Feature Length-Scale Modeling of LPCVD and PECVD MEMS Fabrication Processes

Lawrence C. Musson†, Pauline Ho‡, Steven J. Plimpton† and Rodney C. Schmidt†

† Sandia National Laboratories, P.O. Box 5800, Albuquerque, NM 87185-0316
lcmusso@sandia.gov, sjplimp@sandia.gov, rcschmi@sandia.gov

‡ Reaction Design, 6440 Lusk Blvd., Suite D209, San Diego, CA 92121
pho@reactiondesign.com

ABSTRACT

The surface micromachining processes used to manufacture MEMS devices and integrated circuits transpire at such small length scales and are sufficiently complex that a theoretical analysis of them is particularly inviting. Under development at Sandia National Laboratories (SNL) is Chemically Induced Surface Evolution with Level Sets (ChISELS), a level-set based feature-scale modeler of such processes. The theoretical models used, a description of the software and some example results are presented here. The focus to date has been of low-pressure and plasma enhanced chemical vapor deposition (LPCVD & PECVD) processes. Both are employed in SNL's SUMMiT V technology though as of this writing the PECVD process model includes only unbiased wafers. Examples of step coverage of SiO_2 into a trench by each of the LPCVD and PECVD process are presented.
Keywords: MEMS, CVD, LPCVD, PECVD, level-set method, feature scale.

1 SOME CHALLENGES IN MEMS SMM TECHNOLOGY

In the surface micromachining (SMM) approach to the fabrication of MEMS devices three-dimensional (3D) structures are formed by deposition and etching of thin films. Careful construction of the lithographic masks that control these steps and the application of a final selective "release" etch permits the creation of a variety of free-standing movable parts. SMM fabrication can involve a wide variety of chemical processes in the deposition and etching steps. For example, deposition processes in the SUMMiT V [1] technology developed by Sandia National Labs include low-pressure chemical vapor deposition (LPCVD) of undoped polysilicon, P-doped polysilicon, silicon dioxide from TEOS [$Si(C_2H_5O)_4$], and Si-rich silicon nitride from $SiCl_2H_2$ and NH_3, as well as steam oxidation for the initial SiO_2 layer and the plasma deposition (PECVD) of SiO_2 from SiH_4 and O_2. Etching processes include a plasma etch of oxide and nitride using C_2F_6 and CHF_3, of polysilicon using Cl_2, He, and/or HBr, and a wet etch using aqueous HF.

Many of the above mentioned deposition and etching processes can result in non-ideal device geometries at the feature scale. For example, CVD processes give near-conformal films, which yield rounded corners and dimples. Step coverage can range from perfectly conformal to non-conformal, and lower step coverage can result in sloped sidewalls. Under some conditions non-uniformities and irregularities in surface coverage occur. The unexpected appearance of any of these types of geometric irregularities can be particularly costly in the design, analysis, and batch fabrication cycle associated with the development of a new MEMS device. Thus a thorough understanding of the detailed chemistry and physics which lead to these geometric variations is essential to the development of improved SMM fabrication equipment, higher yield and more reliable fabrication processes, and more useful MEMS designs.

2 THEORETICAL MODELING AT THE FEATURE SCALE WITH ChISELS

Theoretical modeling of the detailed surface chemistry and concomitant surface evolutions during microsystems fabrication processes is recognized as having a great potential for improving SMM process fabrication technologies. The viability of computational simulations for these types of problems has been clearly demonstrated by earlier researchers and advances have been made in developing transport models, chemical mechanisms, and surface evolution modeling (*e.g.*, see [2] [3] [4]). However, currently available computer codes have not been designed to use massively parallel architectures efficiently, nor fully exploit all of the modeling advances that different researchers have made. Thus speed and robustness factors have unduly limited the size and complexity of problems that can be treated with available tools.

To overcome these limitations, we are developing a computer code called ChISELS (Chemically Induced Surface Evolution with Level-Sets), a parallel, 2D and fully 3D feature-scale modeler to explore the time development of material deposition/etch on patterned wafers at low pressures. ChISELS can be viewed as a platform to build and improve on previous simulation tools

while taking advantage of the most recent advances in dynamic mesh refinement, load balancing, and highly scalable solution algorithms.

There are three inter-related aspects to modeling the overall physics of the problem: (1) transport of chemical species, (2) gas phase and surface chemistry, and (3) the dynamic evolution of the solid surface.

Currently, all gas-phase transport is assumed to occur in the free-molecular flow regime (i.e., particle-particle collisions are negligible). In ChISELS, we adopt the ballistic transport and reaction model (BTRM) developed and described by Cale and coworkers [2] [5]. An important aspect of this method is the need to calculate view-factors for each surface element of the discretized feature surface. Chaparral [6], a radiation heat transfer modeler, is used for this purpose. The flux of species k to surface element i is computed from

$$F_{ik} = F_{ik}^0 + G_{ij} \left(F_{jk} - R_{jk} \right) \quad (1)$$

where F_{ik}^0 is the direct flux from the bulk of the reactor, G_{ij} is the view factor between surface i and j, F_{jk} is the flux of species k to surface j, R_{jk} is the reaction rate of species k on surface j, and by Einstein's convention repeated indices in the product imply summation.

Deposition or etching occurs through the chemical reaction of gas phase species with bulk and surface phase species at the feature surface. The thermodynamics and heterogeneous surface chemistry of these reactions are modeled in ChISELS by coupling with Surface Chemkin [7]. This requires the specification of a chemical reaction mechanism for each surface reaction to be modeled in the simulation.

Feature scale microsystem fabrication modelers such as ChISELS are at heart topology modelers, *i.e.* they model the evolution of a free boundary according to the physics that cause it to move. ChISELS uses an implicit surface-tracking approach called the level set method [4]. In the level-set method, a domain-spanning function, ϕ is defined; the zero-value contour, or level set, of which conforms to the feature surface. The level-set function is evolved by solving the scalar partial-differential equation,

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0 \quad (2)$$

over the volume and integrating through time. The velocity, $\mathbf{v}$ is called the extension velocity and is defined over the entire domain. The extension velocity must be chosen so that the level set of ϕ evolves in such a way that it mimics the evolution of the feature surface; *i.e.* it is chosen based on the velocity of the surface—the deposition or etch rate. The level set method avoids the debilitations of explicit conform-and-track methods because the mesh which is used to solve Equation 2 does not deform, so distortion effects are avoided. Likewise, because a volume-defined function is evolved, merging surfaces do not create problems in the method. Equation 2 is solved by an augmented method of characteristics [8].

Additional details of the methods and models that ChISELS uses can be found in [9] or on the ChISELS web site, http://www.cs.sandia.gov/~wchisels.

3 EXAMPLES

Two two-dimensional examples are provided here of ChISELS results. One is of the deposition of SiO_2 into a 10x1 trench using silane by a PECVD process. The other is the deposition of SiO_2 into an identical trench using TEOS. In each case, the deposition rate as a function of depth in the trench is presented.

3.1 PECVD of SiO_2 from SiH_4

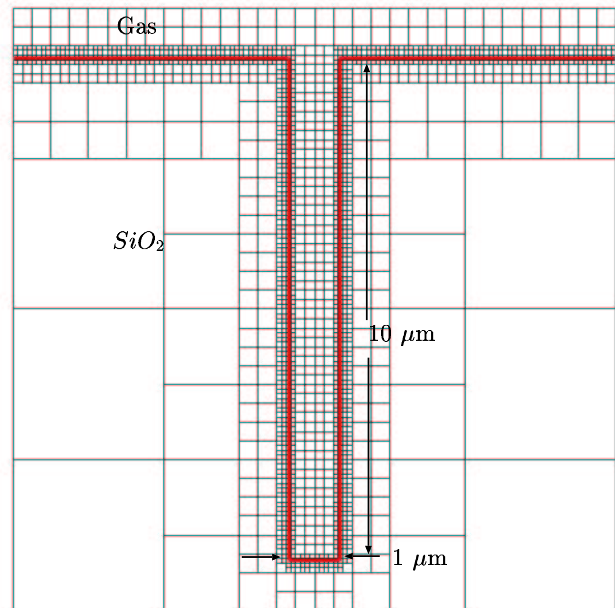

Figure 1: The trench used in the examples is 1 μm wide and 10 μm deep.

The deposition of silicon dioxide into a trench of aspect ratio 10:1 (*cf.* Figure 1) from a mixture of SiH_4, O_2, Ar and derivative compounds in a high-density plasma reactor is modeled by ChISELS. The grid used to model the process is also shown in Figure 1. In this case, there is no biasing of the substrate, so, as a first approximation, ions and electrons approach it in a diffuse way just as the neutrals do.

The chemistry mechanism used in this model is a subset of the one published by Meeks *et al.* [11]. All the reactions in their mechanism are used except for the ion sputtering reactions. This leads to a system with

46 gas-phase species, 13 surface-phase species and 185 surface reactions.

The gas composition in the reactor immediately above the wafer surface is a required input to ChISELS. Because that composition is unlikely to be identical to that introduced into the reactor, a reactor-scale model must be employed to provide the mole fractions of the introduced reactants and their products near the wafer. In this case, Aurora, a a zero-D reactor-scale modeler and Reaction Design product, part of the Chemkin suite, was used to determine those compositions.

The inlet conditions provided to Aurora are a temperature of 300K, and mole fractions of 0.0097, 0.0223 and 0.9680 respectively of SiH_4, O_2 and Ar at a total flow rate of 0.0028 g/s. The output of Aurora is the mole fractions of all reactants and products at the wafer as well as surface, ion and electron temperatures. All of these are inputs to ChISELS.

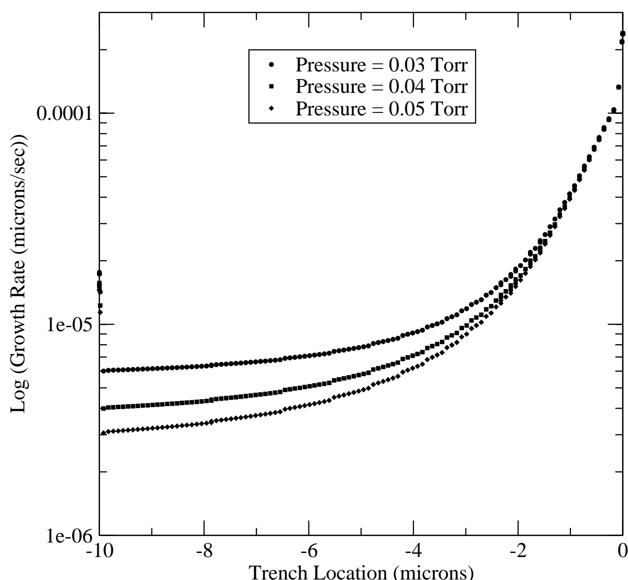

Figure 2: Growth rates as a function of depth of SiO_2 in a PECVD process using SiH_4 and O_2.

Figure 2 shows the deposition rate in the trench as a function of its depth for the indicated pressures of 0.03, 0.04 and 0.05 Torr. As shown in the figure and perhaps contrary to intuition, the lowest pressure of 0.03 Torr actually produced the highest growth rate of all pressures tried. This is due to the difference in the gas-phase composition at the reactor due to a change of reactor pressure. This underscores the importance of coupling ChISELS to a reactor-scale model.

As Figure 2 shows, the deposition rate, and thus step coverage, in this process is not uniform. The deposition rate in the bottom corner of the trench is about two orders of magnitude smaller than that at the top. The source of this non-uniformity is most likely due to the plasma forming highly reactive radicals that get depleted almost entirely near the top of the trench and are hardly present near the bottom. Note also that there are some higher growth rates on the ordinate of Figure 2. These points correspond to surface elements near the center of the bottom plane of the trench. These higher growth rates are owed to greater visibility of the reactor and its constituents above.

3.2 LPCVD of SiO_2 from TEOS

The second example is the deposition of SiO_2 into a trench from TEOS. The trench geometry and grid are identical to the first example. There are two chemistry mechanisms used in this example. The first is a mechanism published by Coltrin *et al.* [12], and the second by IslamRaja *et al.* [13]. Once again, Aurora is used to compute gas-phase composition. The mechanism used in Aurora is Coltrin's. The IslamRaja mechanism is defined only for heterogeneous reactions. The input conditions are a reactor temperature of 1003K—the temperature at which the IslamRaja mechanism was tuned and the only temperature for which it is truly valid—pressures of 0.3, 0.4 and 0.5 Torr and an inlet flow rate of 0.046 g/s of TEOS and N_2 with mole fractions of 0.13 and 0.87 respectively.

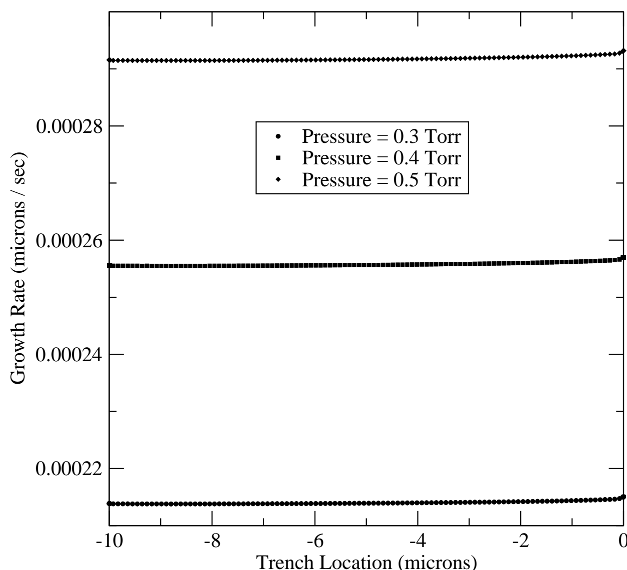

Figure 3: Growth rate as a function of depth of SiO_2 in a LPCVD process using TEOS—Coltrin's chemistry.

Figures 3 and 4 show the deposition rate of SiO_2 as a function of the depth in the trench. Unlike the previous example, the deposition rate as predicted by both mechanisms increases with the reactor pressure. The difference between the two TEOS mechanisms is the mag-

nitude and uniformity of the deposition rate. Coltrin's mechanism predicts a lower overall rate and one which is exceptionally uniform. The IslamRaja mechanism produces a very non-uniform deposition rate varying two orders of magnitude from the bottom of the trench to the top.

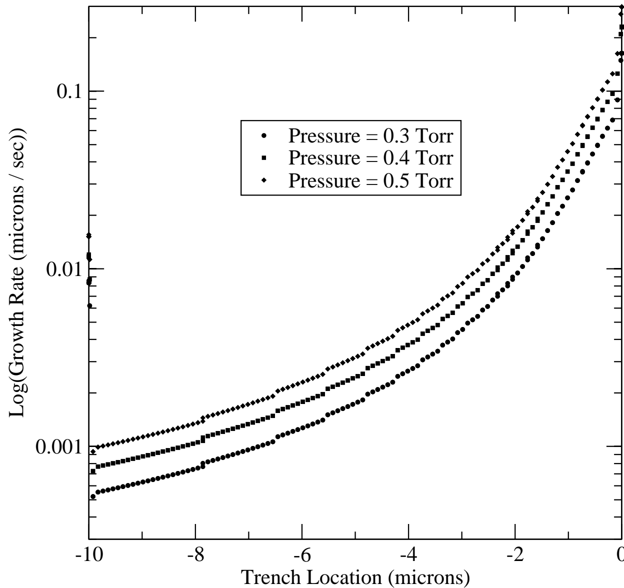

Figure 4: Growth rate as a function of depth of SiO_2 in a LPCVD process using TEOS—IslamRaja's chemistry.

Experiments have shown the deposition of SiO_2 indeed to be non-uniform. So Coltrin's mechanism clearly does not work at the feature scale though it has been shown to work on the reactor scale. The IslamRaja mechanism is not even defined on the reactor scale, so there is no way to couple ChISELS to a reactor-scale model with that mechanism in use. The next step is to refine Coltrin's mechanism so that it remains working on the reactor scale and also produces realistic growth rates at the feature scale.

SUMMARY

A cursory description of the ChISELS feature length-scale modeler has been given. Two examples were discussed of the deposition of SiO_2 by LPCVD through TEOS and by PECVD through silane and oxygen in plasma. Step coverages for each process and how they are affected by reactor operating conditions were shown. More details of the ChISELS software can be found in [9] and [10].

4 ACKNOWLEDGEMENTS

The authors would like to thank Sandia National Laboratories and the Department of Energy for supporting this work. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

REFERENCES

[1] M. S. Rodgers, J. J. Sniegowski, "Designing Microelectromechanical Systems-on-a-Chip in a 5-Level Surface Micromachine Technology," 2nd Int. Conf. Eng. Design and Automation, 1998.

[2] T. S. Cale, T. P. Merchant, L. J. Borucki and A. H. Labun, Thin Solid Films, 356, 152-175, 2000.

[3] A. H. Labun, H. K. Moffat and T. S. Cale, J. Vac. Sci. Technol. B., 18, 267-278.

[4] J. A. Sethian, "Level Set Methods", Cambridge Univ. Press, Cambridge, 1996.

[5] T. S. Cale and V. Mahadev, in Thin Films: Modeling of Film Deposition for Microelectronic Applications, Vol. 22, Ed. S. Rossnagel, Academic Press, 176-277, 1996.

[6] M. W. Glass,"CHAPARRAL: A library for solving enclosure radiation heat transfer problems", Sandia National Laboratories, Albuquerque, NM, 2001.

[7] SURFACE CHEMKIN: A Software Package for the Analysis of Heterogeneous Chemical Kinetics at a Solid-Surface – Gas-Phase Interface Interface, Reaction Design Inc. 2001 (See also: CHEMKIN@ReactionDesign.com).

[8] J. Strain, J. Comput. Phys., 161, 512–528, 2000.

[9] Musson, Lawrence C., Plimpton, Steven J., and Schmidt, Rodney C. MEMS Fabrication Modeling with ChISELS: A Massively Parallel 3D Level-Set Based Feature Scale modeler, Technical Proceedings of the 2003 Nanotechnology Conference and Trade Show, Volume 3 Nanotech 2003 Grand Hyatt San Francisco, San Francisco, CA, U.S.A.February 23-27, 2003

[10] http://www.cs.sandia.gov/~wchisels

[11] Ellen Meeks, Richard Larson, Pauline Ho, Christopher Apblett, Sang M. Han, Erik Edelberg and Eray S. Aydil, J. Vac. Sci. Technol. A, 16(20), 544–563, 1998.

[12] Michael E. Coltrin, Pauline Ho, Harry K. Moffat and Richard J. Buss, Thin Solid Films, 365, 251–263, 2000.

[13] M. M. IslamRaja, C. Chang, J. P. McVittie, M. A. Cappelli and S. C. Saraswat, J. Vac. Technol. B 11(3), 720–726, 1993.