Simulations of nanostructured surfaces obtained by passivity and growth.

Łukasz Bartosik

Supervisors: D. Sc. Janusz Stafiej

D. Sc. Dung di Caprio

Abstract

The presented thesis focuses on the problem of theoretical modeling of nanopore formation during the anodization of a metallic surface. The introduction covers models of formation and growth of porous layers of metal oxides. Theoretical working having substantial contributions to our understanding of how nanopores are created is described. The gaps in our knowledge regarding the process are also highlighted. Subsequently the topic of cellular automata is introduced. Cellular automata are the simulation tool of choice of the author. The basic features and possibilities of cellular automata are described and a justification of choosing cellular automata over other simulation methods is given.

The second chapter of the thesis is devoted to a in-depth description of the designed three-dimensional, asynchronous and probabilistic cellular automaton. The states and rules of the automaton are given and a justification for such a selection of states and rules is provided. Next a description of parallel programming techniques used to run the simulation program on Nvidia Tesla cards (GPGPU) is given.

In chapter three a systematic review of the obtained simulation results is presented. A series of model parameters is investigated to identify their influence on the existence and evolution of porous structures. Simulations meaning to replicate real life experiments such as two step anodization or propagating pre-patterned structures are conducted.

In the concluding chapter information from chapter three is gathered and conclusions are made. It is shown that the proposed model accounts for such features of pore growth as: pore initiation, high aspect ratio and good stability of pores, hexagonal symmetry of the obtained porous layer. Also the directions of further research that may stem from this work is suggested.