

Filling In-situ Phosphorous-doped Void-free Polysilicon in High Aspect Ratio Trenches

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Abstract:

In this paper, a discontinuous supply of doped gas (phosphine (PH₃)) was proposed to enable the polysilicon reproduction of the bottom-up filling of the trenches. By systematically investigating the relationship between PH₃ flow rate and the deposition rate of polysilicon, the study elucidates the physical mechanism behind void formation in trenches under the conventional continuous gas supply mode. An innovative discontinuous gas supply method was employed, where PH₃ was introduced into the reaction chamber in stages, successfully achieving void-free filling of polycrystalline silicon films in trench structures with an aspect ratio of 10:1. The concentration of doped gas PH₃ at the trenches bottom was lower than the top during the polysilicon deposition by the fire-new method. The results from scanning electron microscopy showed a void-free polysilicon filling in trenches significantly.

Keywords:

Doped Polysilicon, PH₃, Low Pressure Chemical Vapor Deposition (LPCVD), Aspect Ratio (AR), Void-free Polysilicon Filling

1. Introduction

In semiconductor industry, heavily doped polysilicon is widely used as gate electrodes, emitters, and diffusion sources of shallow junctions [1,2]. It also has been filled in deep trenches as isolation, gate polysilicon or interconnection material in power devices, micro electromechanical systems (MEMS) and memory components [2]. However, it was not easy to fill deep trenches without forming voids [3,4,5]. There is a lower deposition rate at the bottom of the trenches than the surface due to less precursor gas transported to the bottom, which results in the early closure of trenches and the formation of voids [5,6]. R. Singh et al. [5] developed a pulsed laser annealing technique to enhance the filling uniformity of polysilicon in high-aspect-ratio TSVs, effectively preventing void formation. C. Heitzinger et al. [9] established a multiscale simulation framework to predict dopant segregation in 3D-NAND memory channels, revealing significant arsenic concentration gradients along high-aspect-ratio structures due to interface trapping dominance. Complementarily, the void-free fabrication method claimed in [7] utilizes sequential doping cycles with laser annealing to achieve uniform resistivity in trenches with AR > 20:1. Some studies to widen the opening width and slope of the trenches have been examined

[3,4,5]. These approaches have been well established for filling void-free polysilicon in trenches. However, the applications are limited with the aspect ratio (AR) of the trenches increasing.

In this paper, a void-free polysilicon was fabricated to fill in high AR (10:1) trenches by low pressure chemical vapor deposition (LPCVD). A discontinuous supply method was used to introduce PH_3 into reactor during polysilicon deposition. The relation between the deposition rate of polysilicon and the flow rate of doped gas PH_3 was investigated. And the polysilicon filling in trenches with AR (10:1) under three supply mode of doped gas was studied. The results provide reference knowledge of the polysilicon filling in high AR trenches by this fire-new technique.

2. Experimental Section

P-type (100) silicon wafers were used to study the relation between the deposition rate of polysilicon and the doping concentration during deposition process. And pre-patterned p-type (100) silicon wafers with trenches of 1 μm width, 10 μm depth and 88-89 °C slope were used to investigate the filling voids of polysilicon. The in-situ phosphorous-doped polysilicon of thickness 1200 nm was prepared on a thermal oxide film of thickness 100 nm which was pre-deposited on the wafers. Sample preparation was conducted in a low-pressure chemical vapor deposition (LPCVD) system (TEL Alpha-8SE) at a pressure of 0.75 torr and a growth temperature of 530 °C. The precursors were SiH_4 at a flow of 1200 sccm, PH_3 at a flow of 40 sccm.

In the study of deposition rate and doping concentration, more than a dozen of experiments of different doped gas PH_3 concentration had been carried out. The flow rate of PH_3 was varied from 25 sccm to 400 sccm. Three experiments of different PH_3 supply mode were examined to investigate the polysilicon filling in trenches. The first one used a conventional supply mode that doped gas PH_3 was continuously intruded into chamber with flow rate of 40 sccm, which was the most widely used in semiconductor industry. In the second/third experiments, the doped gas PH_3 supply has many cycles and each cycle included two steps: supply/stop for 20 s/5 s and 5 s/5 s. Fig.1a displays the the gas supplied curves of SiH_4 and PH_3 in the third experiment. The deposition rates of polysilicon were around 1.0 to 1.8 nm/min, as measured by spectroscopic ellipsometry. The content of doped impurities in polysilicon was characterized by X-ray fluorescence (XRF). The microstructure and morphology of the polysilicon filling were characterised by scanning electron microscopy (SEM).

3. Results and Discussion

Figure 1b shows the relation curve between the deposition rate and the flow rate of PH_3 . The deposition rate of polysilicon decreases gradually with the increasing of the flow rate of PH_3 , which is approximately an inverse relationship. This is because an inhibition layer forming with the increasing of the dopant PH_3 partial pressure reduces the deposition rate of polysilicon [3]. The phosphorus concentrations in polysilicon of three experiments are $1.28 \cdot 10^{20}$, $1.16 \cdot 10^{20}$ and $0.9 \cdot 10^{20} \text{ cm}^{-3}$ respectively. It gets down gradually with the decreasing of PH_3 gas quantity.

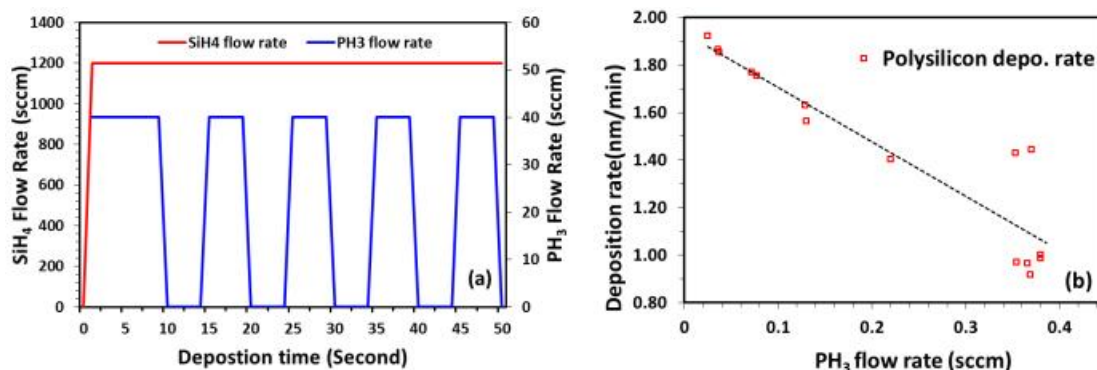


Figure 1. (a). The curve of PH₃ were supplied for 5 s then stopped 5 s, (b) The relation curve between deposition rate and PH₃ flow rate.

To characterize the microstructure and morphology, SEM was used to investigate the polysilicon filling in the trenches. Figure 2a-c display the SEM images of the polysilicon filling voids of the three experiments. Figure 2a shows the width of voids in trenches is 0.221 μm with the conventional supply mode. As shown in Figure 2b, the width of voids in trenches is 0.077 μm with the discontinuous supply mode: supply/stop for 20 s/5 s. The polysilicon filling voids in trenches was significantly improved by the discontinuous supply method of PH₃. In the third experiment with the supply condition: supply/stop for 5 s/5 s, it is found that the voids are almost disappeared, as shown in Figure 2c.

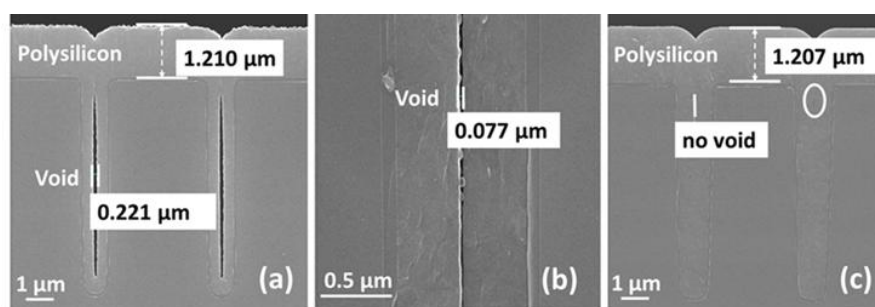


Figure 2. Polysilicon filling with PH₃ supply (a) A continuous supply mode of PH₃, (b) PH₃ was supplied for 20 s then stopped for 5 s, (c) PH₃ was supplied for 5 s then stopped for 5 s.

In the conventional process condition, a laminar flow with a maximum velocity of 5 meter per second (m/s) surrounded the wafer as a result of the temperature distribution and the low-pressure conditions reflected in a Reynolds number of 67 [1]. And as a result of the diffusion-controlled behavior no flow influences occurred, reflected by Peclet numbers for each species of less than 0.01 between the wafers, and of approximate 30 in main flow direction [1]. A hypothesis of the gas transport during the polysilicon deposition process was described as two phases. In the first phase, the precursor including SiH₄ and PH₃ entered the reactor at the same time and filled the whole reaction chamber in a short time (<1 s) under the action of laminar flow. But it was taken more time (several to dozens of seconds) to diffuse from the surface of the trenches to the bottom, which depending on the temperature, pressure, gas molecular weight and diameter, and the size of trenches, etc. During this period, the deposition rate was mainly contributed by the precursor concentration. Obviously, it was lower on the bottom of the trenches than the surface. In the second phase, after some time (several to dozens of seconds), the dynamic equilibrium of the precursor concentration on the surface and bottom of the trenches was established. The deposition rate was mainly contributed by the partial pressure of gases. The species

concentration exhibited a silane decreasing and hydrogen increasing in reactive areas. However, the hydrogen desorption speed at the bottom of trenches was slower than the surface due to the depth limitation of the trenches, which induced the lower deposition rate at the bottom than the surface. It was the mechanism of the voids formation under a conventional conditions. In the first experiment, the deposition rate on the bottom of the trenches is always lower than the surface, as shown in Figure 3a.

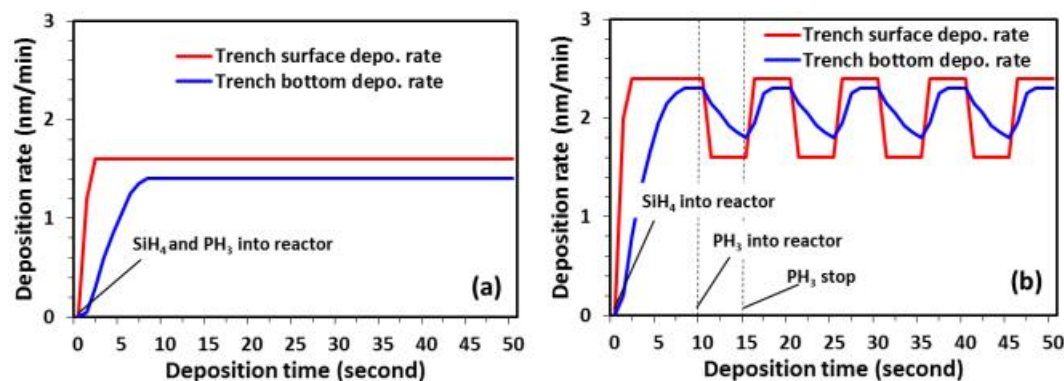


Figure 3. The polysilicon deposition rate (a) PH_3 was supplied continuously, (b) PH_3 was supplied for 5 s then stopped 5 s.

In this paper, we purposed a discontinuous supply mode of doped gas PH_3 . It made the concentration of doped gases on the trench surface always higher than that at the bottom, which caused the deposition rate of the trench surface lower than the bottom. Fig.3b shows the deposition rate curves on the surface and bottom of the trenches with the supply condition: supply/stop for 5 s/5 s. At the beginning of deposition process, only SiH_4 is brought into the reaction chamber. The deposition rate of un-doped polysilicon is around 2.4 and 2.2 nm/min on the surface of the trenches and the bottom, respectively. After that the PH_3 of flow rate 40 sccm is introduced into the reactor and fills the whole chamber in a short time (<1 s), while the PH_3 concentration at the bottom of trenches is almost zero. The deposition rate on the surface decreases rapidly to about 1.5 nm/min, while the bottom is about 2.2 nm/min. And then, the dopant concentration at the bottom of the trenches increases gradually and the deposition rate at the bottom decreases gradually due to the diffusion effect caused by the concentration gradient. Before the deposition rate at the bottom decreases to the surface, the dopant is stopped supply and quickly exhausted from the chamber, and then the chamber returns to the state of the process beginning. By adjusting the time and the cycle number of dopant supply/stop, the average deposition rate at the bottom of the trenches is higher than the surface. The sustained bottom-up filling effect was successfully achieved.

4. Conclusions

In this study, the in-situ phosphorous-doped void-free polysilicon was successfully achieved in high aspect ratio (10:1) trenches using a novel discontinuous supply mode of doped gas PH_3 . The relationship between the deposition rate of polysilicon and the flow rate of PH_3 was systematically investigated, alongside the thickness, dopant concentration, microstructure, and morphology of the polysilicon. These parameters were characterized using spectroscopic ellipsometry, XRF, and SEM measurements. It was observed that the deposition rate of polysilicon decreased gradually with the increasing flow rate of PH_3 , following an approximately inverse relationship. Under the supply condition: supply/stop for 5 s/5 s, a significant reduction in voids was

achieved, with nearly void-free filling observed. Additionally, the mechanism of void formation under conventional conditions was analyzed, and it was demonstrated how this issue is mitigated by the proposed method. These findings provide valuable insights into the polysilicon deposition process and suggest that further studies should focus on refining process parameters to enable consistent and scalable void-free polysilicon filling in high aspect ratio trenches.

Conflicts of Interest

The authors declare that there is no conflict of interest regarding the publication of this article.

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