MONTE CARLO SIMULATIONS OF THE ELECTRODEPOSITION OF COPPER

T. J. Pricer[*], M. J. Kushner[**], R. C. Alkire[*]
[*]Dept. of Chemical Engineering and
Frederick Seitz Materials Research Laboratory
University of Illinois, Urbana, IL 61801

[**]Dept. of Electrical & Computer Engineering
University of Illinois, Urbana, IL 61801

Deposition of submicron features by electrodeposition, used for microelectronics interconnects[1], requires trace amounts of organic additives to obtain desired deposit characteristics. A Monte Carlo simulation has been developed to model the growth of Copper electrodeposits with additives and without additives.

The overall model is a collection of three modules, (a) a Monte Carlo model of nano scale surface growth, (b) a continuum model of the macro scale bulk solution and (c) an overall electrochemical control module for the linked Monte Carlo and continuum model. These modules are incorporated into a web base interface.

The Monte Carlo module of the simulation is a 3-D kinetic model of the electrochemical growth of a surface region in which the simulation space is a cubic lattice that represents the substrate, deposit and solution near the surface. Various mechanisms are modeled including diffusion in the bulk solution, adsorption, desorption, surface diffusion, dissolution and incorporation. Additives can also be introduced into the simulation which can also adsorb, desorb, diffuse and be incorporated into the deposit. The variable, initial substrate geometry can contain trenches and vias.

The continuum model is linked to the Monte Carlo model to provide information about the bulk solution at the macro scale. The continuum model module can be anything from a simple 1-D finite difference model of diffusion or a more complex model of diffusion, migration and fluid flow. Figure 1 compares the concentration profile from a linked Monte Carlo and finite difference simulation and with the theoretical concentration profile found form the diffusion equation.

The model results are validated using three methods. The first method compares qualitatively AFM images of electrodeposited copper with Monte Carlo simulation results. Figure 2 shows a simulated surface that agrees well with Figure 3 of an AFM image of electrodepositied copper. The second validation method uses Scaling Analysis of the Interface Width[2,3]. Experimental scaling results are obtained from AFM images of copper surfaces and are compared to scaling results found from the Monte Carlo simulations. The final validation technique is the comparison of electrochemical responses of the model and experiments.

Acknowledgments:
This work was supported by the U.S. Department of Energy, Division of Materials Science grant DEFG02-96ER45439 through the University of Illinois at Urbana-Champaign, Frederick Seitz Materials Research Laboratory.

References:

1. P. C. Andricacos, C. Uzoh, J. O. Dukovic, J. Horkans, and H. Deligianni, *IBM Journal of Research and Development*, **42**, 567-573 (1998).

2. W. U. Schmidt, R. C. Alkire, A. A. Gewirth, *Journal of the Electrochemistry Society*, **143**, 3122-3132 (1996).

3. W. M. Tong, R. S. Williams, *Annual Review of Physical Chemistry*, **45**, 401-438 (1994).

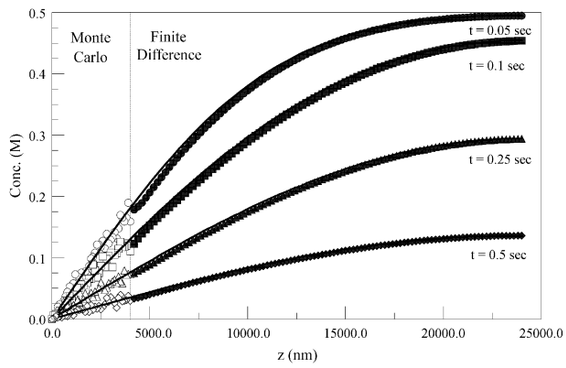

Figure 1: Concentration profile across linked models. Monte Carlo model from 0 to 4000 nm and a 1-D Finite Difference model from 4000 nm to 24000 nm. Consumption of all material at z = 0 and no flux condition at z = 24000 nm. Open symbols are concentrations from the Monte Carlo model, solid symbols are concentrations from the Finite Difference model. The line is the solution to the diffusion equation using Fourier Series.

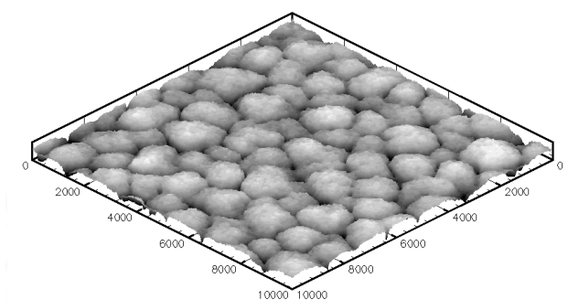

Figure 2: Image of 10 μm × 10 μm area simulated by using the Monte Carlo model.

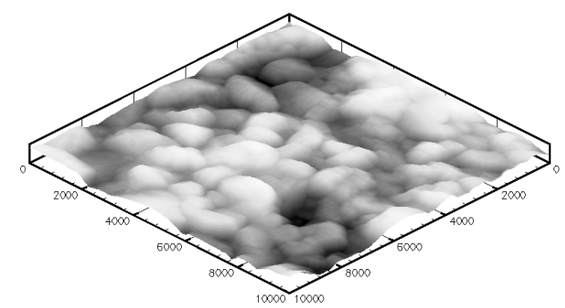

Figure 3: 10 μm × 10 μm AFM image of Cu deposited at 2 mA/cm^2 for 2000 seconds from a 0.05 M $CuSO_4$ + 0.5 M H_2SO_4 solution.