A toy model simulations for passivation on metallic surfaces based on stochastic cellular automata

D. di Caprio[a] and J. Stafiej[b,a]

[a] *ENSCP, University Paris 6, 4, Pl. Jussieu, 75252 Paris, Cedex 05*
E–mail: di_caprio@upmc.fr

[b] *Institute of Physical Chemistry of the Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland E–mail: accjst@ichf.edu.pl*

Passivity of metals has been widely investigated for more than 150 years. Passivity is the reason for metastability of most metallic materials otherwise extremely unstable in usual conditions. The paradox of passivity is that the metal resists corrosion better in more reactive environment. Here we describe a simple approach to account for and explain this paradox. The complicated kinetic models of passive layer in the literature describe an existing passive layer in a quasi 1-dimensional fashion. In contrast, we get information on its roughness and different regimes of morphology and functioning using a discrete lattice discrete time approach of stochastic cellular automata. We use 2-D lattice and assume that the surface metal sites in contact with environment disappear with a probability P_{cor} during one time step forming a product that can diffuse into the environment. We suppose a monotonous relation of $P_{cor} \propto -\log(V)$ on the anodic polarization describing aggressivity of environment. The diffusion is described by asymmetric exclusion random walk which amounts to a kinetic Ising model. The probability $P_{inter}^{N_{broken}}$ of the random step depends on the net number of bonds broken so that at sufficiently high density the walkers produced form a phase as predicted by the Ising model. To avoid problems with awkward boundary conditions we assume that a single walker surrounded by environment sites a has a finite life time and disappears with a given probability of dissolution P_{die}. With this model we reach steady state conditions and reproduce the qualitative shape of polarization curves. In some range of parameters we find a sharp transition from active to passive state marked by a maximum on the polarization curve. We describe the morphological changes of the passive layer induced by polarization.