Numeric simulations of the passive layer morphologies at the metal electrode surfaces

Abstract of the PhD thesis
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The topic of this work is the spatiotemporal self-organisation in complex and out-of-equilibrium systems. The thesis is based on the example of a metal electrode which passivates in an electrolyte solution. I consider potentiostatic (constant voltage) and galvanostatic (constant current) conditions. The process of passivation is described using a simple model, a stochastic cellular automaton. This model is studied with computer simulations using graphics processing units.

On the basis of the simulation results, I claim that the model predicts the self-organised phenomena similar to those observed experimentally. They include oscillations of the electrode potential or corrosion current, as well as periodic surface morphology changes that accompany the oscillations.

The primary advantage of the model is the fact that it enables us to watch the electrode surface evolution in three dimensions during the ongoing process. Other modelling methods, including differential equation systems, provide such possibility to a very limited degree. In the experiments, *in situ* observation of the surface evolution is difficult as well.

The motivation of my research is as follows: First, the simulations will give us better understanding of physical, microscopic mechanism of corrosion and passivation of metals. Second, I strive to increase our knowledge about how simple discrete models generate complex, nonlinear behaviour. And third, the research on the self-organisation could have an influence on the engineering of nanomaterials. Perhaps by regulating electric current or potential we will be able to create surfaces with desired features. This includes adsorptive or catalytic properties.

Chapter 1 – *Introduction* – discusses cellular automata, their history and applications. Next, there are a few words about the history of theoretical research on the surface growth and the growth of layers. Models based on kinetic equations, and discrete models (cellular automata) are quoted. This is followed by an introduction to nonlinear dynamics, applied to the self-organisation in chemistry. The chapter ends with the discussion of the aims of the thesis.

Chapter 2 – *Model for the Passive Layer Growth* – contains an exhaustive description of the cellular automaton used by me as a model for the passivation of metals.

Chapter 3 – *Simulations and Results* – Describes the simulations and the types of data collected. It presents the most important results: oscillations of potential and current, as well as the surface structure changes that go together with the oscillations.

Chapter 4 – *Conclusions* – contains a short summary of the most important findings, and also a discussion of the future research directions.

The thesis is concluded with the list of references.

Warsaw, February 8, 2021