Simulation of Copper Electroplating in Damascene Feature

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Shape evolution was studied numerically during electrodeposition of copper in microtrenches. Two numerical methods incorporating adaptive meshing capabilities were developed. The models, based on finite element and finite difference, handle transport by diffusion, migration, convection, fluid flow and homogeneous reactions. The shape change behavior of this system was investigated, resulting from variation of the feature's aspect ratio, bulk composition and level of additive components. Filling without creating a void or a seam was related to process parameters, enabling to generate safe maps. The tool is incorporated in a collaborative Web-based modeling environment providing a friendly interface for linking models at a variety of scales.

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Introduction

Copper electroplating inside microtrenches and vias currently represents the preferred process technology for on-chip interconnection fabrication. The capability of electroplating copper preferentially in the bottom of the feature leading to void and seam-free deposits is a critical factor in evaluating the chemistry of the plating solution. Additive compounds to the plating bath may impart remarkable shape control and deposit properties. In previous works[1,2] numerical simulations were presented for moving boundary problems in electrochemical systems.

A mathematical model is presented for the general transport balance in electrochemical systems subjected in an appropriate set of initial and boundary conditions. A modified Butler-Volmer equation that takes into account the additive effect is used to describe the kinetic behavior of the system, based on the assumption that additive compounds are consumed on the wafer surface and suppress the kinetics. The model is applied to copper electrodeposition in single trenches and combinations of them.

Mathematical Model

The continuum model of the electrochemical system consists of coupling the associate species balances with electroneutrality. The transport equation includes diffusion, migration and convection. Appropriate initial and boundary conditions complete the mathematical model; the active part of the domain consists of a cathodic surface where current is represented by a Butler-Volmer expression, which is modified to account for the influence of the solution additives. Furthermore, the solid boundary is moved along the local normal to the surface by using a material balance at the solid-liquid interface undergoing electrodeposition. In terms of mathematical formulation[3]:

$$\frac{\partial C_i}{\partial t} = -\vec{\nabla}\cdot(D_i \vec{\nabla} C_i) - z_i F \vec{\nabla}\cdot(\upsilon_i C_i \vec{\nabla}\Phi) + \vec{\nabla}(\vec{V}\cdot C_i) + R_i \qquad (1)$$

$$\sum_i z_i C_i = 0 \qquad (2)$$

Figure 1 illustrates boundary conditions imposed on the top and side bulk boundaries, as well as on the active surfaces (thick lines) for the reacting copper ion, the additive and the non-reacting species.

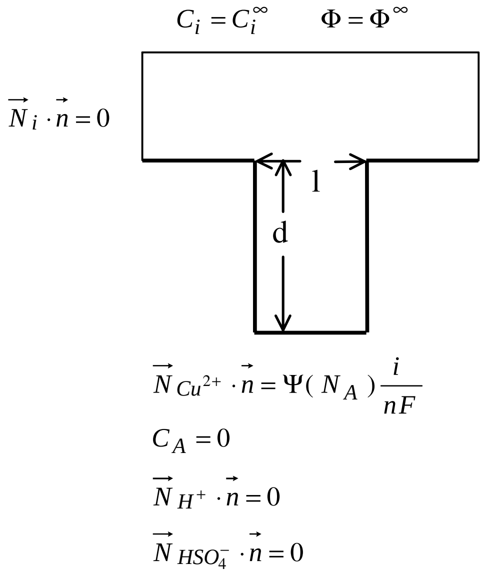


Figure 1 - Schematic drawing of geometry cross-section and boundary conditions

The current is given by :

$$i = \left(\frac{C_{cu^{2+}}}{C^{\infty}_{Cu^{2+}}}\right)^{\gamma} . \left(i_{o_a}\, e^{\left(\frac{\alpha_a n F}{RT}(U_M - \Phi_o - E^{\infty})\right)} - i_{o_c}\, e^{\left(-\frac{\alpha_c n F}{RT}(U_M - \Phi_o - E^{\infty})\right)}\right) \qquad (3)$$

and electroneutrality condition completes the equation set.

Two numerical methods were used for the simulation needs: ERMES, a high-end research code based on finite difference for general curvilinear coordinates was developed for approximating the continuum equation involving diffusion, migration, convection and reaction terms in arbitrary, complex geometries of multi-component systems including moving boundaries. In addition, a finite element method based on the standard Galerkine discretization scheme for the continuum model that accommodated migration contribution, both in the bulk fluid as well as on the cathodic surface, complex geometry and adaptive meshing was developed. In both methods, shape evolution is simulated using the adaptive meshing capability of the codes. At each time step, the solid boundary was moved along the local normal to the surface undergoing electrodeposition a distance corresponding to the volume of metal deposited according to the local current density, resulted from the computation of the boundary Cu^{2+} flux at this time step. Moving boundary simulations assume a mass transport quasi-steady state, i.e. concentration transients relax much faster than the moving of the electrode boundary.

Results and Discussion

In the following, results are presented for variations of the aspect ratio of 0.25µm trenches, of the electrolyte composition and of the additive content. These results are associated with the nature of the additive and the plating bath chosen in this study.

Aspect Ratio

Figure 2 shows shape evolution at sequential times for trench aspect ratios of 0.5 (a), 1 (b), 2 (c) and 4 (d,e) in a 0.25 M $CuSO_4$ + 0.1 M H_2SO_4 plating solution containing 10^{-4} M of additive.

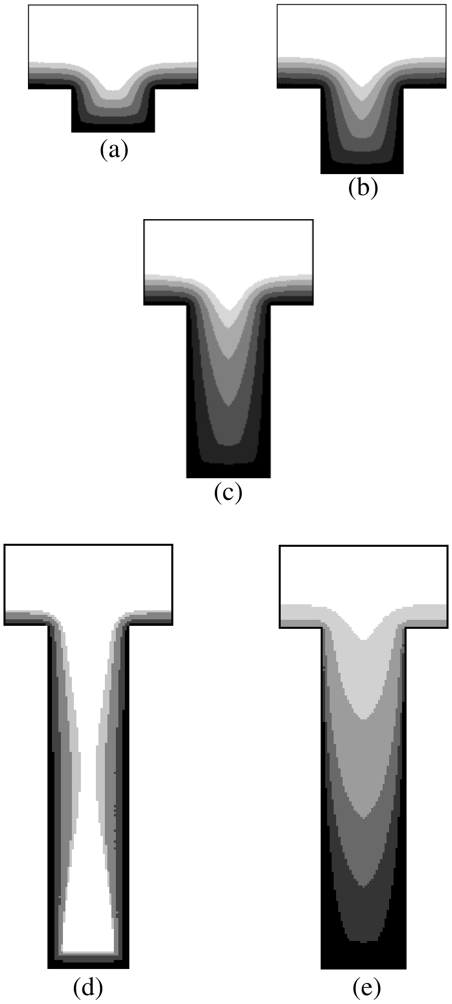

(a)
(b)
(c)
(d)
(e)

Figure 2 - Shape evolution in 0.25 µm trenches

It can be seen that void-free plating resulted for aspect ratios up to 2 at these additive and bulk conditions (Fig. 2a - 2c), whereas plating in a ratio of 4 trench would lead to void formation (Fig. 2d). This behavior is attributed to the fact that as the trench depth increases, the lower realms are less accessible by the additive, which in turn exert less suppression on the copper electrodeposition kinetics leading to void formation. However, by choosing an alternative additive, void-free plating can be obtained for the aspect ratio of 4, as it can be seen in Fig. 2e. Figure 3 illustrates this result by displaying the initial deposition rate of copper along the plated surfaces for aspect ratio 4 and different baths; the rate is noticeably less uniform under void-free conditions (Fig. 2e).

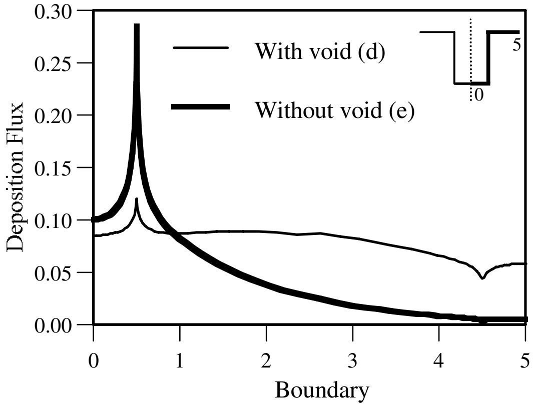
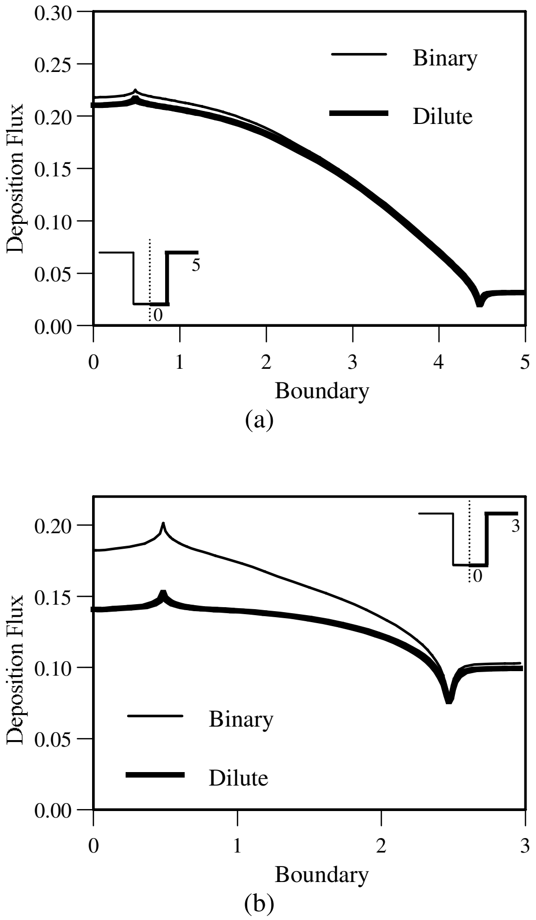


Figure 3 - Deposition rate of copper at initial time for aspect ratio 4 and different baths

Electrolyte Composition

It was found that shape evolution in solutions with copper concentration of 0.25 M $CuSO_4$ and supporting electrolyte contents ranging from 0.005 M to 5 M H_2SO_4 results in void-free plating. Depending on the geometry size, migration in solutions with less electrolyte content may be more important and thus transport of cupric ions to the plating surfaces may be larger compared to solutions with excessive electrolyte. Figure 4 illustrates the migration effect for different geometry sizes, by displaying the initial deposition rate of the cupric ion along the plated surfaces of the trench at 0.005 M H_2SO_4 (binary solution) and 5M H_2SO_4 (dilute solution). As shown, the deposition rate is higher in the binary solution due to the migration effect of the positively charged cupric ion for trenches with width of 2.5 µm (Fig. 4b), while there is no substantial migration contribution for the 0.25 µm case (Fig. 4a).



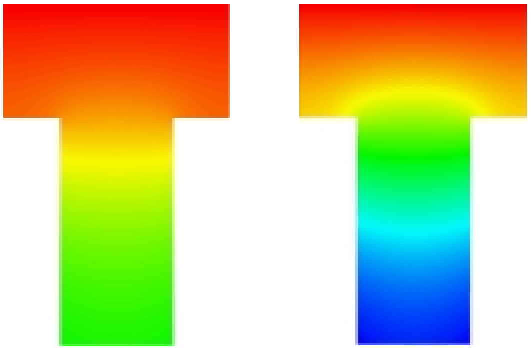
(a)

(b)

Figure 4 - Deposition rate of copper at initial time for dilute and binary bath

(a) aspect ratio 4, 0.25 μm trench width

(b) aspect ratio 2, 2.50 μm trench width



(a) (b)

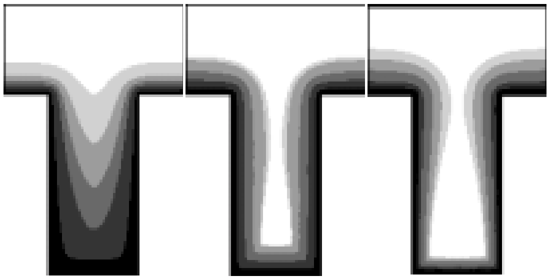
Figure 5 - Concentration contours of copper at initial time for aspect ratio 2, 2.5μm trench width

(a) binary **(b) dilute**

The distribution of copper concentration inside a trench is illustrated for the binary and the dilute solution in Fig. 5. As shown, the copper concentration is higher in the bottom of the trench for the binary solution (Fig. 5a) compared to the dilute solution (Fig. 5b), since copper is more attracted to the plated surfaces due to the migration effect in solutions with limited electrolyte content. This result applies for trenches with 2.5 μm width.

Additive content

Figure 6 shows shape evolution for aspect ratio of 2 at additive concentrations of 10^{-4}, $0.5x10^{-4}$ and $0.25x10^{-4}$ M. It is seen that plating proceeds with void formation at $0.5x10^{-4}$ M and $0.25x10^{-4}$ M cases (Fig. 6b - 6c), whereas it results at void-free plating at 10^{-4} M additive concentration (Fig. 6a). This is attributed to the suppressive activity that the additives exert on the kinetics of electrodeposition; as the content of additives in the plating solution increases, the suppression is stronger and the copper is deposited with a preferential direction to the more remote to the additives interior surfaces.



(a) (b) (c)

Figure 6 - Shape evolution in 0.25 μm trenches

(a) 100% of nominal additive content

(b) 50% of nominal additive content

(c) 25% of nominal additive content

Array of trenches

Copper plating occurs in features that are combinations of trenches with various sizes and aspect ratios. Figure 7 shows simulated shape evolution for copper electrodeposition in a geometry combining two trenches with substantially different opening widths and aspect ratios 4 and 0.5. The width of the trench is governing the filling time since plating occurs from the sides as well; the depth of the feature is responsible for void formation depending also on the rest process parameters.

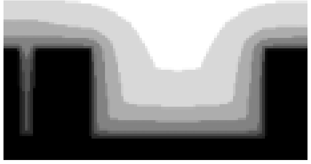


Figure 7 - Shape evolution in an array of trenches

Conclusions

In this work shape evolution during electrodeposition of copper in single trench and multi-trench geometries was studied. A numerical model that predicts shape evolution in electrochemical systems was demonstrated. The model handles diffusion, migration, convection, nonlinear boundary conditions, and complex geometries. Void-free plating was numerically obtained for 0.25 M $CuSO_4$ with 10^{-4} M additive content and 0.5 to 4 aspect ratios. In addition, migration was found to assist the deposition rate at relatively high opening widths of the trenches and small electrolyte contents in the plating bath.

The present study emphasized in the ability to perform complicated simulations in electrochemical systems. The tool is directly applicable in the copper plating process for manufacturing of interconnections. Its built-in features permit the future investigation of the influence of fluid flow, and of more complex reaction mechanisms.

References

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