Monitoring Arsenic In-Situ Doping with Advanced Models for Poly-Silicon CVD

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Abstract

Experiments of As-doped poly-silicon deposition have shown that under certain process conditions step coverages > 1 can be achieved. We have developed a new model for the simulation of As-doped poly-silicon deposition, which takes into account surface coverage dependent sticking coefficients and surface coverage dependent As incorporation and desorption rates. The additional introduction of Langmuir type time-dependent surface coverage enabled the reproduction of the bottom-up filling of the trenches. In addition the rigorous treatment of the time-dependent surface coverage allows to trace the in-situ doping of the deposited film. Simulation results are shown for poly-Si deposition into $0.1\,\mu$m wide and $7\,\mu$m deep, high aspect ratio trenches.

1 Introduction

State-of-the-art memory cells are based on deep trench fabrication technologies. Thereby void-less filling of the deep trenches is one of the crucial process steps. Experiments of As-doped poly-silicon deposition have shown that under certain process conditions step coverages > 1 can be achieved. This means that the deposition rate down at the bottom of the trench is higher than at the feature opening which leads to an unexpected but highly desired bottom-up filling of the trench.

In order to trace the origin of this phenomenon and for a controlled application of this special behavior we have developed a new simulation model for As-doped poly-silicon deposition. The model takes into account surface coverage dependent sticking coefficients, surface coverage dependent As incorporation and desorption rates, and Langmuir type time-dependent surface coverage. In addition the in-situ doping of the deposited film is traced.

2 Model Setup

The model is based on the coupling between topography simulation and diffusion and reaction modeling carried out with the partial differential equation solver AMIGOS [1]. The most important expansion to the former works presented in [2] is the introduction of a time-dependent surface coverage. Due to the special surface chemistry of the process, assumptions for a fast achievement of a steady-state surface coverage did not hold any longer and a rigorous time-dependent calculation of the surface coverage was required. In contrast to the concentrations of the reactive gas species, the surface coverage is only defined and meaningful at this boundary of the simulation domain, which represents the feature surface. Therefore an overall formulation of the model was designed, where the surface coverage process is specified in a separate boundary model.

The relevant gas species for the poly-silicon deposition process are AsH_3, SiH_4, and SiH_2. Transport of the reactants in the high-pressure regime of some 10 Torr is charac-

terized by the diffusion equation

$$\frac{\partial c_i}{\partial t} = \frac{\partial}{\partial x}(D_i \frac{\partial}{\partial x} c_i), \tag{1}$$

where i stands for the three types of reactants. The deposition velocity is governed by an adsorbed arsenic inhibition layer. The kinetics of the layer formation are given by

$$\frac{\partial C_s}{\partial t} = \eta_{\text{AsH}_3} \Gamma_{\text{AsH}_3} - k_s C_s - k_d C_s, \tag{2}$$

where C_s is the arsenic surface coverage, and η_{AsH_3} and Γ_{AsH_3} denote arsenic sticking coefficient and flux, respectively. k_d is the rate constant of arsenic desorption from the protective layer and k_s the incorporation rate of arsenic from the layer into the deposited poly-silicon film. The sticking coefficients for AsH_3 and SiH_4 are defined as

$$\eta_{\text{AsH}_3} = \eta_{\text{AsH}_3}^0 (1 - C_s/C_0) \qquad \text{and} \qquad \eta_{\text{SiH}_4} = \eta_{\text{SiH}_4}^0 (1 - C_s/C_0), \tag{3}$$

where $\eta_{\text{AsH}_3}^0$ and $\eta_{\text{SiH}_4}^0$ are the clean surface sticking probabilities and C_0 is the number of available surface sites for arsenic adsorption. The sticking coefficient of SiH_2 was assumed to be unity. The final deposition rate has three contributions, namely poly-Si deposition from surface reactions of SiH_2 and SiH_4 at the unprotected surface and the incorporation of As from the adsorption layer. Thus, the resulting deposition rate DR is given by

$$\text{DR} = \eta_{\text{SiH}_4} \Gamma_{\text{SiH}_4} + \eta_{\text{SiH}_2} \Gamma_{\text{SiH}_2} + k_s C_s. \tag{4}$$

Again, η_i denote the sticking probabilities and Γ_i the corresponding fluxes. Coupling between gas concentrations c_i within the reactor space and the fluxes Γ_i towards the surface is given by the relations

$$\Gamma_i = \frac{1}{4}\nu_i c_i \qquad \text{with} \qquad \nu_i = \sqrt{\frac{8kT}{\pi m_i}}. \tag{5}$$

Thereby, ν_i is the average molecular velocity of gas species i with a molar mass m_i.

The modeling equations described above result in a set of partial differential equations for the concentrations of the reactants and the surface coverage which is iteratively solved for the profile evolving with time. Most importantly, by tracing the actual surface coverage the model allows to monitor the arsenic incorporation into the poly-Si film and thus to trace the in-situ doping of the deposited layer.

The boundary condition for the model are the concentrations of the reactants on top of the simulation domain. Since the presence of arsenic determines the protective film formation and thus the behavior of the deposition rate, the most important influence is given by the AsH_3 partial pressure.

3 Simulation Results

The simulation results for a 0.1 μm wide and 7 μm deep trench in Fig. 1 demonstrate the effect of increasing AsH_3 partial pressure (from left to right) which is controlled by the AsH_3 flow.

When no or little AsH_3 is present (left) no inhibition of the surface reaction is given and the usual step coverage < 1 and severe void formation are observed. With addition
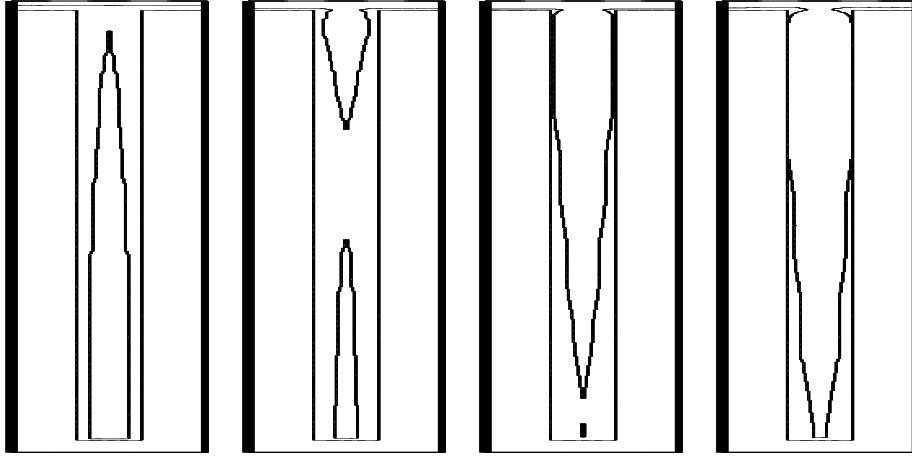
Fig. 1: Profile evolution of As-doped poly-Si deposition with AsH_3 partial pressure increasing from left to right. Note the distorted aspect ratio of the figures, originally it is 0.3 to 7.35 μm.

of AsH_3 an inhibiting layer is formed at the trench opening, lowering the deposition rate but shifting the effect of void formation to a lower region in the trench. With an even higher addition of AsH_3 the deposition is retarded in the complete trench but in the upper part with the higher As concentration more than in the lower part. Bottom-up filling is reached. Still increasing the AsH_3 partial pressure amplifies this effect but the possibility of the formation of a small overhang at the trench opening is given by SiH_2 contributions which under these process conditions become the predominant fraction of the deposition rate. Note that increasing the AsH_3 partial pressure results in stronger inhibition layer formation which reduces the deposition rate. Therefore longer deposition times are necessary to obtain a film thickness of 100 nm, to which the simulations are scaled. The deposition times range from 15 s to 180 s.
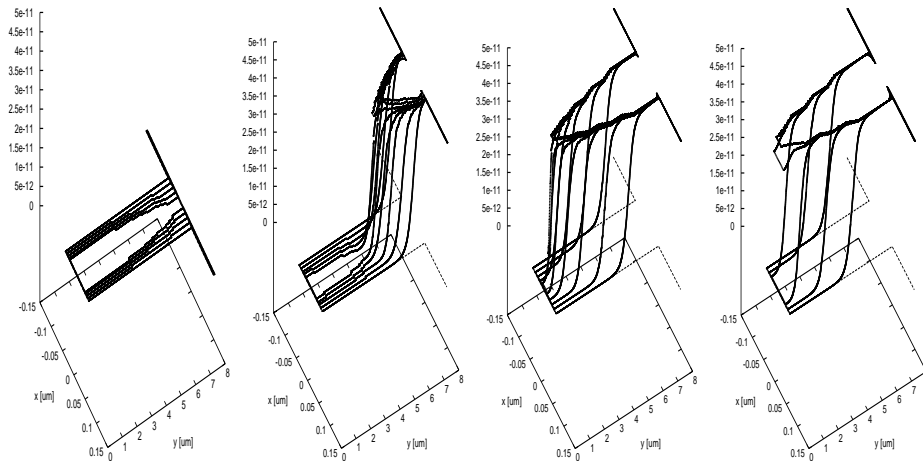

Fig. 2: As incorporation rates corresponding to the profiles from Fig. 1

In Fig. 2 the As incorporation rate corresponding to the profiles from Fig. 1 is shown. It is proportional to the surface coverage prevailing in the different trench regions and represents a measure for the in-situ doping of the deposited film. The figures also suggest that for low AsH_3 flows the surface coverage is concentration limited, whereas it is time limited for higher flows. Concentration limited (the two figures on the left hand side) means that the available As is completely consumed by the layer formation in the upper region of the trench. Even for longer times no significant surface coverage can be observed at the bottom of the trench. Time limitation for higher flows (two figures on the right hand side) means that enough As is present for covering the complete trench, just it takes some time until the As has diffused into the lower regions of the trench.

4 Discussion

The simulation results from above clearly show that the formation of a surface coverage layer has the strongest influence on the profile evolution. The surface layer formation is determined by the amount of As reaching the surface, which in the presented model is determined by three parameters, namely the concentration of AsH_3 on top of the simulation domain (Dirichlet boundary condition), the height of the simulation domain and the transport velocity, given by the diffusivity. Assessing these parameters is crucial for the simulation. In addition, the simulation domain has been split up into two regions for Knudsen diffusivity within the trench (the characteristic diffusion length is determined by the trench diameter) and regions with higher diffusivities outside the trench (boundary layer). This should allow for a more realistic approach of the transport phenomena and for an easier calibration of the parameters.

The simulations shown above demonstrate the fundamental effects of surface layer formation on profile evolution and therefore assume only a very thin boundary layer. Thus the ideal AsH_3 flow obtained from the simulations slightly differs from the experimentally observed one. It should be possible to further reduce this difference by an accurate calibration of the transport parameters from reactor scale (AsH_3 inlet gas flow) to the feature scale concentrations in the boundary layer and close to the trench surface.

5 Conclusion

We have shown that by introducing Langmuir type time-dependent surface coverage into CVD modeling it is possible to simulate the bottom-up filling behavior of As-doped poly-silicon trench filling. Furthermore, the rigorous treatment of the time-dependent surface coverage allows for a monitoring of the in-situ doping of the deposited film, which is meaningful for the characterization of the electrical properties of the deposited poly-Si film. Bottom-up filling can be achieved by increasing the AsH_3 fraction in the process gas. On the other hand this increase in the AsH_3 fraction also reduces the overall deposition velocity of the process. In order to obtain a satisfactory profile evolution the right balance between decreasing void formation probability and the reduction in deposition velocity with respect to manufacturing throughput has to be found.

Acknowledgment

[1] M. Radi, E. Leitner, and S. Selberherr, "AMIGOS: Analytical Model Interface & General Object-Oriented Solver," *IEEE J.Technology Computer Aided Design*, 1999. http://www.ieee.org/products/online/journal/tcad/accepted/radi-feb99/.
[2] W. Pyka, P. Fleischmann, B. Haindl, and S. Selberherr, "Three-Dimensional Simulation of HPCVD—Linking Continuum Transport and Reaction Kinetics with Topography Simulation," *IEEE Trans.Computer-Aided Design of Integrated Circuits and Systems*, vol. 18, no. 12, pp. 1741–1749, 1999.