

An efficient, scalable numerical algorithm for the simulation of electrochemical systems on irregular domains

Matthew Buoni ^{a,*}, Linda Petzold ^b

^a *Mechanical Engineering Department, University of California, Santa Barbara, 6750 El Colegio Road, Apt. 420, Goleta, CA 93106, United States*

^b *Mechanical Engineering Department and Computer Science Department, University of California, Santa Barbara, CA 93106, United States*

Received 27 July 2006; received in revised form 12 February 2007; accepted 22 March 2007
Available online 7 April 2007

Abstract

We present a projection method for the solution of the diffusive transport and reaction equations of electrochemical systems on irregular time-dependent domains. Specific applications include electrodeposition of copper in sub-micron trenches, as well as any other electrochemical system with an arbitrarily shaped bulk region of dilute electrolyte solution. Our method uses a finite volume spatial discretization that is second-order accurate throughout, including a nonuniform region used as a transition to the far-field chemical concentrations. Time integration is performed with a splitting technique that includes a projection step to solve for the electric potential. The resulting method is first-order accurate in time, and is observed to be stable for relatively large time steps. Furthermore, the algorithm complexity scales very respectably with grid refinement and is naturally parallelizable.

© 2007 Elsevier Inc. All rights reserved.

PACS: 82.47.a

Keywords: Electrochemical systems; Irregular domain; Splitting method; Projection method

1. Introduction

1.1. Overview

The purpose of this paper is to present a novel methodology for solving the governing equations of electrochemistry under conditions of dilute electrolyte solution. Such systems, with irregular and moving boundaries, are of interest in copper electrodeposition and play an important role in the fabrication of interconnects for the next generation of computer processors [1] (see Fig. 1).

Our interest is to simulate copper infill of sub-micron scale trenches. This problem is inherently multiscale because the chemical reactions at the copper surface represent a length scale of nanometers (surface

* Corresponding author.

E-mail address: mjbuoni@gmail.com (M. Buoni).

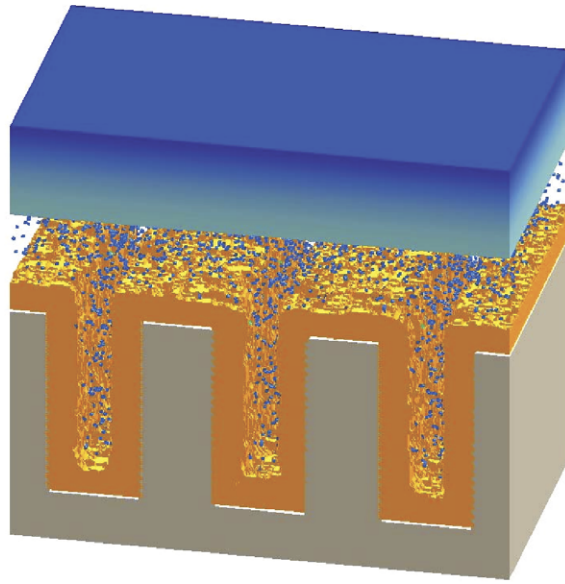


Fig. 1. Schematic of a multiscale simulation of the electrochemical process for manufacturing on-chip copper interconnects. The dots represent Cu^{2+} ions in solution, with the film on the surface being metallic copper.

roughness) and a timescale of nanoseconds to microseconds, while the diffusion and migration processes in the electrolyte solution occur at the micrometer to millimeter length scale and millisecond to seconds time scale [2]. A hybrid simulation methodology was proposed and implemented in [3] and was used to study trench infill. This approach consisted of two codes linked together: a finite difference code in the electrolyte region and a kinetic Monte-Carlo code at the copper surface. Subsequent refinements of this method have been made including the development of finite volume spatial discretization to address unphysical numerical errors (negative chemical concentrations) [6] and control systems analysis of code linkage to minimize instabilities and improve accuracy [4].

Despite the progress that has been made, these simulation methods still suffer from high computational cost. Two-dimensional simulations of modest resolution (100×100) take days to perform, scale poorly with grid refinement and are not readily parallelizable [3]. Specifically, the simulation in the electrolyte region has been a serious bottleneck. In this paper, we will present a numerical method which takes advantage of the structure of the problem to achieve a considerable gain in efficiency.

This paper is organized as follows. In Section 2, we describe the governing equations for the electrolyte region, and discuss the existing numerical approaches and their observed shortcomings. In Section 3, we derive our numerical method directly from the governing equations. This is done in two parts: first the spatial discretization is derived by integrating the governing equations over grid-sized cells; second the temporal discretization is derived by splitting the total time derivative into groups of physically related terms, and applying the Implicit Euler method to two terms and a projection method to the third term. Section 4 briefly addresses issues involved in the implementation. We assess the performance of our method in Section 5 by studying three sample problems. The order of accuracy is confirmed and a point is made about the spatial and temporal refinement required to achieve a given accuracy of the numerical solution. Also, we measure the computational complexity of our method for these three problems, and find that it scales very well as the grid is refined. We conclude the paper by summarizing our findings and highlighting areas of possible future work.

2. Governing equations

The governing equations are stiff nonlinear partial differential equations with algebraic constraints [10]. These equations describe the time evolution of the concentrations of each chemical species, c_k . They are derived by conservation of mass with chemical reactions, diffusion and migration due to electric fields,

Download English Version:

<https://daneshyari.com/en/article/522932>

Download Persian Version:

<https://daneshyari.com/article/522932>

[Daneshyari.com](https://daneshyari.com)