Linking Three-Dimensional Topography Simulation with High Pressure CVD Reaction Kinetics

W. Pyka, P. Fleischmann, B. Haindl, and S. Selberherr

Institute for Microelectronics, TU Vienna
Gusshausstrasse 27–29, A-1040 Vienna, Austria

Abstract

We present a three-dimensional model for the simulation of continuum transport and reaction determined high pressure CVD processes. Our approach allows simulations over arbitrary geometries such as structures resulting from non-uniform underlying PVD films. This enables the examination of film profile variations across the wafer for multi-step processes consisting of low and high pressure parts such as Ti/TiN/W plug-fills. Additionally the model allows a very flexible formulation of the involved chemistry and can easily be extended to arbitrary CVD processes including gas phase reactions of precursors as observed in the deposition of silicon dioxide from tetraethylorthosilicate (TEOS).

1. Introduction

A variety of three-dimensional topography simulators provides facet motion, cellular, level-set or Monte-Carlo algorithms in combination with macroscopic models for the simulation of low pressure deposition processes determined by ballistic transport. However, for increasing process pressure leading to diffusion determined mass transfer, up to now only two-dimensional simulations are available [1].

To close the gap of missing high pressure models in three-dimensional topography simulation we have extended the two-dimensional continuum transport and reaction model and present a fully three-dimensional model for the simulation of arbitrary chemistry, multiple species high pressure chemical vapor deposition (CVD) processes. Together with the low pressure models for our simulator presented in [2] all tools for an integrated three-dimensional back-end process simulation including across wafer non uniformities of ballistic transport and diffusion determined processes are now available.

2. CVD-Model

As shown in Fig. 1 the model consists of a combination of specialized tools which are called automatically from a controlling instance. After extracting the surface of the initial geometry, a three-dimensional mesh of the gas domain above the considered structure is generated. The differential equations describing the mass transfer and the reaction kinetics are set up and evaluated with a general object-oriented solver which operates on the previously generated unstructured mesh. The resulting deposition rates are transfered to the topography simulator which works on a cellular material representation. The surface propagation for each time step is deduced by applying

structuring elements to the actual surface [3]. The size of the structuring elements correspond to the deposition rates calculated with the continuum transport model. The topography simulator also controls the time step, which is especially important, when features close and voids are formed. To avoid the underestimation of the size of such a void by choosing a too large time step, the topography simulator reduces the time step in such a case until the first closure of the void is observed. Again the surface of the resulting geometry is extracted and the procedure is repeated for each time step until the control instance observes the completion of the overall simulation time. Fig. 2 shows the information transfered between the single modules for CVD into a circular shaped via.

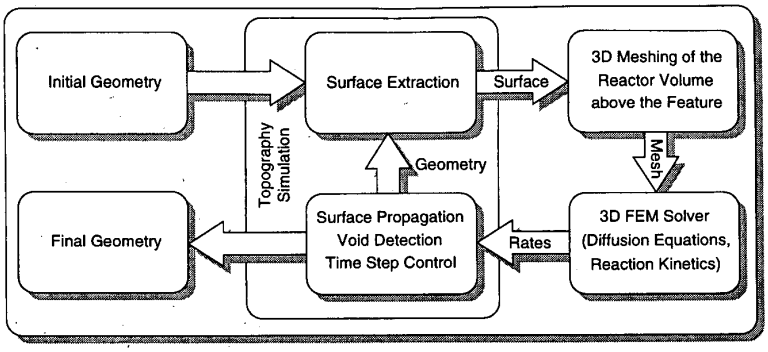

Figure 1: Flow diagram for the high pressure CVD model

The parameters for the meshing tool and the description of the rate model are set up in control files and remain unchanged during all time steps. In this way the process runs fully automatic without any further user interaction.

Several aspects have to be considered for the single modules: The topography simulation is based on a cellular material representation. Therefore, the surface has to be extracted in a triangular format suitable as input for the meshing tool. For the tetrahedralization the dimensions of the gas space above the feature have to be specified and additional points within the volume are inserted. The meshing tool uses a modified advancing front algorithm to generate a three-dimensional unstructured tetrahedral mesh [4].

The chemistry model is set up with AMIGOS [5] which provides an analytic interface for discretizing and solving differential equations. The governing principles for the CVD model are surface reactions $-D_i \frac{\partial c_i}{\partial n} = R$ and diffusion of gas species in the plasma $\frac{\partial c_i}{\partial t} = \nabla(D_i \nabla c_i)$. For the CVD model we only calculate the time independent steady state with $\frac{\partial c_i}{\partial t} = 0$. Transient calculations have revealed that the steady state is reached after a few μs and that the steady state assumption for each single time step is correct.

3. Applications and Results

As shown in Fig. 3 this model is applied to the simulation of tungsten CVD used for a Ti/TiN/W plug-fill process [6]. The chemistry model used for the high pressure CVD process assumes that W is reduced from WF_6 using H_2 and forming HF as by-product. The three gas species diffuse in the feature and the reduction takes place at the feature surface. The assumed process conditions cause a depletion of WF_6 in the feature and a characteristic overhang in the layer profile. The simulated structure is

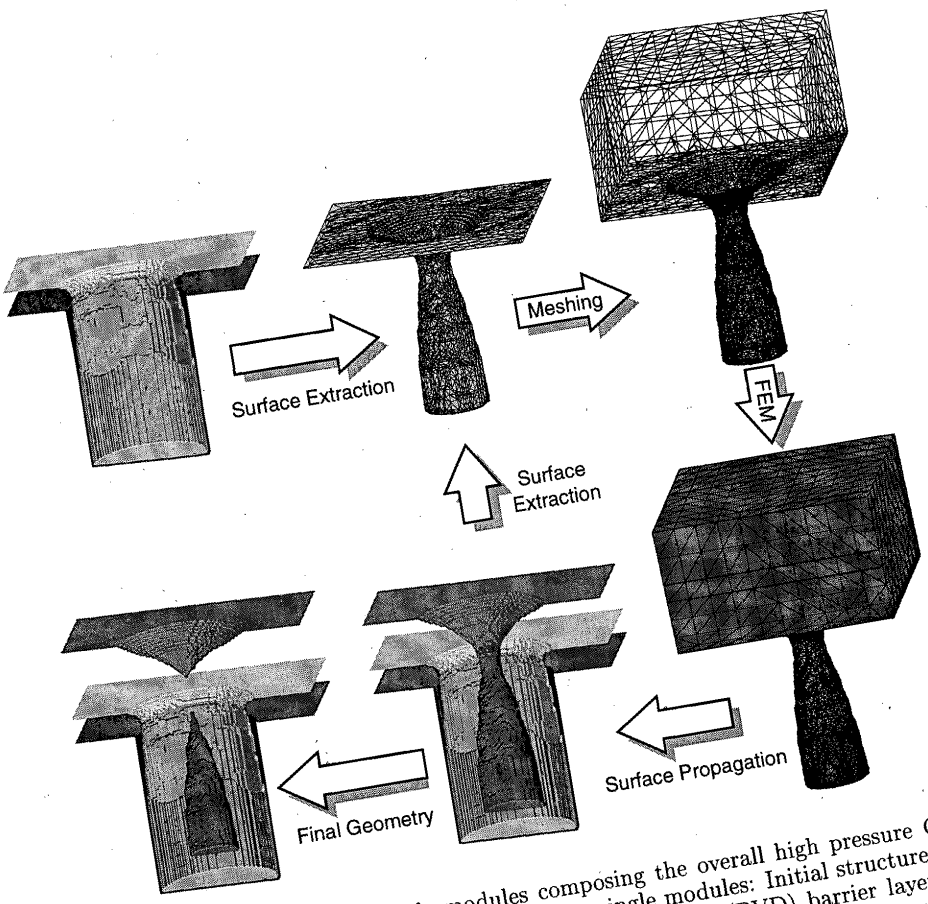

Figure 2: Results of the single modules composing the overall high pressure CVD model and information transfered between the single modules: Initial structure consisting of a circular via with a physical vapor deposition (PVD) barrier layer, extracted surface at an intermediate time step, three-dimensional mesh, final geometry, propagated surface, and distribution of the reduced gas species resulting from the continuum transport and reaction simulation.

located at an off center position of the wafer. Thus the TiN layer, formed by sputter deposition prior to the tungsten CVD is strongly asymmetric requiring the rigorous three-dimensional simulation of the CVD film formation.

The required CPU time for this example, simulated with a DEC 600/333 workstation is approximately 10 min for each time step of the automatically controlled simulation sequence, including surface extraction, meshing, calculation of the deposition rates, time step control, void detection and surface propagation. Depending on the size of the structure between 10.000 and 30.000 tetrahedra were used for the continuum transport model.

4. Acknowledgments

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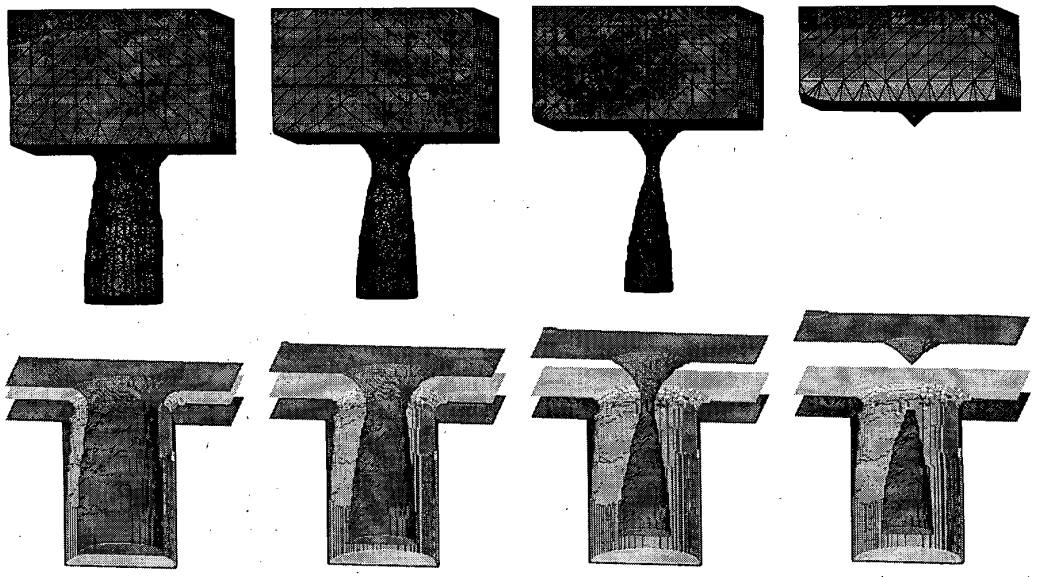

Figure 3: The volume meshes used for the continuum transport model and the corresponding three-dimensional film profiles for a sequence of time steps of a Ti/TiN/W plug-fill process. The profiles in the lower row show from bottom to top the initial circular via, the TiN PVD layer formed by sputter deposition and the growing W CVD layer.

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