Fast Model for Deposition in Trenches using Geometric Advection

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***Abstract*—We have developed and implemented a model for deposition in a trench, applicable to highly reactive chemistries with high sticking probabilities (∼1). The presented model calculates the final deposited thickness for all relevant points inside the trench by finding the view-factor dependent surface rates and integrating those over the entire simulation time. The model also takes into account the shrinking view-factor due to deposition at the top of the trench. Subsequently, the calculated thicknesses along the trench are used to generate the final physical structure by geometric advection in a Level Set framework. We show that our model, combined with the geometric advection framework, can accurately generate the expected physical shape of the deposited film at simulation times 100 times faster than alternatives with iterative schemes. The method was compared to models using top-down ray tracing with Engquist-Osher and Lax-Friedrichs iterative advection schemes.**

I. Introduction

The ability to simulate semiconductor device fabrication using process technology computers aided design (TCAD) has become essential in the device design cycle. Process TCAD simulators are commonly equipped with many physics-based and empirical models which are able to describe the evolution of surfaces during deposition or etching. More recently, however, there has been an increased interest in process emulation as an alternative to full-fledged process simulators [1]. Emulation allows for a very fast structure generation since it does not rely on the time discretized advection of the surface, minimizing computational effort and enabling the process-aware generation of large surfaces and many devices simultaneously. The most well known commercial tool which applies emulation in their structure generation is Coventor SEMulator3D [2].

The currently available process emulation tools rely on the discretization of the simulation domain using voxels, while most process simulators are based on the Level Set (LS) framework and most device simulators rely on tetrahedral meshes. While conversion from a LS to a tetrahedral mesh is quite straight forwardly achieved using fast marching methods [3], [4], converting voxels to device simulation-ready tetrahedral meshes is challenging and can result in errors [5]. Therefore, the use of voxels for geometric advection limits the ease of integration of the generated geometries with physics-based models in process simulators and subsequent complex device simulations. Recently, we have developed a process simulation and emulation framework, ViennaLS, which is built on LS-based spatial discretization [6]. The framework allows for the direct integration of geometric advection models with full-fledged physical models without the need for conversion or re-meshing.

II. View-Factor based Deposition Model

In this manuscript, we present a physical model for the deposition of a species with a high sticking coefficient (∼1) in a trench, which is simulated using the ViennaLS geometric advection framework, thereby allowing for very fast and very accurate simulations. The high sticking coefficient means that the only determinant to the growth rate at any surface point s is the view-factor, or the portion of the source seen from s and the angles between the view-factor and the respective surface normal directions. Although the sticking coefficient of most commonly used chemical vapor deposition (CVD) processes are not that high, there is nevertheless often a need to model the result of this process during low pressure chemical vapor deposition (LPCVD)

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with multiple precursors. One such example is the deposition of SiO_2 from tetraethylorthosilicate (TEOS), where one of the two involved precursors was shown to have a very high sticking coefficient [7], [8]. Another example is silicon LPCVD from SiH_4 which dissociates into SiH_2: A highly reactive molecule with the wafer surface, depositing with a calculated sticking coefficient of 1 [9].

The assumption made in feature scale process modeling is that the plane immediately above the surface acts as a source of the molecules, ions, and atoms which contribute to the deposition rate. For a typical trench geometry, we set up the model system as shown in Fig. 1. The rate at a surface point dr/dt at time t is given by the rate at the top of the wafer R_{top} multiplied by the view-factor F which depends on the angle under which the source plane is visible from the surface (from θ_{start} to θ_{end}). The view-factor F is defined as

$$F = \frac{1}{2}\int_{\theta_{start}}^{\theta_{end}} \cos\theta d\theta, \tag{1}$$

which then gives the rate at a surface point as

$$\frac{dr}{dt} = R_{top} \cdot F, \tag{2}$$

where R_{top} is a constant value which depends on the flux of the depositing species. Therefore, to find the final thickness r at the surface, we integrate Eq. (2) in time

$$r = R_{top}\int_0^t F dt. \tag{3}$$

It is important to note that the angles θ_{start} and θ_{end} both depend on the lateral thickness at the top of the trench R which is time dependent and deposits at a rate of dR/dt, which depends on its own view-factor to the source θ_R. This interdependence results in the integral in Eq. (3) not having an explicit solution, meaning it must be solved numerically. Therefore, for every time step, we first find the rate at the top of the trench, which impacts the visibility angles inside the trench. These new visibility angles are then used to calculate the rates inside the trench. Finally, all rates are used to obtain the growth distance at the top and inside the trench for the current time step. This procedure is repeated for all time steps until the simulation is completed and the final thickness for all points inside the trench is found.

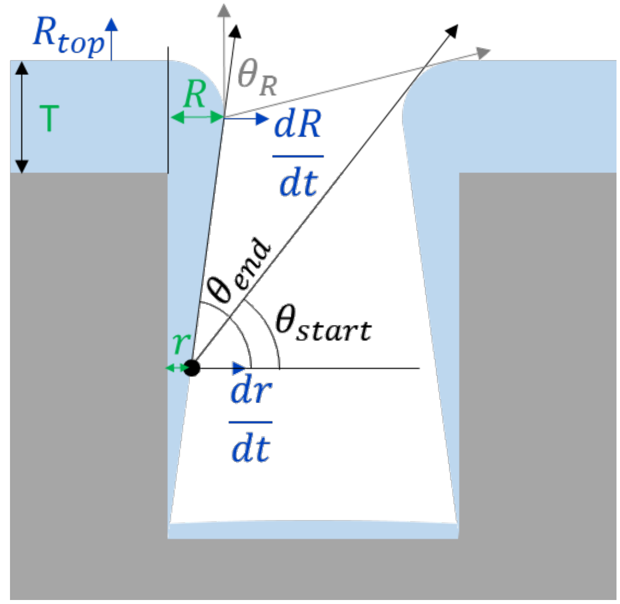

Fig. 1. Schematic of a typical trench geometry during view-factor based growth. To find the thickness in the trench r we integrate dr/dt over time t. However, this rate is impacted by the trench closing rate dR/dt and the visibility angles θ_{start} and θ_{end}. These angles depend on how much the trench has already closed at time t, given by R, so to obtain the closing rate, we also must integrate its growth rate over time.

The calculated thicknesses are geometrically treated as circles (or ellipses) which are then applied inside the geometric advection framework to calculate the LS values, represented as signed distances, which describe the advected surface. For the interested reader, the implementation of the geometric advection method in the ViennaLS framework [6] is described in more detail in [10].

III. Simulation Results and Discussion

A sample geometric advection, which applies the model described above, was performed on a trench with diameter 20 nm and depth 50 nm, shown in Fig. 2. The red surface is the initial trench and the blue surface is the final deposited film. The top rate R_{top} and simulation time t were set to 1 nm/s and 10 s, respectively. The calculated thicknesses are shown in Fig. 2 using circles or ellipses associated with each LS point inside the trench. Each circle (or ellipse) represents one of the geometric advection distributions used to determine the exact location of the new surface.

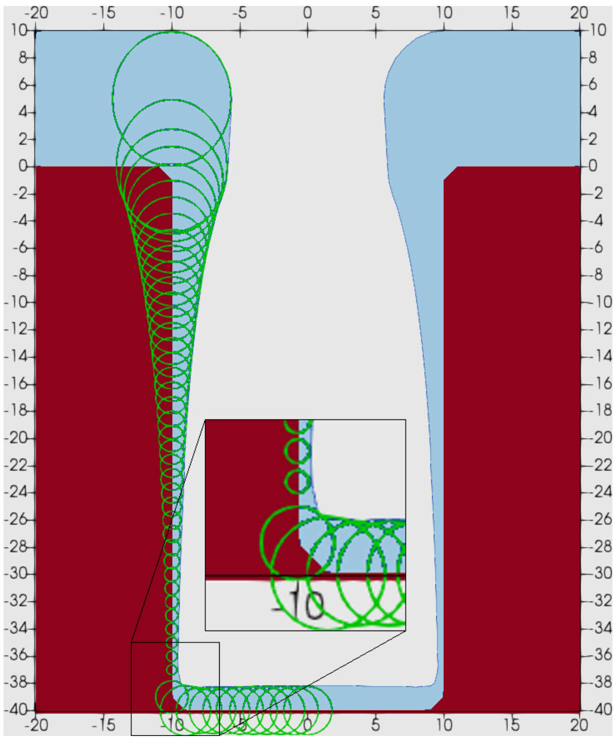

Fig. 2. Result of a simulation of view-factor based deposition using geometric advection. The initial trench is shown in red, the deposited film in blue. Green circles show the geometric advection distributions which are based on the calculated deposition rates and are used to find the new LS values.

The result of the geometric advection simulation was compared to physical simulations which use time discretization and top-down ray tracing Monte Carlo to calculate the deposition rates at each time step, followed by LS advection at each time step. This is the typical way physical simulations of such processes are carried out [11]–[13]. In Fig 3 we compare the result of our geometric advection, presented here, with physical simulations using different schemes: 1st (lighter) and 2nd (darker) order Engquist-Osher (EO) [14] (grey) and Lax-Friedrichs (LF) [15] (black) schemes. We note that qualitatively our results reproduce the physical simulations down the trench, with the exception of the trench top (circled in Fig 3).

At the top, it is likely that the ray tracing simulation is not accurate. Due to the limited resolution of the simulation domain, the top corners of the trench are represented by abrupt changes in the normal. This is not a concern for our implementation of the geometric advection since we do not perform time-stepping on the LS itself, meaning this initial abrupt change in the normal can be ignored in the final generated structure and does not affect how the simulation progresses.

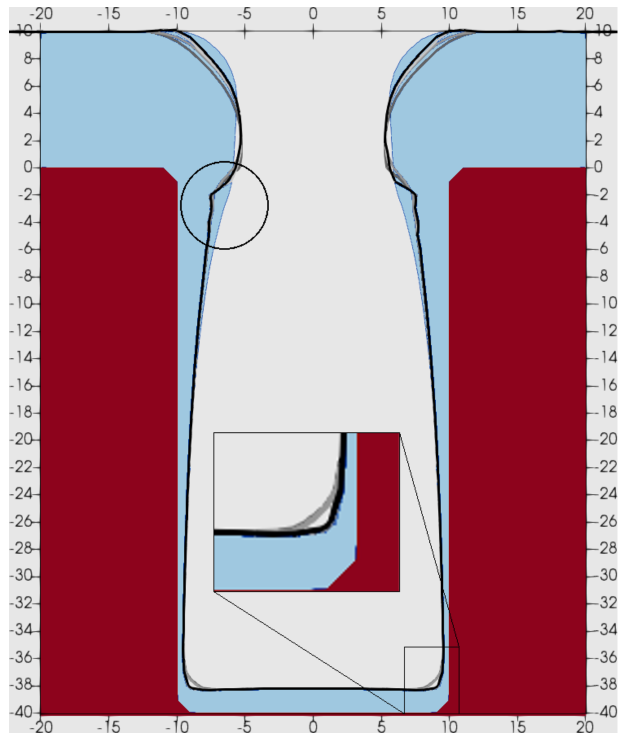

Fig. 3. Comparison of the geometrically advected film (blue) with physical models using 1st (lighter) and 2nd (darker) order EO (grey) and LF (black) iterative advection schemes. Geometric advection can reproduce the bottom trench corners better than physical models based on EO schemes.

From Fig. 3 we also note that, for an accurate representation of the bottom trench corners, we need to involve a more complex iterative advection scheme, such as the LF scheme, since EO results in too much averaging. The EO scheme is known to introduce non-physical geometries, such as flattened corners during deposition [16]. LF schemes produce more accurate results, but are restricted to certain types of velocity functions or LS data structures [17], meaning that the scheme may produce good results for one application, while introducing large numerical discrepancies in others [18]. This also means that the user has to have some previous knowledge about the process itself and the modeling approaches before choosing the correct iterative advection scheme. This is all once again not a concern for our geometric approach, which matches very well with the more complex iterative advection scheme.

TABLE I
SIMULATION TIMES TO GENERATE THE RESULTS SHOWN IN FIG. 3, INCLUDING PARALLEL PERFORMANCE. GEOMETRIC ADVECTION, WHICH IS THE MODEL PRESENTED HERE, WAS MORE THAN 100 TIMES FASTER.

Advection scheme	**Simulation time (s)**		
	1 core	**2 cores**	**4 cores**
Engquist-Osher 1st order	2.95	1.71	1.04
Engquist-Osher 2nd order	3.08	1.76	1.06
Lax-Friedrichs 1st order	3.15	1.85	1.07
Lax-Friedrichs 2nd order	3.24	1.85	1.13
Geometric advection	**0.028**	**0.018**	**0.009**

Finally, we compare the simulation times of our geometric approach with the different iterative advection schemes, with a summary given in Table I. We note that the presented method is more than 100 times faster on both serial and parallel systems. All simulations were carried out on a personal computer with a 4-core Intel i7-10700 CPU with 128 GBs system memory. For the solution of the numerical integration in Eq. (3), forward Euler was applied with time steps of 10^{-4} s. This time step was also used to produce the results in Fig. 3, which shows sufficient accuracy. The number of rays used in the physical simulations can greatly impact the simulation times. In our simulations, 1000 rays per active grid point were generated from the source plane towards the wafer surface. A lower number of rays would result in faster performance at a cost of an increased artificial (non-physical) surface roughness.

IV. CONCLUSION

We present a model for deposition in trenches for highly reactive processes where the sticking coefficient is very high ($\sim$1), meaning that the deposition rate, and thereby final thickness distribution in the trench, is entirely determined by the view-factor from the surface to the source of depositing particles. The model calculates the process-induced thicknesses in the trench and then generates the final surface using geometric advection schemes. The method resulted in a speedup of over 100 times when compared to iterative advection schemes.

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