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Citation: *Applied Physics Letters* **58**, 2147 (1991); doi: 10.1063/1.104988

View online: <http://dx.doi.org/10.1063/1.104988>

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New test structure to identify step coverage mechanisms in chemical vapor deposition of silicon dioxide

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(Received 1 October 1990; accepted for publication 16 February 1991)

A new test structure has been developed to identify unambiguously the main mechanism which determines the profiles of thin films deposited by low-pressure chemical vapor deposition (LPCVD) in structures such as steps, trenches, and via-holes. The two mechanisms considered are reemission due to a low surface reaction probability and surface diffusion. Experimental results using silane, diethylsilane (DES), tetraethoxysilane (TEOS), and tetramethylcyclotetrasiloxane (TMCTS) as the silicon sources for oxide deposition by LPCVD show that indirect deposition from reemission is the major contributing factor in determining the step coverage.

Step coverage of thin films deposited in trenches and via-holes becomes critical as the line width of VLSI circuits decreases. Recently, researchers have greatly improved the step coverage of SiO_2 in both low-pressure chemical vapor deposition (LPCVD) and plasma-enhanced CVD (PECVD) systems by substituting organic silicon sources such as tetraethoxysilane (TEOS) for silane.¹⁻⁶ However, there is considerable disagreement over the main mechanism responsible for this improvement. Figure 1 shows the three mechanisms responsible for precursor transport to device structures: direct transport, reemission, and surface diffusion. Note that at LPCVD operating pressures the mean free path lengths are much larger than the device dimensions; therefore, gas diffusion is unimportant for step coverage. The direct flux arrives from the gas phase without other collision with the surface. Reemission refers to transport by multiwall collisions due to a sticking coefficient (S_c) < 1. The sticking coefficient is the probability that a precursor is chemisorbed on the surface; therefore, reemission includes both reflection and desorption effects. In the reemission case the precursors can leave the surface with different angular distributions, depending on the nature of the surface and the species.^{7,8} At one extreme, the incoming precursors experience strong interaction with the surface and lose all their memory of the incoming trajectory; they then reemit with a cosine distribution.⁷⁻⁹ At the other extreme, the surface acts as a perfectly reflecting wall, and the reemission is characterized by asymmetric specular reflection^{7,8} where the distribution is maximized at an angle equal to the incident angle from the surface normal. The desorption pattern can be a combination of the two patterns mentioned, resulting in a lobular shape distribution with a maximum along the specular reflection angle.^{7,8} Indirect deposition from reemission and surface diffusion allow precursors to reach areas less accessible to direct flux such as sidewalls and trench corners.

Although Becker *et al.*,¹ and Levin and Evans-Lutterodt² used reemission to explain the improvement of step coverage of undoped glass films and borophosphosilicate glass (BPSG) films from TEOS, other authors have attributed the improvement to high surface mobilities of deposited particles from organic sources (such as TEOS) as

compared to those deposited by silane.³⁻⁵ In their research on step coverage of undoped and phosphorus-doped SiO_2 glass films, Levin and Evans-Lutterodt⁶ state that the existence of porous lines of oxide (deposited with TEOS) at the base of $1 \mu\text{m}$ trenches indicates that the surface diffusion length is not much larger than $1 \mu\text{m}$. Yet, the scanning electron micrograph (SEM) photos in the paper show very conformal step coverage of films in trenches $50 \mu\text{m}$ deep and $4 \mu\text{m}$ wide, suggesting a surface diffusion length of at least $15 \mu\text{m}$. Similar contradictions can also be observed for simulation programs such as SAMPLE¹⁰ which apply surface diffusion to simulate CVD profiles. Such simulations often require different surface diffusivity to fit oxide profiles in trenches of different aspect ratios, which is unrealistic. Recently, researchers including us, have employed indirect deposition due to reemission to simulate CVD step coverage.¹¹⁻¹⁵ Lack of direct evidence to support either mechanism has led to the different viewpoints in the literature. In this work, we present a test structure with a cavity and overhang capable of determining the dominant mechanism.^{14,15} CVD and sputtering were the two deposition techniques studied. Figure 2 shows the test structure, possible mechanisms of near surface mass transport and schematic of the resulting profiles. By studying these profiles we can determine the contribution of each mechanism.

The area under the overhang is shielded from direct flux; therefore, no deposition should occur there if direct deposition is the dominant mechanism. Deposition in this region can only occur through indirect deposition due to either reemission or surface diffusion. We use two features of the test structure to separate reemission from surface diffusion. First, the area under the long overhang serves as

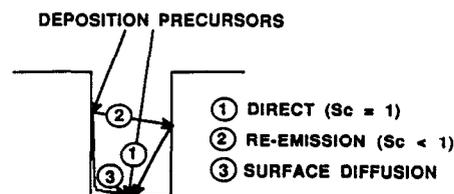


FIG. 1. Near-surface mass transport and deposition mechanisms.

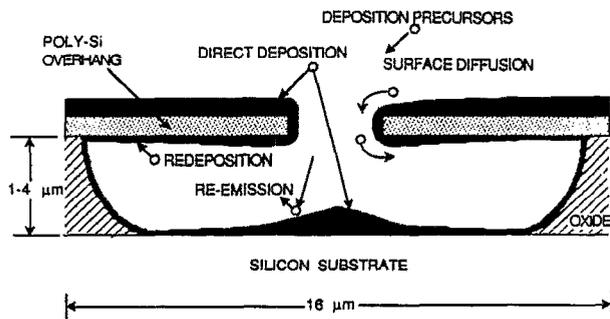


FIG. 2. Overhang test structure and different deposition profiles due to the mechanisms described in Fig. 1.

a sink for surface diffusion whereas the top surface near the opening of the overhang acts as the source. If surface diffusion controls step coverage, we should observe a decrease in thickness on the top surface near the opening as shown schematically in the right side of the overhang in Fig. 2. Second, variation of the height of the cavity should not affect the deposition profiles under the overhang when surface diffusion dominates unless the diffusion length significantly exceeds the length of the overhang, which is unlikely.⁶ On the other hand, if reemission dominates, changes in the cavity height would effect the flux of reemitted particles reaching the area under the overhang. In the left side of Fig. 2 we see that as the cavity height increases both cosine and specular reemission distributions will tend to drive the precursor flux deeper under the overhang, and thus improve thickness uniformity. This can be seen if we first focus on the direct flux distribution in the cavity, which would only be on the bottom surface with a maximum at the center of the opening. The final distribution can be extrapolated by including single and multiple re-emissions from the direct flux. As cavity height increases, the reemission angle (to the surface normal) for the particles from the central region on the bottom surface to reach the far corner under the overhang decreases. Since for a cosine reemission distribution the emission probability increases as the reemission angle decreases, the flux to the far corner increases with the height increases. The trend is also true for the specular reflection case, where the reemission of the direct flux of the same incident angle also penetrates further under the overhang as the height increases.

We fabricated test structures to test this theory on two deposition techniques, sputtering of Al and CVD of SiO₂. The test structures were fabricated by first depositing 1–4 μm of undoped SiO₂ onto 4 in. silicon wafers; this oxide thickness determines the cavity height. After depositing 5000 Å of polysilicon and patterning, lines of different widths were dry etched through polysilicon, followed by a 6:1 HF wet etch into the CVD SiO₂. This isotropic etching of SiO₂ forms the cavity. Aluminum was sputtered onto the test structure at 61 °C. SiO₂ from various sources was deposited onto the test structure in a horizontal-tubular hot-wall LPCVD system. The oxide film thicknesses were kept at 5000 Å. The different silicon sources investigated in-

TABLE I. LPCVD oxide deposition sources and conditions.

Si source	Temperature (°C)	Pressure (mTorr)	O ₂ /source flow ratio
Silane	370–430	150–190	1.1–2
DES	380–440	750	2
TMCTS	560	850	25
TEOS	700	300	...

cluded silane (SiH₄), diethylsilane (DES), tetramethylcyclo-tetrasiloxane (TMCTS), and tetraethoxysilane (TEOS). The deposition conditions as shown in Table I range in temperature from 370 to 700 °C. The liquid TEOS source was introduced into the reaction chamber by bubbling nitrogen gas through it. The O₂/source flow ratio could not be accurately determined.

Figure 3 illustrates the profile of Al deposited by sputtering near room temperature (61 °C) on the test structure. It is clear that there is no deposition in the areas covered by the overhang except where the Al flux can reach directly. There seems to be no evidence of surface diffusion or indirect deposition due to reemission. We can conclude that the sticking coefficient (*S_c*) is nearly 1 in this case.

The four silicon sources studied fall into two groups, slightly conformal films (silane and DES) and near conformal films (TEOS and TMCTS). Even in the latter case, the test structure was capable of showing some nonuniformity. For brevity, we use only the silane and TEOS source results to demonstrate the use of the test structure. Figure 4(a) shows a SEM cross section of a test structure with a 2-μm-wide opening, an 8-μm-long overhang, and a 1.4-μm-high cavity height after oxide deposition from a silane source. The structure in Fig. 4(b) has a cavity height of 4.3 μm. As expected, the deposited oxide layers in Figs. 4(a) and 4(b) are not conformal. The uniform thickness of the oxide on the top surface indicates a lack of any significant surface diffusion. This is further demonstrated by the fact that the oxide thickness on the underside of the overhang and on the bottom surface tapers off more rapidly in the 1.4-μm-high cavity than in the 4.3-μm-high cavity. In Fig.

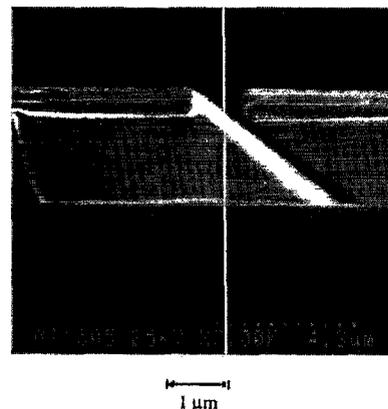


FIG. 3. Al sputtering (61 °C) deposition on the test structure.

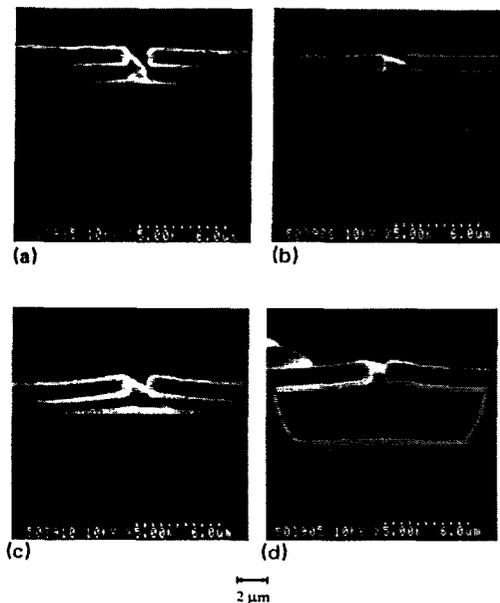


FIG. 4. Silane source oxide deposition on the (a) $1.4\ \mu\text{m}$ and (b) $4.3\text{-}\mu\text{m}$ -deep test structure; TEOS source oxide deposition on the (c) $1\ \mu\text{m}$ and (d) $4.3\text{-}\mu\text{m}$ -deep test structure.

4(a), the oxide thickness on the underside close to the opening exceeds the thickness in the far corner by 275%, compared to 25% in the taller cavity, shown in Fig. 4(b). We can explain the difference in the degree of tapering if we assume reemission dominates. The larger source angle of the shorter test structure leads to the greater oxide thickness in the central region of the bottom surface, and as a result of this thicker oxide and shorter height of the cavity, more precursor is reemitted and deposited on the underside of the overhang near the opening. We conclude from the experimental results that reemission dominates over surface diffusion in controlling step coverage. For the temperature range we studied for silane and DES sources, a temperature increase leads to only a small improvement in step coverage. Also for the pressure and flow ratio ranges we studied for silane source, the deposition profiles do not significantly change.

Figure 4(c) shows a SEM cross section of a test structure with a $2\text{-}\mu\text{m}$ -wide opening, an $8\text{-}\mu\text{m}$ -long overhang, and $1\text{-}\mu\text{m}$ -high cavity after a TEOS-source oxide deposition. The structure in Fig. 4(d) has a cavity height of $4.3\ \mu\text{m}$. Similar to the deposition from silane, we observe a constant thickness on the top surface, a larger gradient in oxide thickness under the overhang, and a thicker oxide on the center of the bottom surface for the shorter cavity (25% compared to 11%). This shows that changing the height changes the deposition profiles under the overhang,

which implies that reemission is important. Besides, the thickness above the overhang is twice the thickness under the overhang away from the opening. If surface diffusion significantly contributed to the conformal deposition inside the cavity, the thickness of oxide under the overhang away from the opening would be very close to the thickness above the overhang; however, the large difference in the thickness indicates that surface diffusion is not the significant factor in step coverage improvement. TEOS-source oxide depositions are more conformal than silane-source depositions due to the lower sticking coefficient of TEOS-source precursor than silane-source precursor. The low sticking coefficient results in more collisions of the precursor with the walls of the structure allowing it to reach less accessible area; therefore, there is more deposition in the cavity for the TEOS case.

In summary, the results show that the test structure unambiguously identify the main mechanism determining step coverage. For the LPCVD oxide films studied which include silane, TEOS, DES, and TMCTS sources, deposition into shallowed regions of steps is controlled by reemission (sticking coefficient < 1). The results indicate that surface diffusion does not play a significant role in step coverage improvement.

The authors gratefully acknowledge financial support from SRC and DARPA. The authors also thank David L. O'Meara from J. C. Schumacher for his help in doing the TMCTS and DES sources oxide deposition on the test structures.

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