

Modeling and Simulation of Redox Titration of Metal Oxides at Porous Microelectrodes

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Abstract

In the past two decades, highly porous nanostructured materials have been investigated and used for a large variety of applications, such as catalysis, energy conversion/storage, optics, sensing and more. Nanoporous gold (npAu) is one of such materials which have shown great potential as an electrocatalyst due to not only its physical properties but its surface chemistry as well. It presents a controllable and defined porosity which makes it suitable for numerical modeling and analysis.

A 2D axisymmetric geometry was used to describe the system depicted in Figure 1. Digital simulations coupling voltammetry to a two micro electrodes (tip and substrate) SECM setup were accomplished using the multi-physics computer program COMSOL Multiphysics®. The tip is used to reduce the oxidized species of a mediator present in the solution which diffuses to the substrate held at open circuit potential covered by a npAu film where an electrochemically adsorbed species reacts with the mediator to regenerate the oxidized form. Mass diffusion of the mediator is heavily affected by the pore size and structure of the npAu film which can be analyzed by the current response registered at the tip.