

Kinetic Monte Carlo Study of the Effect of Lateral Diffusion on Adlayer Structure during Electrodeposition

Per Arne Rikvold, Stefan Frank, Daniel E. Roberts
Florida State University, Center for Materials Research
and Technology and School of Computational Science
Tallahassee, FL

We use kinetic Monte Carlo simulations to study the effect of the ratio between the rate of adsorption/desorption and the rate of lateral adsorbate diffusion on the structure of submonolayers formed during electrodeposition. In particular we study the time evolution of the island size distribution during potential-step and potential-pulse conditions, in which the electrode potential is brought either permanently or only for a short time beyond the threshold for submonolayer adsorption. In the former case, the adlayer grows monotonically toward saturation, while in the latter the potential is reversed at a partial coverage, after which the adlayer desorbs. Below the critical island size, beyond which islands are more likely to grow than to decay, the size distribution is relatively independent of the lateral diffusion rate and well described by a metastable distribution of lattice animals. For high coverages, the size distribution of large islands is dominated by coalescence. A striking effect of rapid diffusion is to open a "gap" in the island-size distribution, so that the adlayer consists mainly of very large and very small islands. We also note significant differences between the structures of growing and desorbing adlayers at the same coverage.