



3D Cellular Automata modelling of Intergranular Corrosion

Simone GUIZO¹, Dung DI CAPRIO², Jacques DE LAMARE¹, Benoit GWINNER¹

¹ *Den-Service de la Corrosion et du Comportement des Matériaux dans leur Environnement (SCCME), CEA, Université Paris-Saclay, France*

² *Chimie ParisTech, PSL Research University, CNRS, Institut de Recherche de Chimie Paris (IRCP), France*

Intergranular corrosion (IGC) is one of the attacks that a material may suffer. It is characterized by a preferential attack to grain boundaries, which induces an acceleration of the material degradation. As an example, it can concern stainless steels (SS) when exposed to oxidizing media (e.g. HNO₃) as in the chemical industry [1] or in the nuclear fuel reprocessing industry [2]. Fully understand the degradation mechanism is an important challenge. IGC is characterized by the formation of triangular grooves at grain boundary level. Their progression leads, with a certain periodicity, to grain dropping, which causes an acceleration of the corrosion phenomenon [3]. From a quantitative point of view, the description of IGC kinetics is still incomplete: in particular, the IGC evolution at bulk level, is quite uneasy to access by experiments. Numerical simulations can, in this case, provide more information and improve the knowledge. Cellular Automata (CA) can model any complex reality through simple rules and space-time discretization, and are particularly suitable to model IGC [4-5]. The goal of this work is to simulate with CA the kinetics of degradation by IGC, to match as accurately as possible the experimental results in [3]. A hexagonal close-packed (HCP) grid is chosen for the simulations. The granular material structure is modeled through the Voronoi algorithm, while two corrosion probabilities (for grain and grain boundary species) drive the time evolution. With appropriate time and space equivalences, CA simulations are then able to reproduce accurately the experiments in terms of corrosion propagation velocity. The surface morphology reflects the same pattern as in the experiments: after the first transitory phase, grains start detaching from the material and accelerate the IGC process. The material-solution interface is then studied through the time evolution of the solution-grain boundary distribution. Results show an important dependence on the choice of the two corrosion probabilities.

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[2] Fauvet, P., Corrosion issues in nuclear fuel reprocessing plants. Nuclear corrosion science and engineering. D. Feron, Woodhead Publishing. 22 (2012) 679-728.

[3] B.Gwinner et al., Towards a reliable determination of the intergranular corrosion rate of austenitic stainless steel in oxidizing media. Corrosion Science 107 (2016) 60-75.

[4] D.Di Caprio et al., 3D cellular automata simulations of intra and intergranular corrosion. Corrosion Science 112 (2016) 438-450.

[5] C.F. Perez-Brokate et al., Cyclic voltammetry simulations with cellular automata. Journal of Computational Science 11 (2015) 269-278.