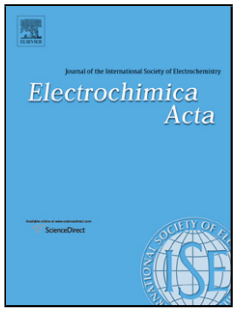

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A Finite Element Simulation of the Electrochemical Growth of a Single Hemispherical Silver Nucleus

Mesfin Haile Mamme[a,*], El Amine Mernissi Cherigui[a], Olga Dolgikh[a], Jon Ustarroz[a], Hans Simillion[a], Herman Terryn[a], Johan Deconinck[b]

[a] *Research Group Electrochemical and Surface Engineering (SURF), Vrije Universiteit Brussel (VUB), Pleinlaan 2, 1050 Brussels, Belgium*

[b] *Department of Electrical Engineering and Power Electronics, Vrije Universiteit Brussel (VUB), Pleinlaan 2, 1050 Brussels, Belgium*

Abstract

Understanding the early stages of electrochemical nucleation and growth is the cornerstone for nanoscale electrodeposition. Although studied since decades, the process is not yet fully understood. In this paper, we introduce a new modelling approach to study the growth of a single hemispherical nucleus: Multi-Ion Transport and Reaction Model (MITReM). This approach takes into account the transport driven by diffusion and migration of all species in the electrolyte together with the electrochemical reactions at the electrode boundary. A Finite Element Method (FEM) is used to solve the balance equations for the concentration of all the active species and the electrolyte potential. In contrast to analytical models or discrete scale modelling techniques, the strength of this approach is that no assumptions on the diffusional or kinetic limitations have to be made. In addition, this novel platform allows to add further levels of complexity, such as multiple nuclei, adatom surface diffusion, aggregation, particle detachment, etc. The simulation results prove that, the initial growth stage of a 10 nm single hemispherical silver nucleus always starts under kinetic control, regardless of concentration and electrode potential. Later on, a transition from kinetic to diffusion control takes place. The time of transition depends on the imposed concentration and electrode potential. Moreover, the simulations clearly show that the growth rate is strongly affected by the imposed concentration and electrode potential, as it has been proven experimentally in countless occasions. Numerical simulation by MITReM proves to be of great interest to gain knowledge towards unravelling the early stages of electrochemical nucleation and growth processes.

Keywords:

Hemispherical nucleus growth, kinetic control, diffusion control, Multi-ion modelling, electrochemical nucleation and growth

*Corresponding author

Email addresses: mesfin.haile.mamme@vub.ac.be (Mesfin Haile Mamme), Olga.Dolgikh@vub.ac.be (Olga Dolgikh), Johan.Deconinck@vub.ac.be (Johan Deconinck)