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Mathematical modeling of electrochemical kinetics of alkaline methanol oxidation

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In this talk we consider a kinetics of alkaline methanol oxidation from mathematical point of view. At first, we describe an algorithm for symbolic conversion of a chemical model to a mathematical model, based on hypergraph theory. The chemical model is given in a form of a list of reagents and reactions, while the mathematical model is presented as a system of differential equations dv/dt=F(v,u). Here v represent surface coverage of the electrode by adsorbed reagents, u is the electrode voltage, which can be either fixed or time-dependent. Solutions of the model possess rich mathematical structure, closely related with the chemical properties of the system. Stationary points are defined by the equation F(v,u)=0. Topological "hedgehog" theorems provide existence of at least one stationary point. By construction, F is a polynomial function of v, and specialized solvers are able to find all its roots. Linearization characterizes the behavior of the system near the stationary point. Eigenvalues of the system matrix are key characteristics, their signs define stability of equilibrium by Lyapunov's criterion, their values define the rate of convergence to the equilibrium, poles of lectroimpedance, structure of Nyquist plots and numerical characteristic of the system, known as stiffness. We show, that in electrochemical alkaline methanol oxidation there are several experimental effects, which can be explained by a high value of stiffness: slow relaxation to the stationary state, observed in the measurements of polarization curves and chronoamperometry, strong hierarchy of electroimpedance spectra and large hysteresis in cyclic voltammograms.

Biography

Dr Igor Nikitin was graduated from moscow institute for physics and technology, where he received his MS in 1991, PhD in 1996 and Doc Sci in 2005. Since 2004 he has been research scientist at the mathematical institute of the university of cologne, as well as associate professor at the moscow institute for physics and technology. Since 2008 he is a research scientist at fraunhofer institute for algorithms and scientific computing, sankt augustin, Germany. He has principal research interests in mathematical modeling, dynamical systems, numerical simulation, computer algebra, differential equations and has more than 100 publications in the field.

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