The Application of Level Set Method for Simulation of PECVD/LPCVD Processes

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Abstract

In this study we present a Chemical Vapor Deposition (CVD) process simulator based on the sparse field method for solving the level set equations. An accurate and efficient tool for tracking the CVD profile evolution is developed, which includes different physical effects of direct deposition and angle dependent ion-induced deposition as well as re-deposition. The simulation results shows that the deposition profiles agree well with the experiment for different opening sizes and various micro structures. It also provides the evidence that this approach is able to describe the complex topographical evolution for PECVD/LPCVD processes.

***Index Terms*— CVD, Level Set.**

I. INTRODUCTION

With the reducing size and increasing complexity of semiconductor chips, the fundamental understanding of the processes occurring at the micron level is the need of the hour. Thin film deposition which is used for device interconnect features is one of the major aspect in the development of semiconductor devices. During the deposition process, conformal step coverage is one of the major requirements, however the deposition at the step is not uniform. Thus the study of deposition techniques is of interest to many researchers. This makes simulation studies of utmost importance as it helps to predict the accurate profile after deposition.

Based on the experimental results, mathematical models are developed which when employed yields results accurately fitting with the experimental results. In this paper simulations for different geometries are generated which are in good approximation with the experimental results. The Level Set method has been used for the simulations owing to its advantages over other methods.

II. PHYSICAL MODEL

The actual reactions taking place at the sub-micron level are very complex, the understanding of which is still not clear. From the experimental results, it has been found out that mainly three phenomenon governs the CVD processes namely Direct Deposition, Re-deposition and Surface Diffusion [1,2]. Also PECVD or Plasma Enhanced CVD processes has high energy ions formed as a result of collisions with the plasma along with the neutral particles while in LPCVD or Low Pressure CVD only neutral particles governs the chemical reactions.

Previous results however have proved that the effect of surface diffusion is not that important and hence is not considered in simulation [1], however the importance of re-deposition have been explained by deposition experiments of overhanging structures. Deposition experiment on an overhang structure shows deposition under the overhang also which are not even visible from the source.

This has been previously explained with the phenomenon of re-deposition where all the complex process occurring has been lumped in the form of Sticking Coefficient (SC), the value of which decides the extent of re-deposition. A value of SC =1 employs no re-deposition and all the particles hitting the surface is assumed to have deposited there, whereas for SC<1 it is assumed that the incoming particles undergoes re-deposition number of times before it finally deposits.

III. SIMULATION MODEL

In this paper we have investigated the simulation of CVD processes where we have considered that the complex process of re-deposition as well as surface diffusion can further be lumped into one parameter that result in an isotropic deposition. In every iteration an isotropic term is added which is itself a weak function of distance from the source. The ion particle is assigned SC=1 as they have high energy and as a result they are assumed to react and deposit as soon as they hit the surface, whereas the neutral particles have a low sticking coefficient thus it is assumed to have undergone many re-emissions before it finally deposits. The phenomenon of re-deposition as modelled previously however requires a lot of computational time and memory. In this study we have assumed that the neutral particles (SC<1) has an equal probability to deposit everywhere in the vicinity even if there is zero visibility angle owing to the re-emissions it undergoes before depositing. This can be very well modeled with the isotropic factor both for PECVD and LPCVD. This not only saves a lot of computation time for modeling re-deposition compared with the previously reported methods but also generates results in good agreement with the experimental data.

This isotropic term of flux is added to the flux calculated for direct deposition or ion-induced deposition (IID). The angular deposition function used for IID is

$$f(\emptyset) = \cos^{10} \emptyset * \sin \emptyset \qquad -(1)$$

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$$Flux = flux_{ion} * \int_{\emptyset_1}^{\emptyset_2} f(\emptyset) \quad -(2)$$

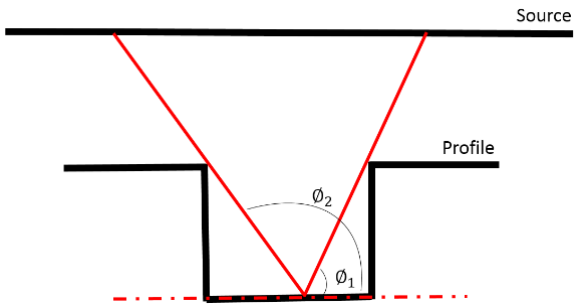

Figure 1 – The model used for simulation

Where Ø is the visibility angle as shown in Figure 1 [6] and equation 2 gives the flux of ion on the surface of the profile.

IV. LEVEL SET METHOD

The Level Set method [7,9] has been used for the evolution of the profile, where the idea is to extract the zero-level set contour after every iteration leading to the advancement of the front as shown in Figure 2 below.

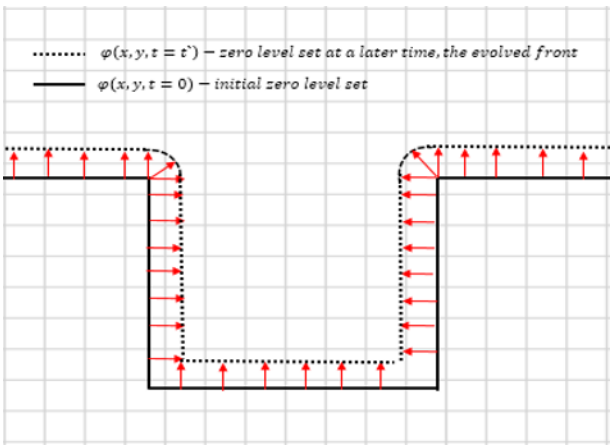

Figure 2 -Schematic of the profile evolution in Level Set

The evolution of the level set is governed by the Level Set equation given by

$$\varphi_t(x, y, t) = vel * |\nabla\varphi| \quad -(3)$$

Where phi is the level set function whose evolution is tracked and vel is the velocity of each point on the front. The Level Set method has many advantages including its ability to handle topological changes naturally [9].

The computation domain is reduced to three rows of cells, one below, one above and the one where the zero level set lies, taking the narrow band method to the extreme (Sparse Field Method [3]) as shown in Figure 3.

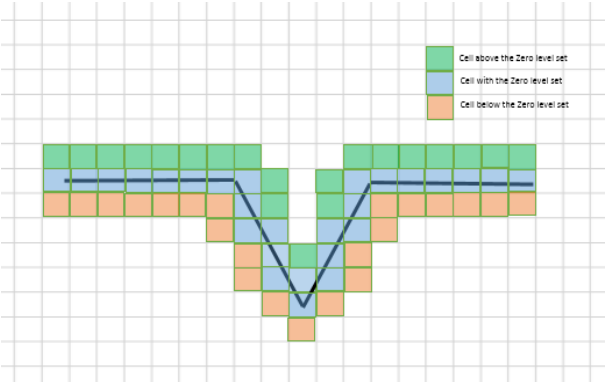

Figure 3-Schematic of the computational domain being restricted to three grid cells. The orange color cells lie below the cells (blue color) containing the level set function, while green colored cells lie above the level set function.

V. THE ALGORITHM

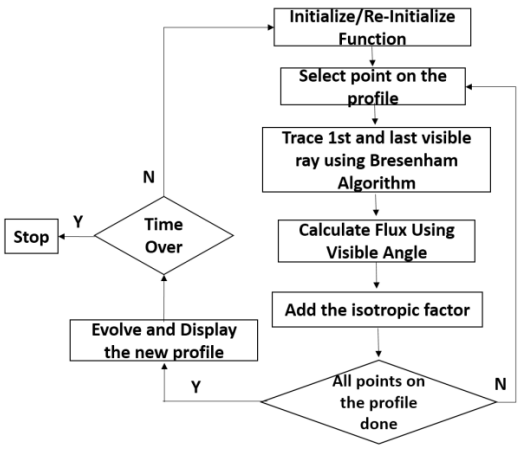

Figure 4-The flow chart of the algorithm

The flow chart of the algorithm is shown in Fig. 4. The Level Set function is re-initialized after a fixed number of iterations, this re-initialization helps the function to be well behaved even after several evolutions [8]. The Bresenham Algorithm is used for tracing the first and last visible ray, where the idea is to find the sign of the Level Set function at every coordinate on the ray joining the point on the profile and the source. The first and the last ray having the same sign (positive) at all the coordinates on the ray under consideration will be the required rays. Using the first and the last traced ray, the visibility angle is calculated as shown in Fig 1 and correspondingly the flux is calculated from equation (2). The isotropic term is then added to the calculated flux which models the re-deposition phenomenon. Then the profile is finally updated based on the flux (velocity) of each point on the profile.

VI. RESULTS & DISCUSSIONS

The simulation results are close to the experimental results with different values of $flux_{ion}$ which changes with the geometry. The reduced computation domain makes the simulations much faster. Simulations are generated for trenches with different aspect ratio and a comparison is made with and without considering re-deposition in Fig 5. The thickness of the deposited profile is in close approximation with the experimental results with a mean relative error of about 5.7% in Figure 8 to 8.05% in Figure 7. The key-points for measuring the mean relative error has been indicated in the simulation results.

VII. CONCLUSIONS

In this study it has been demonstrated that level set method is capable to model the PECVD and LPCVD processes. This method describes the interface more accurately as generated results are in good agreement with the experimental results. Our implementation has been able to predict all the topologies types in PECVD/LPCVD processes with good simulation accuracy. Simple to complex geometries has been simulated efficiently with the level set method as shown in Fig 5,6. This program is also possible to be implemented in a parallel way on a multi-core architecture like GPUs further increasing the efficiency in terms of reduced computational time making it apt for industrial applications. Comparing with the experimental data, this level set approach is an efficient tool for modeling thin film deposition as well as other MEMS processes.

VIII. ACKNOWLEDGEMENT

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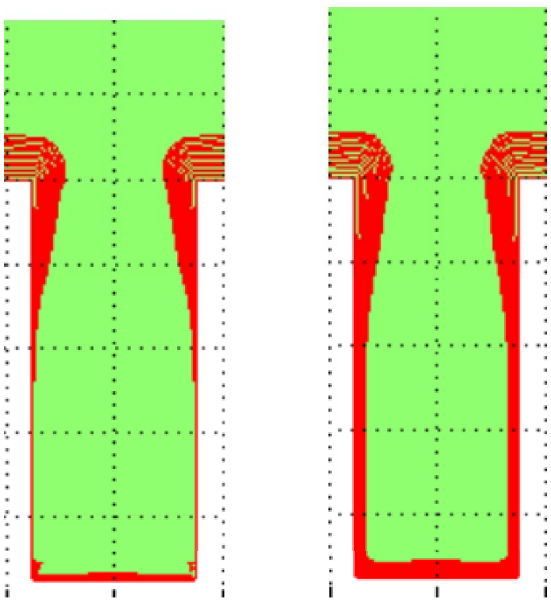

(i) (ii)

Fig 5: (i) Simulation Result when S.C = 1 (Direct Deposition)
(ii) When S.C < 1 Simulated by adding the isotropic term

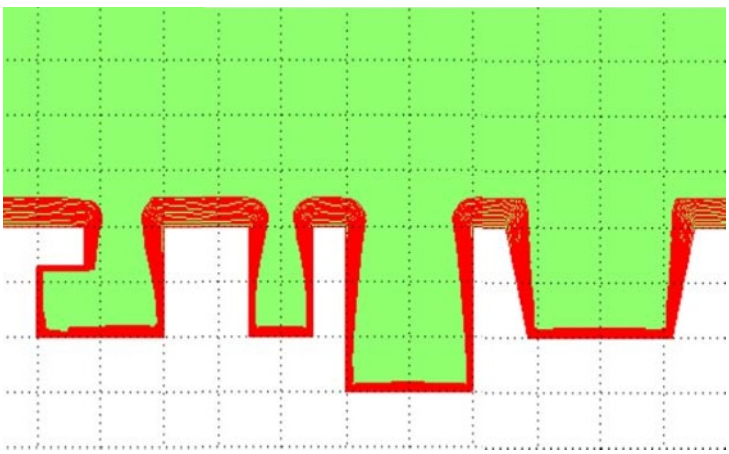

Fig 6: Simulation Results of some complex geometries

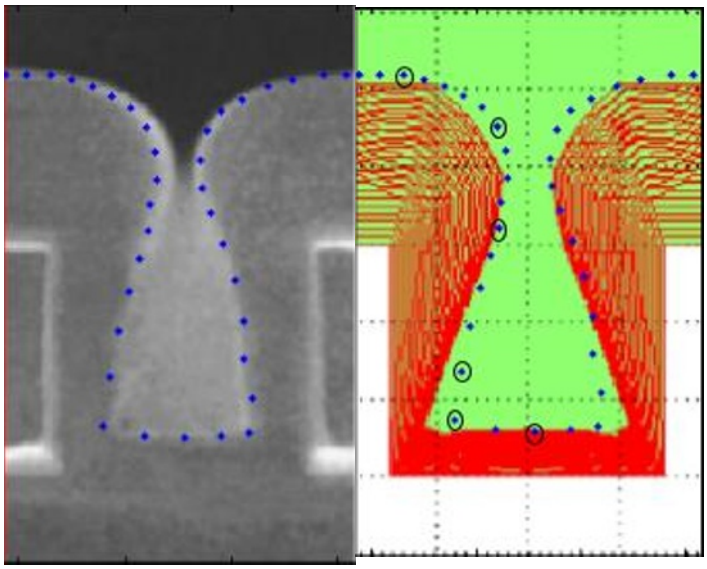

Fig. 7: SEM Results (LPCVD) [4] and Simulation Result. The mean relative error calculated by considering the encircled key-points is 8.05%

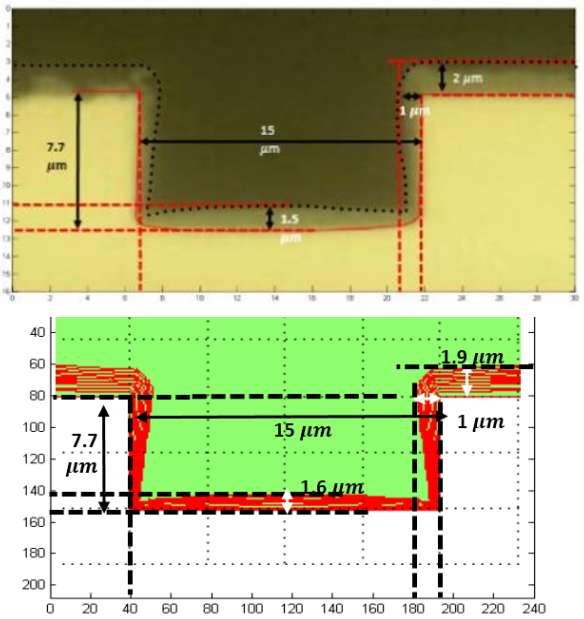

Fig 8 : Experimental(PECVD) and Simulation Results showing close approximation with the experimental picture. The mean relative error is 5.7%.