Cellular automata based approach to nanopore formation in passive layers

L. Bartosik^{*a*}, D. di Caprio^{*b*} and J. Stafiej^{*a*}

^a Institute of Physical Chemistry, Polish Avademy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland, E-mail: jstafiej@ichf.edu.pl

^b LECIME, L'ENSCP, UMR 7575 du CNRS, 4 Place Jussieu, 75005 Paris, France, E-mail: dung.di_caprio@upmc.fr

In this presentation we discuss our attempts to employ the cellular automata (CA) approach to simulate nanopore formation occuring during heavy anodization on many passivating common use metals such as aluminium, titaniun, iron, niobium, vanadium. Because the phenomenon occurs on metals with largely different chemical properties and on the mesoscopic scale we feel that a cellular automata approach can be method of choice to study the phenomenon. In this presentation we show our first results obtained with what we call walker on walker (WOW) model. In this model the layer material is represented by asymmetric exclusion random walkers glued up by an attractive interaction and forming at metal solution interface. There is another kind of random walkers that form at the metal/layer interface, walk on top of layer walkers and bring about dissolution of the layer when stepping into solution. We show that this is enough to repreduce the nanopore formation. However to reduce noise we also use a combination of CA and numerical solution of Laplace equation.