Simulation of Copper Nanostructure Formation by Coupling Kinetic Monte Carlo Simulation, Continuum Models, and the Level Set Method

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A multiscale simulation model has been developed that couples multiple instances of a kinetic Monte Carlo (KMC) simulation code to a moving boundary (MB) level-set continuum simulation code to simulate the filling of on-chip features (trenches) by electrodeposition in the presence of additives. Both the KMC and MB simulations code run dynamically. The KMC code uses surface concentrations calculated by the MB code to compute reaction rates and it simulates the chemistry and physics that occur at the electrode surface. The MB code uses fluxes computed by the KMC code as a surface boundary condition. The MB code simulates the chemistry and physics in the electrolyte in the trench with continuum methods and advances the copper-solution interface with a level-set approach.

The formulation of the KMC simulation model developed here allows users to test additive mechanisms to determine whether their mechanisms correctly predict trench filling behavior. A four-additive electrodeposition bath was used in the studies performed here. The bath consisted of a suppressor (chloride (Cl) and polyethylene glycol (PEG)), an accelerator (bis(3-sulfopropyl)disulfide (SPS)), and a leveler (HIT). Many studies have been performed on the individual components of the bath, especially Cl, PEG, and SPS, as well as on baths consisting of all three of these additives. Some experimental[1,2,3] and simulation[4,5] studies have been performed to understand trench filling behavior with Cl, PEG, SPS, and a leveler. The simulation approach presented here lays the groundwork to make it possible to determine which additive mechanisms presented in the literature most likely explain experimentally observed trench filling phenomena.

There are a growing number of examples of linked simulation codes in the recent literature. Linkage of simulation codes that apply to different length scales is desirable since improvements can then be made in a component code at one scale without affecting the codes at other scales. A linked Monte Carlo and continuum transport/reaction models of boundary layer phenomena was used in a multiscale integration hybrid algorithm to simulate a unimolecular surface reaction.[6] A multiscale metal film growth simulation was created by incorporating molecular dynamic data into a level-set model of the growing film.[7] A molecular dynamics code was coupled to a Monte Carlo code to improve feature-scale simulations of copper ionized PVD in a trench; the molecular dynamics code provided copper ion sticking probabilities to the Monte Carlo code that were a function of the position in the trench, and the Monte Carlo code simulated the trench filling.[8] Linked codes were also used to simulate Metal-Oxide-Semiconductor Field Effect Transistors; a Monte Carlo code calculated an equilibrium density on the device and passed that information to a finite element continuum code that computed a potential field distribution that was passed back to the Monte Carlo code.[9] The code sequence was run until the electron density and the potential field converged. Finally, multiscale low pressure CVD behavior was simulated by linking a reactor scale code, a feature scale code, and a mesoscale code that mediated the linkage between the other codes.[10] The

reactor scale passed concentration, temperature, and pressure information to the mesoscale code, which resolved the information to a finer mesh and passed the information to the feature scale code. The feature scale code returned flux information via the mesoscale code to the reactor scale code. For computational efficiency, the reactor scale code ran multiple iterations before calling the other codes for updated information, a strategy which does not affect the accuracy of the simulations provided that the smaller scale codes are called before too much change has taken place in the reactor scale code.

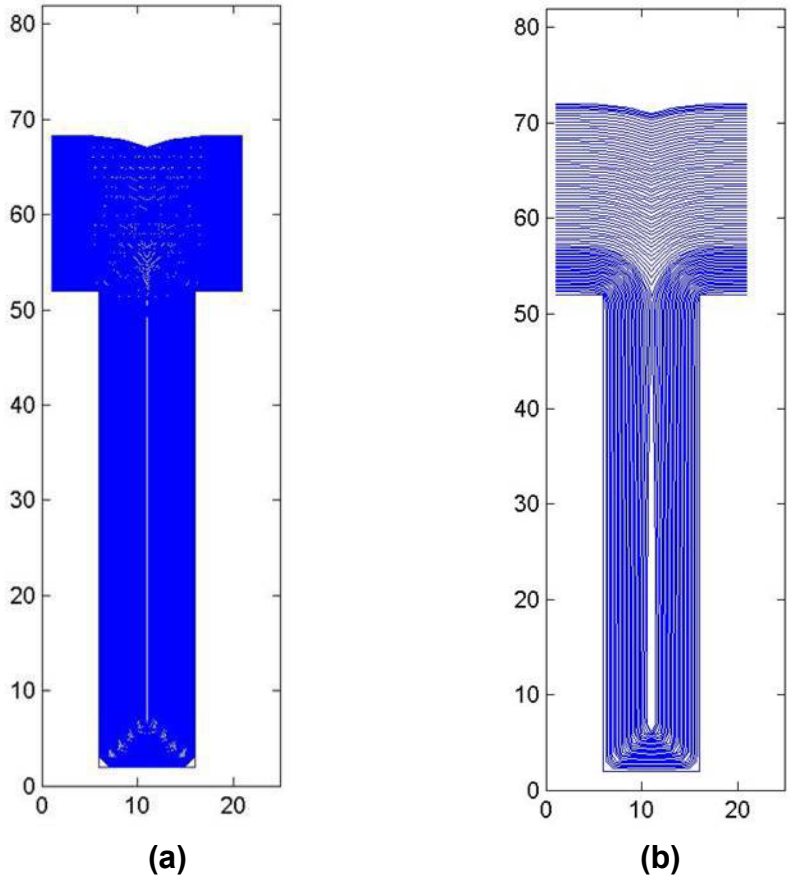

Figure 1. Simulations of additive-free copper electrodeposition into a 0.15 μm trench with 5:1 aspect ratio at an applied overpotential of (a) -0.12 V and (b) -0.25 V. The simulation in (a) required 100 s to fill the trench and the simulation in (b) required 15.4 s to fill the trench.

In the present work, the MB simulation code was linked to multiple instances of the KMC simulation code along the trench to perform multiscale, coupled simulations. The coupled simulation follows a “master-worker” computational paradigm; the MB code is the master code and the KMC codes are the workers. The KMC code simulates the evolution of surface shape and morphology at selected locations on the trench. The locations where the codes were coupled were optimally chosen so as to reduce the interaction between successive KMC simulations, while still providing a sufficient number of points to establish macroscopic

properties profile on the surface. This macroscopic profile serves as the bottom boundary condition for the MB code in the next iteration. Because the number of KMC simulations is less than the number of nodes at the interface in the MB code, the MB code uses a linear piecewise function to interpolate the flux values passed from the KMC simulations on its nodes. Similarly, the MB code uses the same interpolation routine to determine the concentration and solution potential values passed to the KMC codes. Since the trench is approximately symmetric about the vertical axis, only one half of the trench was simulated. Both the MB and KMC simulations treat the passed information as a piecewise constant signal.

A MPI-based management system was developed to manage the information passing between the coupled codes. A KMC terminating mechanism is used in the coupled simulation to terminate individual KMC simulations during feature filling. The KMC simulations terminate at different times according to the manner in which the trench is filling. The termination mechanism ensures that 2 KMC simulations do not simulate growth in the same part of the trench. When the KMC domains meet one another, the termination mechanism shuts one of the KMC simulations off and allows the other to continue its simulation.

It is expected that at low applied overpotentials, in the absence of additives, the void in the trench should be smaller than at high applied overpotentials. At low applied overpotentials, the flux of copper at all points in the trench is relatively constant, where at high applied overpotentials, the flux of copper at the top of the trench can be significantly larger than at the bottom of the trench. In Figure 1, simulations of additive-free copper electrodeposition into a 5:1 aspect ratio, 0.15 μm trench have been performed. The simulations were performed at a low and a high value of the applied overpotential to determine whether the model correctly reproduces the expected results. In Figure 1a, where deposition has been performed at a low applied overpotential, the void is much smaller than in Figure 1b, where deposition has been performed at a high applied overpotential.

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References

[1] J. J. Kelly and A. C. West, *Electrochem. and Solid State Lett.*, **2**, 561 (1999).

[2] J. J. Kelly, C. Tian, and A. C. West, *J. Electrochem. Soc.*, **146**, 2540 (1999).

[3] P. Taephaisitphongse, Y. Cao, and A. C. West, *J. Electrochem. Soc.,* **148**, C492 (2001).

[4] A.C. West, S. Mayer, and J. Reid, *Electrochem. and Solid State Lett.*, **4**, C50 (2001).

[5] Y. Cao, P. Taephaisitphongse, R. Chalupa, and A. C. West, *J. Electrochem. Soc.*, **148**, C466 (2001).

[6] D. G. Vlachos, *AIChE J.*, **43**, 3031 (1997).

[7] U. Hansen, S. Rodgers, and K. F. Jensen, *Phys. Rev. B*, **62**, 2869 (2000).

[8] D. G. Coronell, D. E. Hansen, A. F. Voter, C. Liu, X. Liu, and J. D. Kress, *Appl. Phys. Lett*., **73**, 3860 (2000).

[9] D. Hadji, Y. Marechal, and J. Zimmerman, *IEEE Trans. on Magnetics*, **35**, 1809 (1999).

[10] M. K. Gobbert, T. P. Merchant, L. J. Borucki, and T. S. Cale, *J. Electrochem. Soc.*, **144**, 3945 (1997).