Oxidation of Ferritic Stainless Steel Interconnects: Thermodynamic Assessment and Experimental Validation

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imagination at work

Methodology

Experimental thermodynamic data and "first principles" calculated values at 0K and phase equilibrium data

Appropriate model selection for each phase

Optimization of model parameters

Obtain self-consistent Gibbs energy functions for all the phases in the system (thermodynamic description)

Reproduce experimental diagrams and thermo-dynamic properties of the binaries and ternaries

More importantly – extra-polate the Gibbs energies of lower order phases to those of higher order phases

Oxidation study of interconnect materials GE13L, Stainless steel 441

Furnace held at temperature Testing time: 5min, 30min, 6h, 25h, 100h

Weigh before & after oxidation

X-ray diffraction of surface (oxide)

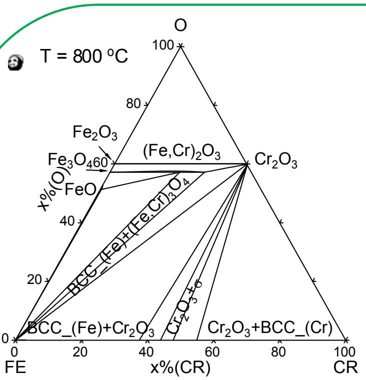
Oxide volume fraction

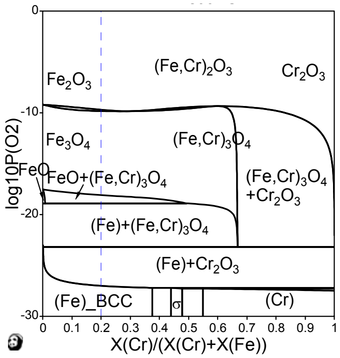
Sample preparation Vacuum impregnated, sectioned, polished

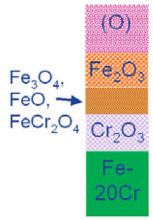
Characterization SEM/EDS

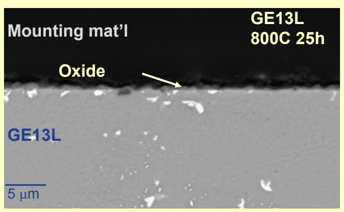
Kinetic evaluation

Fe-Cr-O at 800°C

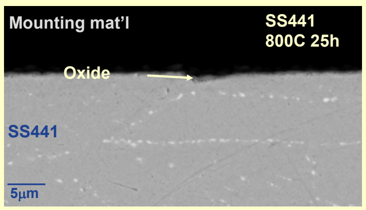








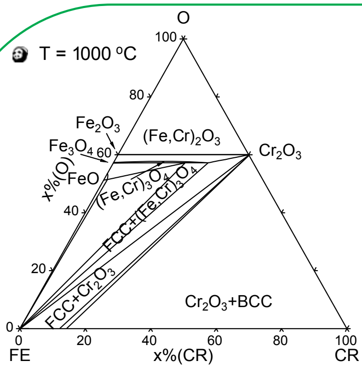
[Wt Change/Area]^2 = 0.00007.time+0.0006; time is in hours

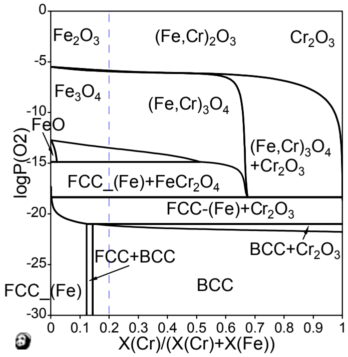


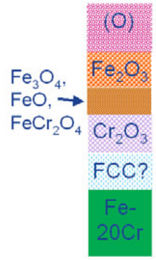
[Wt Change/Area]^2 = 0.0005.time+0.0015; time is in hours

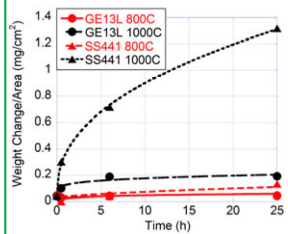
- Very thin oxide observed on both GE13L and SS441
- Parabolic constants are very low indicating slow kinetics
- Chromium oxide indicated in micrograph is a mixture of $(Cr,Fe)_2O_3$ and $(Cr,Fe)_3O_4$

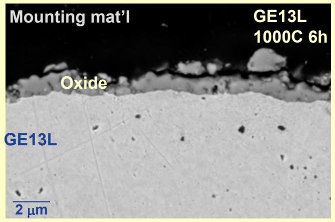
Fe-Cr-O at 1000°C



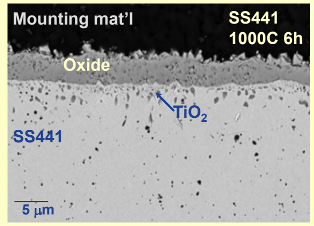








Wt Change/Area = 0.034 ln(time)-0.016; time is in hours



[Wt Change/Area]^2 = 0.0673.time+0.0782; time is in hours

Temperature	Interconnect Materials	Testing Time	Oxide Thickness (μm)	Phases Identified by XRD		
				Hematite-type $(Cr,Fe)_2O_3$	Magnetite-type $(Cr.Fe)_3O_4$	Rutile TiO_2
800 °C	GE13L	25 h	< 0.5	✓	nil	N/A
	SS441	25 h	< 0.5	✓	✓	nil
1000 °C	GE13L	6 h	1.2	✓	✓	N/A
	SS441	6 h	3.9	✓	✓	✓

Conclusions

- High temperature testing (such as those at 1000 °C) can lead to changes in phase equilibria as well as the oxidation kinetics of stainless steels.
- Thermodynamic modeling indicates different phase equilibria exist for 800 and 1000 °C. For Fe-20 Cr alloys, the alloy side (low PO_2) is anticipated to form Cr_2O_3. While on the oxygen side (high PO_2), it is likely that the oxide scale will be Fe_2O_3. In between these two layers, several oxides may form, i.e. Fe_3O_4, FeO, $FeCr_2O_4$.
- The overall PO_2 stability level at 1000 °C is greater than that of 800 °C. This results are in line with the oxidation experimental results.

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