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Cellular automata modelling of localised corrosion.

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Modelling of corrosion has developed to become a precious prediction tool, providing a useful complement to extrapolation of experimental data in order to prevent systems failure. However, it remains presently difficult to develop a comprehensive modelling covering all aspects and processes in corrosion. Such modelling would require simultaneous description of large space and long time scales, characteristic of the systems and their durability as well as atomistic scale description for chemical or electrochemical reactivity and/or atomic scale structure features such as defects or intergranular structures.

In the field of aqueous corrosion, we present a stochastic CA modelling approach of corrosion with spatially separated electrochemical half-reactions, diffusion, acido-basic neutralization in solution and passive properties of the oxide layers. We sum up previous studies whereby starting from different initial conditions, a common framework allows the description of generalized corrosion, localised corrosion [1], reactive and passive surfaces. Different types of corrosion such as pitting [2] or occluded corrosion [3] are described. The model highlights spontaneous spatial separation of anodic and cathodic zones, which is associated with surface state: bare metal and passivated metal on the surface as well as solution properties acidic or basic. This spontaneous change comes together with a much faster corrosion rate. Material morphology shows to be closely related to corrosion kinetics.

Cellular automata appears as an interesting intermediate proposal focusing on the mesoscopic scale, between the discontinuous description of atomistic modelling or molecular dynamics modelling, and the continuous systems at larger scales. Cellular automata can use parameters in relation to reactivity, diffusivity and complements macroscopic deterministic description introducing stochastic events.

[1] C.F. Pérez-Brokate, D. di Caprio, D. Féron, J. de Lamare et A. Chaussé : Probabilistic cellular automata model of generalised corrosion, transition to localised corrosion. *Corrosion Engineering, Science and Technology*, 52:186–193, 2017[2] C.F. Pérez-Brokate, D. di Caprio, D. Féron, J. de Lamare et A. Chaussé : Pitting corrosion modelling by means of a stochastic cellular automata-based model. *Corrosion Engineering, Science and Technology*, 52(8):605–610, 2017[3] C.F. Pérez-Brokate, D. di Caprio, D. Féron, J. de Lamare et A. Chaussé : Three dimensional discrete stochastic model of occluded corrosion cell. *Corrosion Science*, 111:230 – 241, 2016