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Fast step coverage simulation for 3D contact hole with analytical integral.

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Abstract We have developed a high speed Al CVD profile simulator for 3D contact filling using analytical integral for gas phase flux and re-emission flux from contact surface. The analytical integral formulation for 3D circular contact is described in detail. The analytical integral simulator has four times faster simulation speed than that of using numerical integral. The simulation results agree well with observed experimental results except for the bottom coverage.

Ultra Large Scale Integrated(ULSI) circuits require high density multi-layer interconnections with high aspect ratios. CVD profile simulation is useful to develop technology for high aspect ratio feature filling. Many works on profile simulation for LPCVD have been done, using such as the direct simulation Monte Carlo(DSMC) method[1] and analytical mass balance method[2,-3]. However the DSMC method is inefficient in the calculation of flux distribution in the case of the reactive sticking coefficient is very small. The simulation method in Ref [2] was limited to reproduce only initial deposition profiles because shadowing effect was not considered. Although a set of fundamental equations and results for the direct flux and re-emitted flux are shown in Ref [3], the comparison between the simulation and experimental profiles for contact holes were not shown. Detailed filling profiles for contact holes are necessary to develop large aspect ratio contact filling, because the current density though the contact holes has large factor in electro-migration endurance.

We have developed high speed simulator for circular feature. The present profile simulation codes employed an analytical model[3] including the direct flux of precursor species from the gas phase and the indirect flux due to remission from the micro feature surface. Knudsen flow is applied to the Al LPCVD because the device scale sizes are less than the mean free path for collisions between gas molecules. To reduce computational time, analytical integral is employed for 3D contact holes.

The coordinate system was shown in Fig. 1. To evaluate shape factor which determine re-emitting flux between circular surfaces P and Q. Point P and Q on the circular surfaces are defined as $(x_p, 0, z_p)$ and $(x_q \cos\theta, x_q \sin\theta, z_q)$, and normal vectors n_p and n_q are defined as $(n_{px}, 0, n_{pz})$ and $(n_{qx} \cos\theta, n_{qx} \sin\theta, n_{qz})$ respectively.

Re-emitted flux on the point P from contact hole surface is described as follows,

$$J_p = \sum_{q \neq p}^{n} J_q (1 - S_c) \int_{-\theta}^{\theta} \frac{(n_p \cdot r_{pq})(n_q \cdot r_{qp})}{\pi r_{pq}^4} ds_q \qquad (1)$$

where J_q is impinging flux on the point Q on the contact hole surface, S_c is reactive sticking coefficient, r_{pq} is direction vector between points P and Q, and ds_q is area of the re-emitting area around point Q. The integral in Equ. 1 can be analytically integrated as follows.

$$\begin{aligned} I_q(\theta) &= \frac{\beta 1\,\beta_2}{2\,\beta_3}(\alpha_3 - \beta_3)^2\,\theta + \left((\alpha_1 - \beta_1)(\alpha_2 - \beta_2) - \frac{\beta 1\,\beta_2}{\beta_3}(\alpha_3 - \beta_3)^2\right)\frac{1}{\gamma}\arctan\left(\frac{\tan\frac{\theta}{2}}{\gamma}\right) \\ &\quad + \frac{2\,(\beta_1\,\alpha_3 - \alpha_1\,\beta_3)(\beta_2\,\alpha_3 - \alpha_2\,\beta_3)}{\beta_3\,(\alpha_3 - \beta_3)}\frac{1}{2\,\gamma^2}\left(\frac{1}{\gamma}\arctan\left(\frac{\tan\frac{\theta}{2}}{\gamma}\right) + \frac{\tan\frac{\theta}{2}}{\gamma^2 + \tan^2\frac{\theta}{2}}\right) \end{aligned}$$

The constants in the last equation are defined as follows.

$$\begin{aligned} \alpha_1 &= x_p\,n_{px} + (z_q - z_p)\,n_{pz}, & \beta_1 &= x_q\,n_{px} \\ \alpha_2 &= -x_q\,n_{qx} + (z_p - z_q)\,n_{qz}, & \beta_2 &= -x_p\,n_{qx} \\ \alpha_3 &= x_p^2 + x_q^2 + (z_p - z_q)^2, & \beta_3 &= 2x_p\,x_q \\ \gamma &= \sqrt{(\alpha_3 + \beta_3)/(\alpha_3 - \beta_3)} \end{aligned}$$

The region of the integral can be estimated by considering shadowing effect and visibility between points P and Q. Visibility are checked by whether both inner products $(n_p \cdot r_{pq})$ and $(n_q \cdot r_{qp})$ are

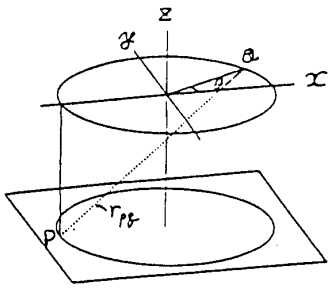


Figure 1: Schematic diagram of coordinate system for re-emitted flux calculation.

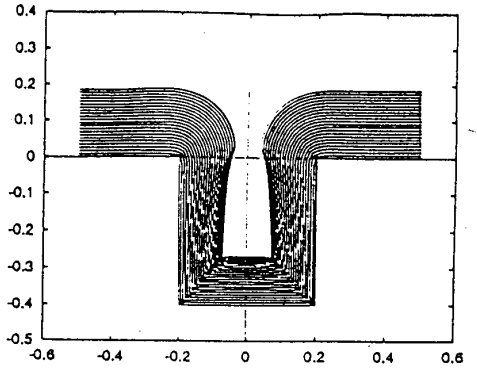
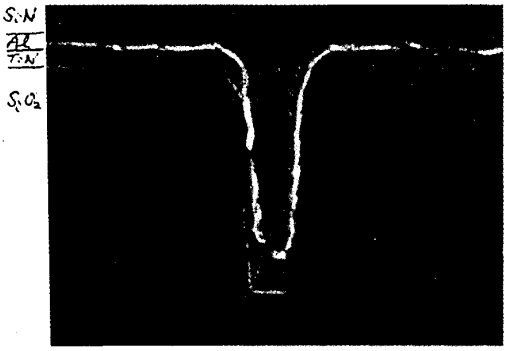


Figure 2: Deposition profile for a circular contact of aspect ratio equal to unity with $S_c = 0.1$



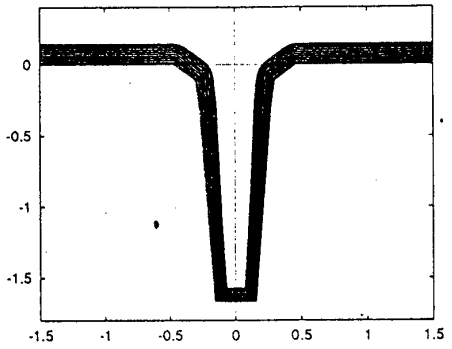


Figure 3: Comparison of results for the experimental results(left) and the simulated profile(right) for Al CVD for a cylindrical contact.

positive. Shadowing effect are also checked by super-imposition between shadow cone made with shadow circle and point P and the cone made with circle Q and point P.

Computational time using analytical integral for the case shown in Fig. 2 was approximately four times shorter than that of using numerical integral with sufficient accuracy. Figure 3 shows the comparison between results obtained with this model and experimental for Al chemical vapor deposition. A reactive sticking coefficient of 0.04 was determined by another comparison between experimental results and 3D trench simulation for trenches with overhang(cantilever type structure)[4]. By the comparison in Fig. 3, the simulated coverage for the circular contact agreed with the experimental result except the bottom coverage. This discrepancy is considered to be attributed to a surface diffusion during Al CVD.

In conclusion, we have developed high speed simulator for 3D contact filling using analytical integral for gas phase flux and re-emission flux from contact surface. The analytical integral formulation for 3D circular contact is described in detail. The analytical integral simulator has four times faster simulation speed than that of using numerical integral. The simulation results agree well with observed experimental results except for the bottom coverage.

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