Understanding Localised Corrosion Phenomena by Using the Synergies of Thermodynamics and Diffusion

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ABSTRACT

Corrosion phenomena represent an important field for modern technologies, ranging from industrial manufacture and waste incineration plants to environmentally friendly energy sources that may help to achieve the ambitious political goals of a green future. Hence, many efforts have been taken to understand the fundamental mechanisms that may lead to material degradation. One major problem, however, is that conditions (temperature, pressure, reactant compositions…) are often quite extreme and the mechanisms are difficult to be observed experimentally.

To overcome such problems and to provide a cost-effective alternative to predict experimental corrosion behaviour, numerical simulation proved to be very efficient. Hence, this presentation emphasises on the development of a two-step based modelling approach *ASTRID* - "Applied Simulations of Thermodynamic Reactions and Interphase Diffusion" [1] that combines element diffusion and local thermodynamic equilibrium conditions via *ChemApp*.

The aim of this presentation is to draw the listener's attention to the local thermodynamic conditions that can adjust in typical corrosion processes. Depending on the experimental conditions, high local activities of a species can either passivate the material by the formation of a protective film or – more severely – may dramatically enhance localised corrosion problems.

Examples will be given for the cases of high temperature oxidation in steels [2, 3, 4] and localised electrochemical corrosion phenomena [5]. Furthermore, novel strategies to minimise corrosive attack, both from an experimental side as well as by theoretical possibilities [6] will be discussed.

[1] M. Auinger, R. Naraparaju, H.J. Christ, M. Rohwerder, *Oxid. Met.* 76 (2011) 247-258.
[2] M. Auinger, A. Vogel, V.G. Praig, H. Danninger, M. Rohwerder, *Corros. Sci.* 78 (2014) 188-192.
[3] M. Auinger, M. Rohwerder, *HTM J. Heat Treatm. Mat.* **66** (2011) 100-102.
[4] J.H. Bott, H. Yin, S. Sridhar, M. Auinger *"Selective Precipitation of Oxides and Nitrides in Fe-Al Alloys"* submitted
[5] M. Auinger, I. Katsounaros, J.C. Meier, S.O. Klemm, P.U. Biedermann, A.A. Topalov, M. Rohwerder, K.J.J. Mayrhofer, *Phys. Chem. Chem. Phys.* **13** (2011) 16384-16394.
[6] M. Auinger *"Hydrogen transport in non-ideal crystalline materials"* submitted