Simple lattice model approaches in electrochemistry

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Lattice models like cellular automata approaches are interesting for modeling in a simple way complex non linear dynamic systems. This approach is versatile and has been used in a wide variety of domains like physics, biology, chemistry, urban traffic as well as trade markets. We apply such approach to domain of electrochemistry.

Here, the lattice sites represent chemical species in liquid or solid state. Reaction and diffusion can be modeled and the stochastic evolution of the system is set by rules which take into account the local environment and probabilities. These may depend on physical parameters like the electric potential. In some cases, the electric field spatial distribution can be dynamically modeled, by a simple analogy with a diffusion process. Electric field spatial distribution combined with reaction kinetics may result in complex morphologies exhibiting sometimes self-organised patterns or different roughness properties. We present applications of the approach in the domains of:

- aqueous corrosion;
- self-organised nanoporous structures by anodisation;
- electrodeposition.

In the different examples, characteristic morphologies are reproduced and correlations between morphologies, kinetics and electric field distribution highlighted.