New Algorithm for Simulation of Electrode Shape Changes in Electrochemical Reactors

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Introduction

The complex behavior of electrochemical plating processes makes the prediction of the shape evolution of the work-piece a difficult task. Different models can be used to describe the electrochemical phenomena occurring in the electrolyte and at the electrode interfaces during an electroforming process.

Most electrode shape change simulations are based on current density distributions that are obtained using the Potential Model (PM), describing ohmic drop effects in the electrolyte. Several authors applied the PM to compute the layer growth rate and compared the obtained results with experiments. Bergh and Alkire [1] applied the Finite Element Method (FEM) to solve the resulting Laplace equation, with nonlinear electrode polarization behavior. Deconinck *et al.* [2,3] discretized the equation using the boundary element method (BEM).

More recently the Multi-Ion Transport Model (MITM) has been used to simulate the electrode shape changes processes. In a given electrolyte, ion transport is computed, and the electrode growth rate (governed by the Faraday Law) becomes proportional to one or more partial ionic current densities [4-6].

Electrode shape change simulations based on current density distributions obtained with the MITM are in general more complicated than PM because they also involve changes, of electrolyte flow over time. Georgiadou *et al.* [6] studied copper deposition in a particular trench geometry. The simulation of the electrode shape evolution is fully coupled with the solution of the MITM based on the Finite Difference Method (FDM).

In all references above the authors use an Euler scheme for the integration of Faraday's law with respect to time, combined with the so called "string theory" [8]: the new electrode shape is obtained by displacing the boundary proportional to the local current density. This method is easy and not expensive in computation time. However practical situations like the overgrowing of insulators or electrodes that grow together, make the practical use of the string-theory quite complicated.

The present paper proposes a new electrode growth algorithm that is based on the Level Set Method (LSM). The basic LSM has shown its strong points as alternative to the string theory [7-8] for applications where the advancing front speed is function of the front curvature or is given by an evolution law. Now the LSM is adapted in order to compute the electrode growth changes for the MITM and will be subsequently called "Boundary Convection Method" (BCM).

MITM-BCM Model Description

The MITM describes mass transport due to convection, diffusion and migration of all ions and neutral species present in the electrolyte [4,5]. For plating applications the ionic current density distributions along the work-piece determine the electrode growth rate as described by Faraday's law.

The BCM uses this local growth rate as the vector speed $\bar{v}$ in the following convection equation:

$$\frac{\partial \Phi}{\partial t} + \bar{v} \cdot \bar{\nabla} \Phi = 0. \qquad (1)$$

Physically this equation means that the electrode boundaries are convected proportional to the local growth rate. Equation (1) is discretized through a residual distribution technique using the multidimensional upwind method [5]. The electrode growth front is found through interpolation of the solution, $\Phi(x, y, t)$, of equation (1) on the FEM mesh.

The main advantage of the BCM is that the interfaces can break up in parts or merge together.

Examples

The MITM-BCM model has been applied to simulate the electrode shape changes for different reactor configurations. As an example, the copper deposition on two parallel wires, in a laminar fluid flow is given in figure 2.

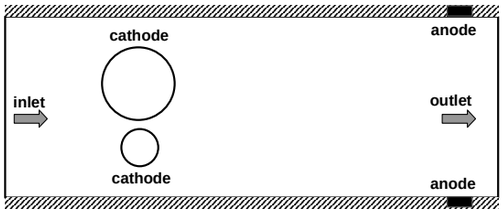

Fig. 1 The plating reactor configuration (2D cross-section)

The results demonstrate how a non-uniform shape change will manifest in time due to the combined effect of mass and charge transfer effects (figure 2).

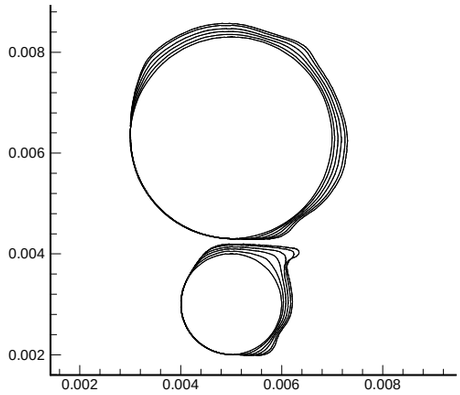

Fig.2 The growth profile for two neighboring wires

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