

Effect of Deposition Conditions on Oxide Parameters of Silicon

Souad Merabet¹, Ahlem Alioua¹ and Bilal Djellil¹

¹Laboratoire des énergies renouvelables, University of MSB Jijel, Way BP 98 Ouled Aissa, 18000 Jijel, Algeria
{smerabet, bdjellil}@univ-jijel.dz, aalioua@univ-jijel.dz

Keywords: Oxide Parameters, Diffusion Coefficient, Activation Energy.

Abstract: In this study, the effect of deposition conditions and the temperature thermal treatment on the oxide parameters of two structures of silicon layers were investigated. The study present the evolution of in situ boron profiles following a dry thermal oxidation in poly-Si/SiO₂/c-Si films deposited at 520°C and 605°C temperatures and thermally oxidized in dry oxygen at respectively temperature 840°C, 945°C and 1050°C for duration $t=1h33'$. The results show that the deposition conditions and the temperature treatment make a very important impact on the obtained films, which affect the redistribution and localization of dopants. It has been observed that the obtained value of the linear and the parabolic rate constant, the diffusion coefficient and the oxidation thickness are higher in the films deposited at $T_d = 520^\circ\text{C}$ than those deposited at $T_d = 605^\circ\text{C}$. Also, the X-ray diffraction is strongly affected by the oxide thickness deposited between poly-silicon layers and crystalline substrates.

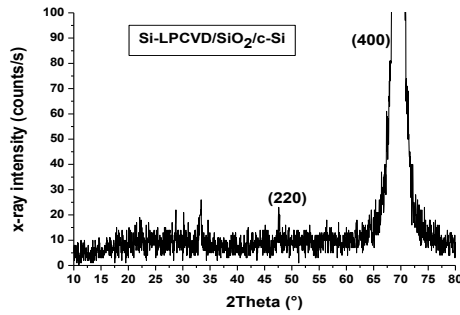
1 INTRODUCTION

Thermal oxidation enables the formation of thin, almost defect-free, and reliable silicon oxide films (Gerlach and Maser, 2016). This is the reason for the dominance of silicon in semiconductor industry in comparison to other materials (Lojek, 2005). In the last years, particular interest has been given to polycrystalline silicon films and their applications in different area such as microelectronics devices and photovoltaic cells (Sandor, Fulton, Engel-Cox, Peck, and Peterson, 2018). Oxidation kinetics in poly-silicon is mainly controlled by the presence of grain boundary and the segregation of dopants towards these boundaries (Yun, Huang, Teal, Kin, Varlamov, and Green, 2016). The oxidation of silicon is based on the migration of oxidation species through the already formed silicon oxide layer and following interfacial reactions, described by two parameters, the linear and the parabolic rate constant, respectively (Fukuda, 1997), (Hashim, et al, 2015), (Kovacevic, Pivac, 2014). These parameters are closely related to the deposition conditions and the initial surface texture of the films.

2 LAYERS STUDY

In this work, the effect of the deposition parameters of poly-silicon films obtained by LPCVD method (low pressure chemical vapor deposition), with 200 nm of thickness and doped with in situ boron ($2 \times 10^{20} \text{cm}^{-3}$), has been studied as function of the characteristics parameters of thermal oxidation such as the linear and the parabolic rate constant for a thermal treatment ranging from 840°C, 945°C and 1050°C, for duration of 1h33'. The structure of poly-silicon films has been characterized by X-ray diffraction. The measure X-ray spectra is shown in figure 1, the XRD intensity exhibit (400) peaks for the poly-silicon films. While the single-crystal was formed according to a <111> crystallographic orientation, this difference may be due to the oxide interface (poly/SiO₂/c-Si).

Figure 1: X-rays diffraction peaks of the poly-silicon layer.



3 THEORETICAL MODEL

The physical mechanism of thermal conductivity in the furnace oxidation is governing by the diffusion of oxidant species in the oxide, and the chemical reactions at the oxide-material interface. The diffusion of oxidant species in the oxide, and the chemical reactions at the oxide-material interface, in this case, the kinetic equation is expressed as (Hemeryck, 2008), (Fabien, 2018):

$$X^2 - (X_0)^2 + A(X - X_0) = B.t \quad (1)$$

Where X is the oxide thickness at time t , and X_0 is the oxide thickness at $t=0$ s.

And the linear rate constant and the parabolic rate constant are expresses by (Fukuda, Yasuda, and Iwabuchi, 1992):

$$\frac{B}{A} = C_1 \times \exp\left(\frac{-E_1}{k_B T}\right) \quad (2)$$

$$B = C_2 \times \exp\left(\frac{-E_2}{k_B T}\right) \quad (3)$$

Where C_1 (Å/s) and C_2 (Å²/s) are the pre-exponential factors depends on the thermal temperature, the thickness of layer and substrate orientation. E_1 and E_2 are activation energies for the linear and the parabolic rate constant respectively. k_B , the Boltzmann constant and T , the oxidation temperature.

The oxide thickness at the thermal oxidation can be described by the solved equation (1), expressed as (Fukuda, Yasuda and Iwabuchi, 1992):

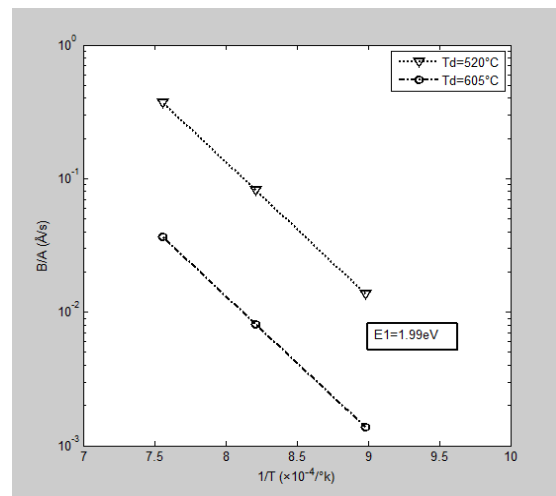
$$X(t) = \left\{ A(T) \pm \sqrt{A^2(T) + 4[X_0^2 + A(T).X_0 + B(T).t]} \right\} / 2 \quad (1)$$

$$(4)$$

4 RESULTS AND DISCUSSION

Figure 2 shows the curves of the linear and the parabolic rate constant versus $1/T$ for the thermal oxidation temperature range of 840-1050°C, for two structures of poly-crystalline silicon films with 200 nm of thickness. The growth rate shows a nearly Arrhenius-like dependence. The activation energies evaluated in curve fitting are $E_2=1.59$ eV for the parabolic rate and $E_1=1.99$ eV for linear rate respectively.

The linear rate constant is dominated by the reaction at the SiO₂/Si interface. The results show that the obtained value of the linear rate constant for films deposited at 520°C are higher than those obtained for films deposited at 605°C. This may be explained by the fact that at the interfacial zone, the first 15 nm thick for films deposited at 520°C, are amorphous. Under thermal treatment those amorphous regions crystallize, this crystallization is favored, moreover, by the higher concentration of dopants which segregate at the grain boundary, increases grain size and produces a less rough surface (Lemiti, Audisio, Mai, Balland, 1989). And the films deposited at 605°C, are polycrystalline with a small grains;



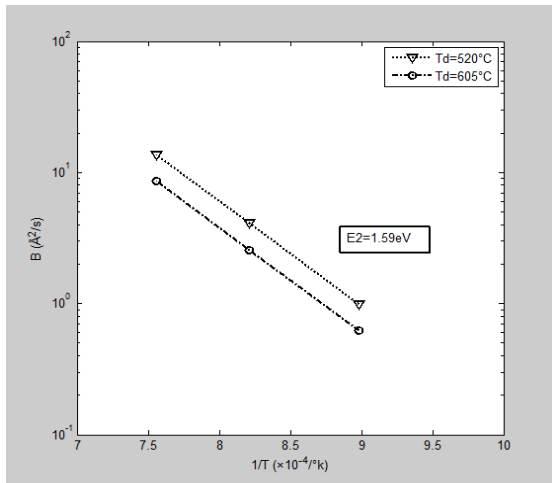


Figure 2: Arrhenius plot for the linear rate constant (B/A) and the parabolic rate constant (B). The activation energies are calculated to be E1=1.59eV and E2=1.99eV.

In figure 3, the calculation of oxide thickness was done based on the linear-parabolic oxidation model. The follow-up of the evolution of these curves shows a variation according to the deposition temperature, this can be explained by the different oxidation rate of the grains and the grains boundaries substantially alter the kinetics of oxidation. The oxidation reaction decreases when the crystalline quality of the films increases, with the decrease in the density and disappearance of the deposits intra-granular zones. Also, the difference increase as function of the temperature thermal treatment increase. For 840°C, 945°C, and 1050°C, the difference is 100Å, 200Å and 300Å respectively.

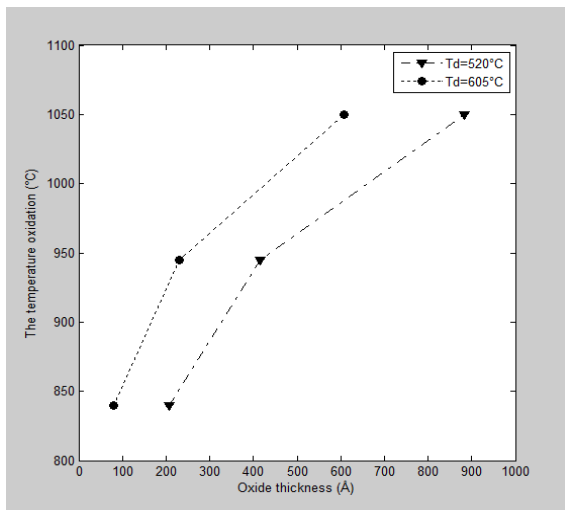


Figure 3: Relationship of oxide thickness and deposition temperature.

In order to examine the relationship between the effect of the dry thermal oxidation and the structure of the films, the in situ boron diffusion coefficient D was estimated by modelling the profiles in figure 4. The dopants will follow the limited-source diffusion process, which is governed by the following equation (Guan, et al., 2015):

$$C(x, t) = C_0(0, t) \cdot \exp\left[-\left(\frac{x}{2\sqrt{Dt}}\right)^2\right] \quad (5)$$

Where C_0 , x , and t represent the initial surface concentration, the diffusion distance, and the annealing time respectively;

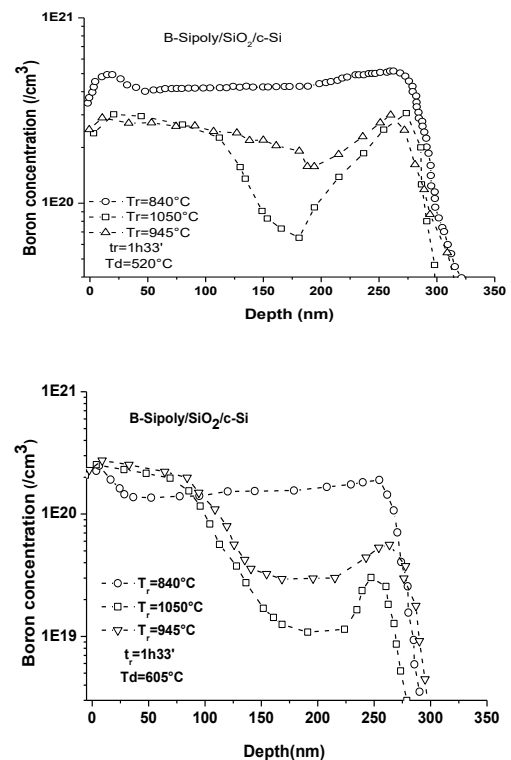


Figure 4: Experimental boron profiles after treatment annealing.

The obtained results of the diffusion coefficient of in situ boron are illustrated in Figure 5. The follow-up of the evolution of these results shows a variation according to the temperature treatment, from 840°C to 1050°C, with clear increase starting from the temperature treatment of 1050°C. Just a small variation is observed when the obtained values are compared in the two structures, but at 1050°C the results are approximately the same. This can be explained by the fact that the structures under high levels of doping and heat treatment evolve to the

same morphological structure. The same results were observed for different durations of treatment in other works (Boukezzata, Birouk, Mansour, Bielle-Daspét, 1997).

According to the results in figure 5, the variation of estimated diffusivities versus the temperature reverse enables to calculate with the Arrhenius expression low, the value of activation energy:

$$D = D_0 \cdot \exp\left(\frac{-E_a}{k_B \cdot T_{ox}}\right) \quad (6)$$

Where D_0 , k_B , and T_{ox} represent the pre-exponential diffusion coefficient, the Boltzmann constant, and the annealing temperature, respectively;

The evaluated activation energies in curve fitting are $E_a=2.32$ eV and $E_a=2.056$ eV for the films deposited at 520°C and 605°C respectively. Previous results reported by (Boukezzata, Birouk, Mansour, Bielle-Daspét, 1997), (Lemiti, Audisio, Mai, Balland, 1989), showed a good agreement with those values.

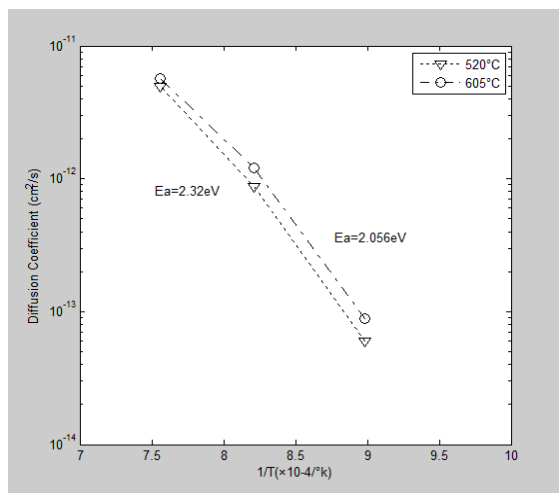


Figure 5: Relationship of diffusion coefficient and oxidation temperature.

5 CONCLUSION

In this work, we have examined the dry oxidation of poly-Si/SiO₂/c-Si layers deposited through LPCVD and doped in situ with boron. The structure of layer affect the localization and redistribution of dopant, it has been found that the value of the diffusion coefficient is more important in layer deposited at 520°C than the layer deposited at 605°C , and by comparing the obtained values for several temperatures treatment, just a small variation is observed between the two structures, and when the temperature treatment is higher (1050°C) the results are

approximately the same; this was explained by evolve structure in the same structural morphologies.

ACKNOWLEDGEMENTS

The author would like to thank Mr. M. Boukezzata for his services. This work has been supported by ministry of higher education and scientific research of Algeria.

REFERENCES

- Gerlach, G., Maser, K., 2016. A Self-Consistent Model for Thermal Oxidation of Silicon at Low Oxide Thickness, *Advances in condensed matter Physics*, Article ID 7545632
- Lojek, B., 2005. *History of semiconductor Engineering*, Springer, Berlin, Germany
- Sandor, D., Fulton, S., Engel-Cox, J., Peck, C., and Peterson, S., 2018. System Dynamics of Polysilicon for Solar Photovoltaics: A Framework for Investigating the Energy Security of Renewable Energy Supply Chains, *Sustainability* 10(1), 160
- Yun, J., Huang, J., Teal, A., Kin, K., Varlamov, S., and Green, M. A., 2016. Correlation of the crystal orientation and electrical properties of silicon thin films on glass crystallized by line focus diode laser, *Thin Solid Films*, 609 pp.12-18.
- Fukuda, H., 1997. Growth kinetics of nanoscale SiO₂ layer in a nitric oxide (NO) ambient, *Applied Surface Science*, 113-114 pp.595-599.
- Hashim, U., et al, 2015. Comparison of Deal Grove Model growth rate with Dry thermal oxidation process for ultra-thin Silicon Dioxide film, Conference paper, DOI: 10.1109/COBE.2015
- Kovacevic, G., Pivac, B., 2014. Structure, defects, and strain in silicon-silicon oxide interface, *J. Applied Physics*, vol. 115, n°4, Article ID 043531
- Hemeryck, A., 2008. Modélisation à l'échelle atomique des premiers stades de l'oxydation du silicium : Théorie de la Fonctionnelle de la Densité et Monte Carlo cinétique, Doctorate thesis, Université Toulouse III – Paul Sabatier
- Fabien, R., 2018. Study of Thermal Oxidation of SiGe for Advanced CMOS FD-SOI Technologies, Doctorate thesis, Université de Grenoble Alpes
- Fukuda, H., Yasuda, M., and Iwabuchi, T., 1992. Kinetics of Rapid Thermal Oxidation of Silicon, *Journal of Appl. Phys.* Vol. 31 pp.3436-3439
- Lemiti, M., Audisio, S., Mai, C., Balland, B., 1989. Evolution de la taille des grains du silicium polycristallin pendant des traitements thermiques ou oxydation, *Revue Phys. Appl.* 24 pp.133-141
- Guan, B., et al., 2015. Nanoscale Nitrogen Doping in Silicon by Self-Assembled Monolayers, *Scientific Reports* | 5:12641 | DOI: 10.1038/srep12641

Boukezzata, M., Birouk, B., Mansour, F., Bielle-Daspet, D., 1997. Structural and electrical changes in polycrystalline silicon thin films that are heavily in situ boron-doped and thermally oxidation with dry oxygen, Chem. Vap. Deposition vol. 3, n°5, pp.271-279