Modeling of Deposition Process by Level Set Method

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ABSTRACT

In this paper, we report a novel method for effectively reducing the amount of calculation for a deposition rate at a specific level-set node. The proposed algorithm makes it possible to reduce the number of level-set nodes for the same accuracy and convergence. Furthermore, the total CPU time for simulating the surface evolution on the wafer during the plasma deposition process has been reduced approximately by one-ninth of the required CPU time with comparison to the traditional level-set method.

The increased number of level-set nodes with closer grid spacing is generally required for the representation of a curved surface such as a contact hole for multi-level interconnections. However, the CPU time for the level-set calculation of the speed function F increases by $O(n^2)$ as we increase the node density by $O(n)$.

Keywords: Level set method, process simulation, modeling

1 INTRODUCTION

Despite many efforts to accurately model the topographical evolution of a complex structure on the substrate, it is still a challenge to figure out the topography on the wafer after a series of semiconductor processing steps by computer simulation.

An advantage of the above-mentioned cell method is the stability of the topography representation. In addition, the cell method can support quite a complex structure having a region that is completely disconnected from other region. But, despite the practicality of cell method for 3D simulation, they suffer from a lack of accuracy by using the method fixing the time step interval. The raggedness of the resulting profiles and the difficult of representing the actual advancing surface due to partially etched/deposited cells remain in shortcoming.

The surface advancement method, another method to representing the evolving surface, doesn't have several problems arising in the cell method [1]. But, this method has some difficult problems concerning the control of the segments and nodes, like as the node density, the size and loops of segments.

A level set method has been investigated in an effort to minimize the discretization errors and/or the occurrence of a rough surface, which was originally developed by Sethian [2]. Level set method calculates the propagation of a surface by updating the value of each grid point, which corresponds to the motion of the surface. The correct solution of the topological change can be obtained from the differential equations when the front either merges with itself or forms a cup or a stable edge. However, the traditional surface evolution from the level set requires a huge amount of computational time. Narrow band method was proposed for overcoming this problem, but it can't main key to reduce the computational time [2, 3].

In this paper, we employ the level set method with novel method to investigate the fast modeling of the topography evolution for process modeling

2 DESCRIPTION OF ALGORITHM

To calculate a deposition rate of each surface patches, one point B in patch was selected. Figure 1 shows that all intersection points between edge of cell and zero level set were selected. In case the zero level set is located on the edge of cell, both vertexes of edge were selected as the intersectional points. In Fig. 1, the center point A was calculated using four intersectional points and then the nearest point B from center point A was found in zero level set. The nearest point B was used for the calculation of the deposition rate of each surface patches.

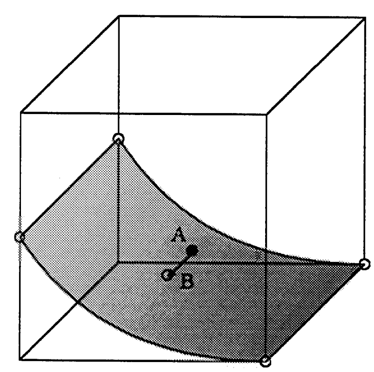


Figure 1: The selection of point B for the calculation of a deposition rate of each surface patches.

In Fig. 2 is shown a schematic cross-sectional view illustrating a particle transport with consideration of visibility and surface reflection. The visibility test consists of a procedure of checking a sign of the level set function defined on the line between the source and field points [2]. The probability of the reflection of the incident particle is modeled as *(1-Γ)* where *Γ* is the sticking coefficient. In this case, the distribution of the reflected particles is modeled as a cosine function with a normal axis on the surface [3].

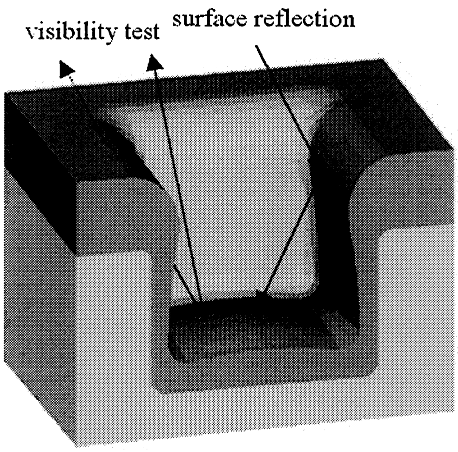


Figure 2: A schematic diagram of the particle transport.

The equation (1) shows the direct deposition rate of particles ejected from source and the equation (2) shows the re-deposition rate of particles reflected from surface of deposition target. Total deposition rate of each nodes was determined by the summation of equations (1) and (2).

$$F_{direct} = \int\int D(\theta,\phi)\Gamma(\theta,\phi)\cos\theta' d\theta d\phi \qquad (1)$$

$$F_{reflection}(\vec{r}_1) = \int \frac{\Gamma(\vec{r}_1,\vec{r}_2)}{\pi|\vec{r}_2-\vec{r}_2|^2} F_{incoming}(\vec{r}_1)\cos\theta'\cos\theta'' dS \qquad (2)$$

In equation (1), $D(\theta,\phi)$ is the distribution of incident particles from source to target and $\Gamma(\theta,\phi)$ is the visibility function of incident particles with θ,ϕ angles. $\Gamma(\theta,\phi)$ return 1 for visible node and 0 for non-visible node. Using the visibility function, the deposition rate variation due to the shadow effect, which determined the possibility of deposition of the incident particles with θ,ϕ angles, can be applied to our deposition simulation. In Fig. 3, θ' which is the angle between the incident particle and the vertical vector at surface node, was used for the calculation of direct incident flux of particles.

In equation (2) present $\Gamma(\vec{r}_1,\vec{r}_2)$ for a visibility function of ions which were reflected at $\vec{r}_1$ and then absorbed at $\vec{r}_2$, γ for sticking coefficient, $F_{incoming}$ for a calculated flux of ions at previous step. θ' is the angle between vertical vector at $\vec{r}_1$ and $\overrightarrow{r_1r_2}$ line, and θ'' is the angle between vertical vector at $\vec{r}_2$ and $\overrightarrow{r_1r_2}$ line. Because the surface roughness is so great compared to the size of ions, we assumed that incident ions were reflected with the cosine distribution at surface.

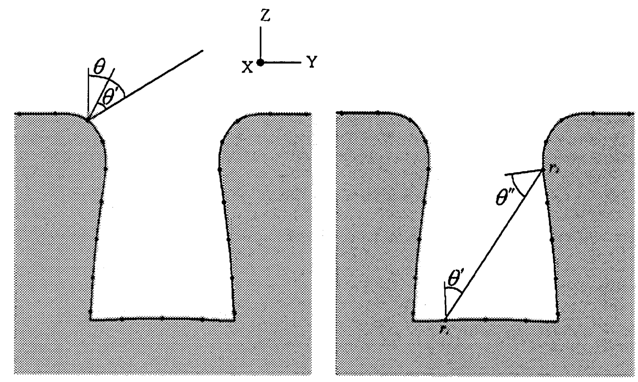


Figure 3: A schematic diagram of angles was used for calculating the deposition flux.

In the simulation of deposition process with low sticking coefficient, as we assumed the reflection with cosine distribution at surface, the ratio of the flux at i-th and i+1-th reflection would converge to a constant value. Therefore the deposition rate at arbitrary position can be calculated when the convergence is generated at n-th reflection. Equation (3) presents the calculation of deposition rate at arbitrary position

$$F = F_{direct} + \sum_{i=1}^{n} F^{i}_{reflection} + \frac{F^{n+1}_{reflection}}{1 - F^{n+1}_{reflection} / F^{n}_{reflection}} \qquad (3)$$

We put the speed function for calculation of level set equation at each grid equivalent to the deposition rate of cell including a nearest surface point from (i, j, k) grid. And then the speed functions at all grid of narrow band are determined.

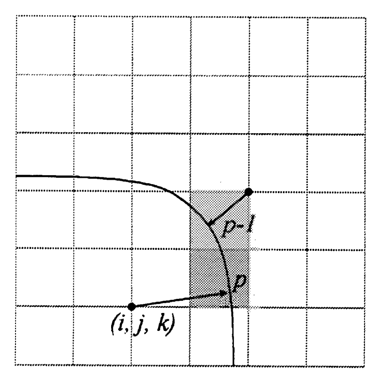


Figure 4: the method of determining the speed function of level set function.

In table 1 the number of points used for calculation the deposition rate are given for various sizes. In case width of narrow band is twice grid width, the number of points is about five times more than presented method. For N points, it requires N^2 evaluation that the calculations of the deposition rate by surface reflection take. Therefore, twenty five times evaluation is required.

Table 1: A table illustrating the calculated thickness of the deposited layer and its ratio.

Grid Size	20×20 ×20	30×30 ×30	40×40 ×40	50×50 ×50	60×60 ×60
Old Method	4073	8365	14737	22794	32107
New Method	628	1480	2720	4132	6284

3 RESULTS

Figure. 5 depicts a cross-sectional view illustrating the simulation for a sputter-deposition process into a contact hole having an aspect ratio of 0.67. Referring to Fig. 5, the surface designated by B denotes a deposited profile with taking the surface reflection into account, whilst the surface designated by A exhibits the profile without considering the surface reflection into account.

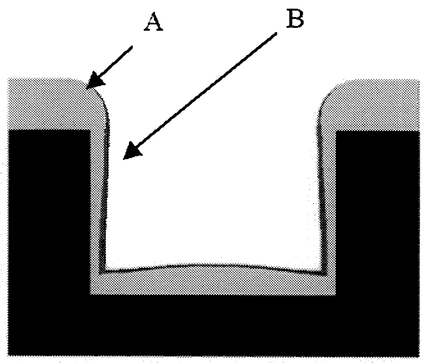


Figure 5: A result showing the deposition rates by (A) direct flux and (B) reflected and re-sputtered flux.

Figure. 6 shows a cross-sectional view illustrating the simulation for LPCVD of SiO2 from DES/O2 source of 380°C. Table1 shows thickness on each position of preceding process simulation. Figure. 7 shows the cross sectional view illustrating the simulation of sputter deposition in a rectangular via having an aspect ratio of 2. Fig. 8 shows the SEM and the cross sectional view illustrating the simulation of PECVD deposition.

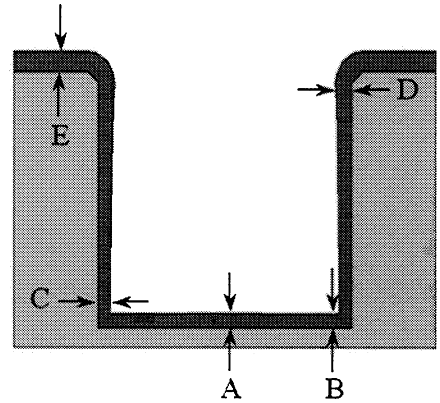


Figure 6: A plot showing the simulated profile for LPCVD deposition of DES/O_2 with an aspect ratio of unity.

Table 1: A table illustrating the calculated thickness of the deposited layer and its ratio.

A (in µm)	B (in µm)	C (in µm)	D (in µm)	E (in µm)
0.035	0.033	0.030	0.040	0.050
C/B	B/A	D/C	E/A	
0.94	0.95	0.78	0.70	

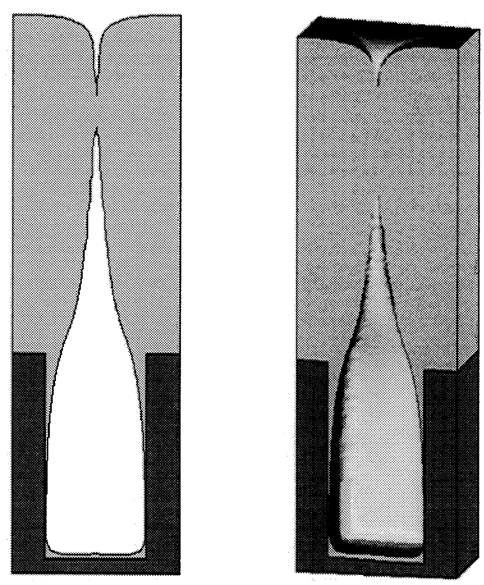
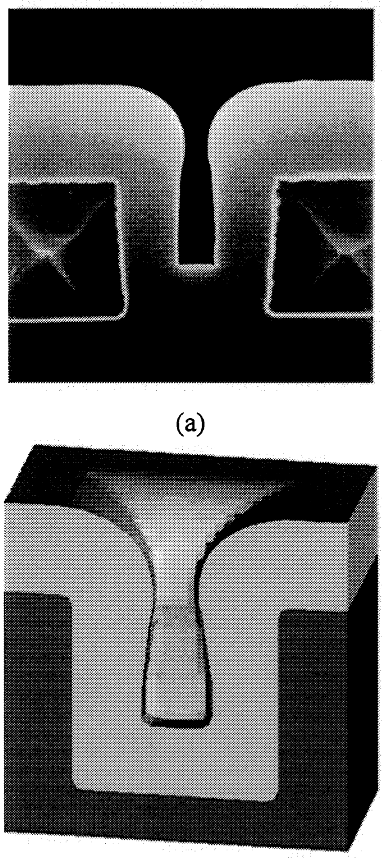


Figure 7: Plots showing the simulation results of sputter deposition in a rectangular via.



(a)

(b)

Figure 8: PECVD SiN deposition. (a) The SEM. (b) The cross sectional view of simulated result.

4 CONCLUSION

A deposition modeling method using level set method was presented. In case level set method was used for modeling semiconductor modeling, it is demonstrated that using points on zero level set is more efficient than using nearest points from grids for calculation of a deposition rate. Examples of various deposition processes are presented. And calculated results are explained by using simulation model.

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