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Solving partial differential equations on irregular domains with moving interfaces, with applications to superconformal electrodeposition in semiconductor manufacturing ☆

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Abstract

We present a numerical algorithm for solving partial differential equations on irregular domains with moving interfaces. Instead of the typical approach of solving in a larger rectangular domain, our approach performs most calculations only in the desired domain. To do so efficiently, we have developed a one-sided multigrid method to solve the corresponding large sparse linear systems.

Our focus is on the simulation of the electrodeposition process in semiconductor manufacturing in both two and three dimensions. Our goal is to track the position of the interface between the metal and the electrolyte as the features are filled and to determine which initial configurations and physical parameters lead to superfilling.

We begin by motivating the set of equations which model the electrodeposition process. Building on existing models for superconformal electrodeposition, we develop a model which naturally arises from a conservation law form of surface additive evolution. We then introduce several numerical algorithms, including a conservative material transport level set method and our multigrid method for one-sided diffusion equations. We then analyze the accuracy of our numerical methods. Finally, we compare our result with experiment over a wide range of physical parameters.

Keywords: Semiconductor process; Level set methods; Multigrid methods; Superconformal electrodeposition; Conservative material level set methods; Immersed interface methods

1. Introduction

In this article, we will design a numerical algorithm to solve partial differential equations on irregular domains with moving interfaces. This approach is considerably faster than existing ones: most of the calculations are performed only in the desired domain instead of in an extended rectangular domain, aided

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by the use of a one-sided version of the multigrid method to solve the corresponding large sparse linear systems. Our method has been tested to give accurate numerical solutions for problems defined on domains with convoluted geometries, including thin fingers and sharp corners.

Our focus application is the simulation of the electrodeposition process. Electroplating (see [6]) is deposition process that permits filling of high-aspect ratio features without seams or voids through the process of superconformal deposition, also called superfilling. Our goal is to track the position of the interface between the metal and the electrolyte as features are filled in order to determine numerically what initial configurations lead to superfilling.

Building on existing models for superconformal electrodeposition, we develop a model which naturally arises from a conservation law form of surface additive evolution. This model allows us to perform a careful analysis of how superfilling depends on the choice of physical parameters, with close comparison to experiment.

In order to successfully compute the solution to this model, several new computational techniques are developed in this paper. These include:

1. A new conservative material transport level set method in two and three dimensions for interfaces that carry scalar fields as they evolve.
2. An immersed interface type method for building one-sided difference operators for complex interfaces with thin arms and fingers.
3. A multigrid method in two and three dimensions for solving one-sided diffusion equations with irregular moving interface.

The outline of this paper is as follows. Section 2 briefly describes some existing work on electrodeposition, and then describes a general overview of some related numerical methods. Section 3 describes the underlying physics of the electrodeposition process and also the determination of some of the parameters used in our model. The basic equations that need to be solved for modeling the deposition process are derived based on previously existing models. However modifications are made so that the model is physically more reasonable.

Section 4 presents the finite difference methods for level set equations, conservation laws, and diffusion equations. In this section, most of the discretizations are done in two space dimensions. We discuss in Section 5 how to solve large linear systems in an efficient way and details of the one-sided multigrid method. The last section is devoted to numerical results, conclusions, extension to the three-dimensional case, and suggestions for future work using the methods described in this article.

2. Background material

2.1. Target application: electrodeposition

Electrodeposited copper can be used as the material for on-chip trenches and vias. The process of copper electrodeposition (see Fig. 1) depends on the use of additives that affect the local deposition rate and this leads to superconformal filling of trenches.

Fig. 1. An image of copper deposited from electrolyte. Voids are apparent in the trenches. The picture is taken from [29].