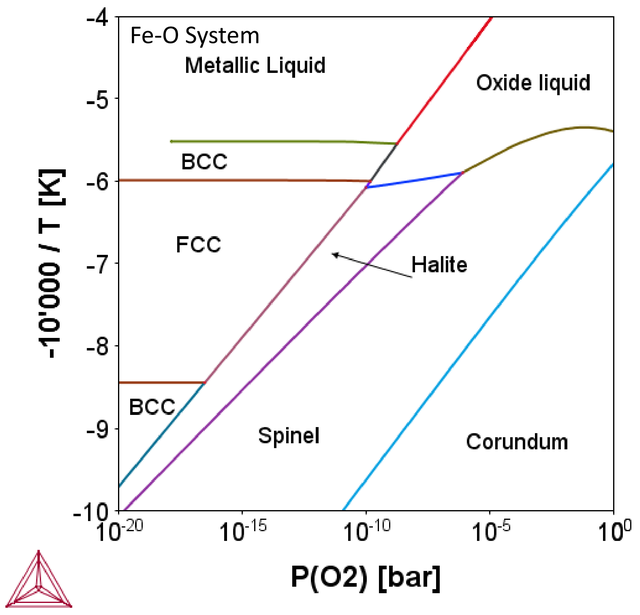
Applications

- ✓ Oxidation, scale formation
- ✓ Internal oxidation
- ✓ Sulfidation
- ✓ Nitridation
- ✓ Carburization, metal dusting
- ✓ Gas turbines, combustion engines
- ✓ High temperature pressure vessels
- ✓ Petrochemical industry
- ✓ Chemical Engineering
- ✓ Molten salt nuclear reactors
- ✓ Concentrated Solar Power (CSP) systems

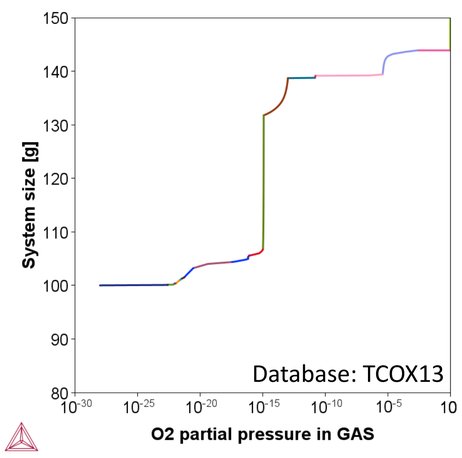
--- and many more

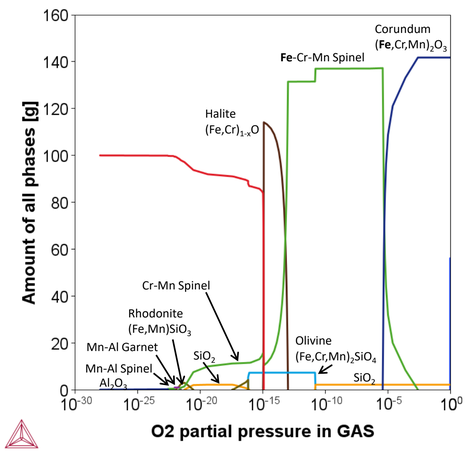
Oxygen



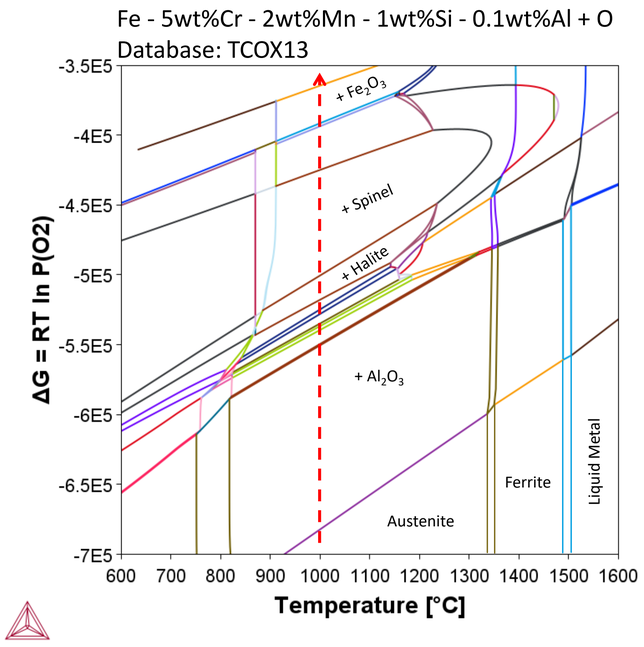


The sequence of oxide phases forming can be calculated by varying oxygen partial pressure while keeping temperature fixed. The thickness of the layer package is more difficult to calculate as it requires simulating diffusion through oxide layer (top).
A useful representation is to plot temperature in function of oxygen partial pressure, mapping out the stability fields of the various phases (right). This diagram is closely related to the Ellingham diagram.

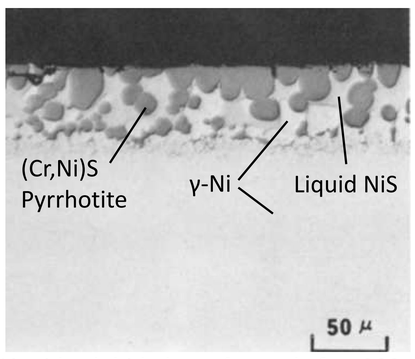




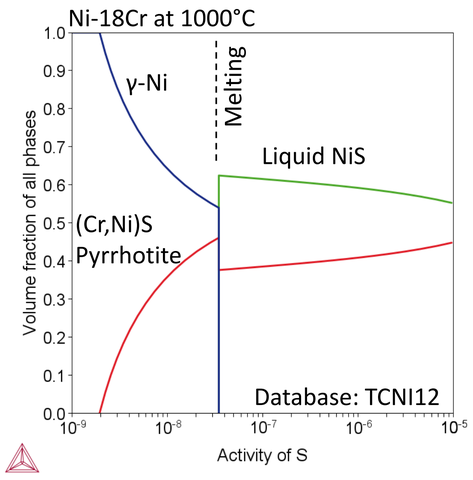
For multi-component alloys the oxidation sequence becomes very complex. The stability diagram on the right is calculated with the same axes as a typical Ellingham diagram and shows that Ellingham diagrams only poorly represent reality. Thermodynamic calculations also provide additional information, such as stability of complex oxides and composition of oxides in function of $p(O_2)$.

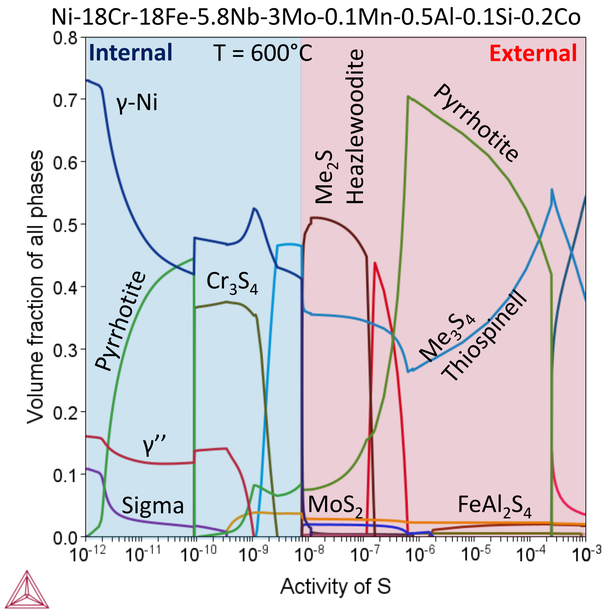


Sulphur



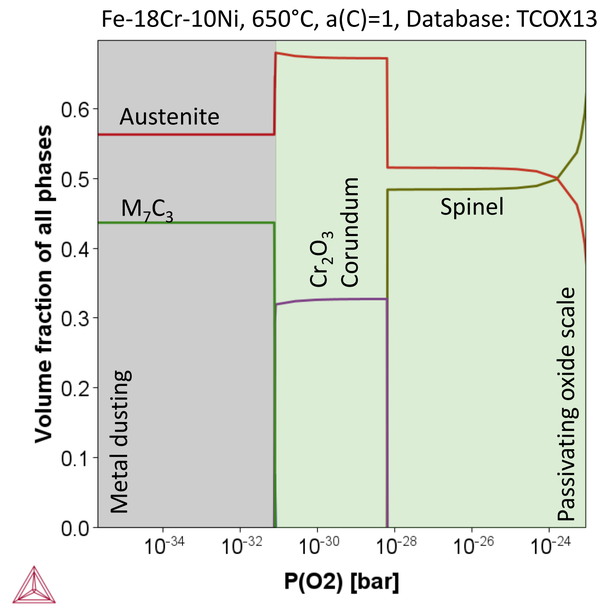
Liquid sulphide layer formed after 200s on Ni-18Cr at high S-activity (from *Goebel and Pettit, Met. Trans 1970,* ***1)***



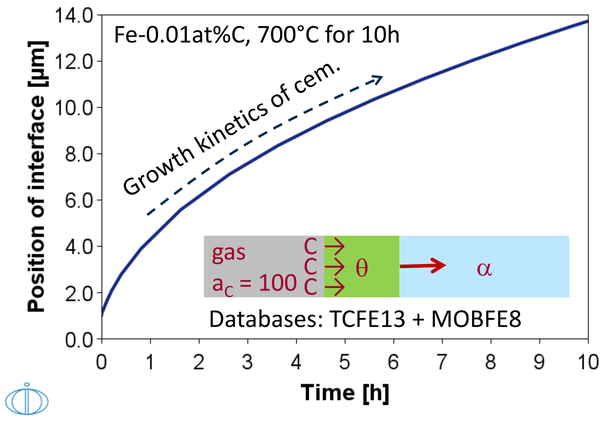


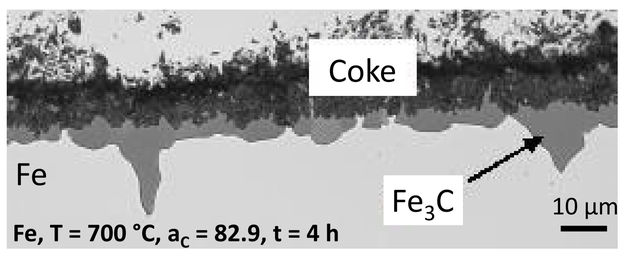
Natural gas or crude oil can have high levels of sulfur that originates from the organic plant or algae from which it was formed. At high temperatures this can lead to corrosion by the formation of a complex array of sulfide compounds both on the surface and also penetrating inside the original surface.

Carbon



At adequately high oxygen activity, a protective oxide layer forms on the alloy. Below a critical level, the oxide is dissolved and rapid disintegration of the steel can follow (top).
Growth kinetics of the carbide layer can be simulated with DICTRA. Example below is for the simple case of pure iron.





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