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Simulation of Doped Si Oxidation in Nano-dimension Scale

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Introduction

The fabrication of microelectronic structures and devices vitally depends on the thermal oxidation for the formation of gate dielectrics, device isolation. Particularly, the precise control of silicon dioxide thickness as device geometries continues to scale to nano dimensions [1].

In semiconductor manufacturing process observed that thickness of SiO_2 layer getting uneven when oxidizing doped Si areas by various dopants. It was defined that boron, phosphorus, arsenic determinate SiO_2 formation in thermal oxidation technological process [2].

Dimension is very important parameter in nano-technologies therefore doping dependent oxidation makes additional problems when forming nano-structures.

By using mathematical simulation program ATHENA was performed mathematical simulation of Si thermal oxidation, and was evaluated the Si substrate doping dependent oxidation.

Doping Dependent Oxidation

Experimental results explain that SiO_2 formation on highly-doped n-type and p-type substrates can be enhanced compared to SiO_2 formation on lightly-doped substrates. The dependence of silicon dioxide growth kinetics on doping concentration is manifested as part of the linear rate constant, where the physical significance of the high doping levels has been explained primarily as an electrical effect. This factor in the linear rate constant is given by

$$\left(\frac{B}{A}\right)_{doping} = \left[1 + B_{K0} \cdot \exp\left(\frac{-B_{FE}}{k_b T}\right)\left(V^* \frac{V^*}{V_i^*}\right)\right], \qquad (1)$$

where V* is the equilibrium vacancy concentration in silicon at the Si/SiO_2 interface. Vi* is the equilibrium vacancy concentration in intrinsic silicon. B_{K0} and B_{KE} relates to the doping dependence of the oxidation rate.

The equilibrium vacancy concentration, composed of vacancy defects in different charged states, depends on the Fermi level location and is given by

$$V^* = V_i^* \left\{ \frac{1 + \left(\frac{n_i}{n}\right)\phi^+ + \left(\frac{n_i}{n}\right)^2 \phi^{++} + \left(\frac{n}{n_i}\right)\phi^- + \left(\frac{n}{n_i}\right)^2 \phi^=}{1 + \phi^+ + \phi^{++} + \phi^- + \phi^=} \right\}, \qquad (2)$$

where n is the electron concentration and n_i is the intrinsic carrier concentration, and φ+, φ++, φ−, and φ= are fractions of the vacancy concentration which are positively, double positively, negatively, and double negatively charged respectively.

Figure 1 shows a plot of at for common silicon dopants. Notice that for n-type dopants (V^*/V_i^*) increases as the doping concentration increases, but V^*/V_i^* remains essentially constant for the p-type dopant. The increase in V^*/V_i^* for n-type dopants increases the linear rate constant. This ultimately leads to thicker oxides when oxidizing highly-doped n-type substrates due to a higher availability of unoccupied silicon lattice sites (vacancies) for oxidant molecules to be incorporated.

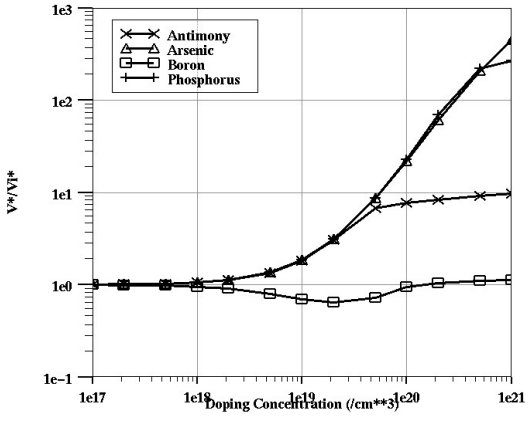


Fig. 1. Simulated V/V_i ratio versus doping concentration

The oxide thickness trend is shown in Fig. 2, where the SiO_2 thickness is plotted versus doping concentration for common silicon dopants [3].

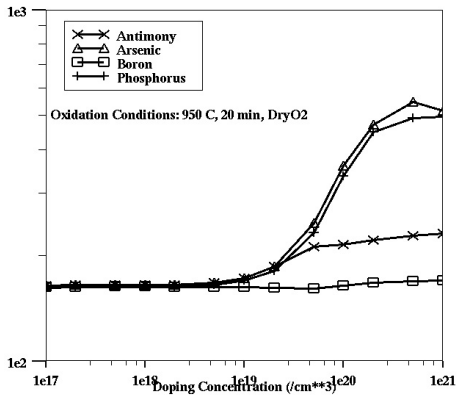


Fig. 2. Simulated silicon dioxide thickness vs. doping concentration for common silicon dopants

Oxidation of equal Si substrate

By using mathematical simulation program ATHENA [4] was performed mathematical simulation of oxidation technological process of undoped Si substrate and phosphorus doped Si substrate. Mathematical simulation results presented at Fig. 3 – 6.

Ion implantation technology was used to dope Si by phosphorus. To analyze dopants influence to SiO_2 formation, it was doped one side of Si substrate by using Si_3N_4 mask. Ion implantation dose is $3 \cdot 10^{15}$ C/cm^2, energy – 10 keV. Ion implantation mathematical simulation results presented at figure 4. Mathematical simulation results (Fig. 4) demonstrate that phosphorus dopants concentrate at right corner of Si substrate.

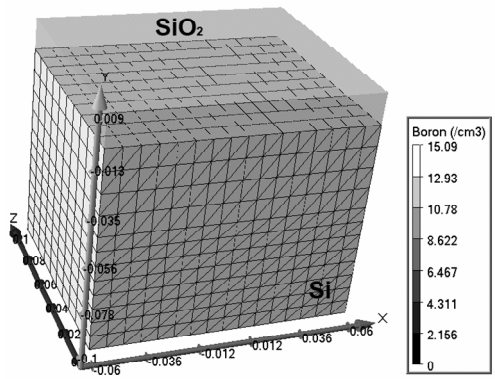


Fig. 3. Mathematical simulation results. Undoped Si oxidation: oxidation time – 1min., temperature - 1000 ^oC, ambient – wet O_2

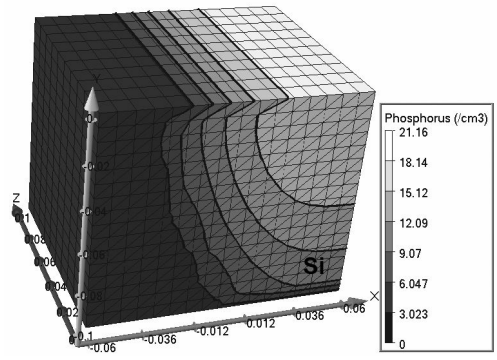


Fig. 4. Mathematical simulation results. Phosphorus implantation in to Si substrate: ion implantation dose – $3 \cdot 10^{15}$ C/cm^2, energy – 10 keV

Next step – Si surface oxidation in wet O_2 ambient. Oxidation reaction time is 1 min., temperature – 1000 ^oC. Mathematical simulation results presented at Fig. 5.

During oxidation growing SiO_2 expand up and deep in to Si substrate. This effect is very important in integral elements forming technological process.

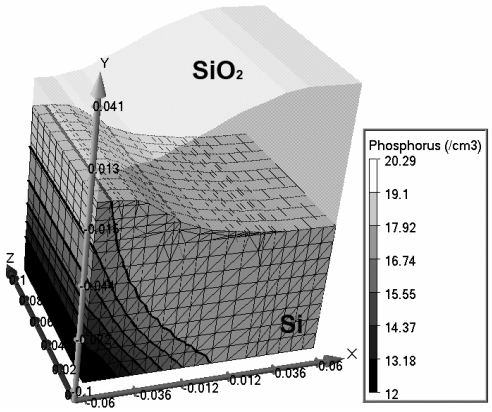


Fig. 5. Mathematical simulation results. Phosphorus doped Si oxidation: oxidation time – 1min., temperature - 1000 ^oC, ambient – wet O_2

Fig. 6 demonstrate comparison of mathematical simulation results of phosphorus doped and undoped silicon oxidation.

Mathematical simulation results demonstrate (Fig. 3-6), that dopant in Si substrate influent to SiO_2 growing form and to SiO_2 layer thickness – very important parameter. After phosphorus doped Si oxidation process formed SiO_2 thickness is ~ 60nm bigger than oxidizing undoped Si.

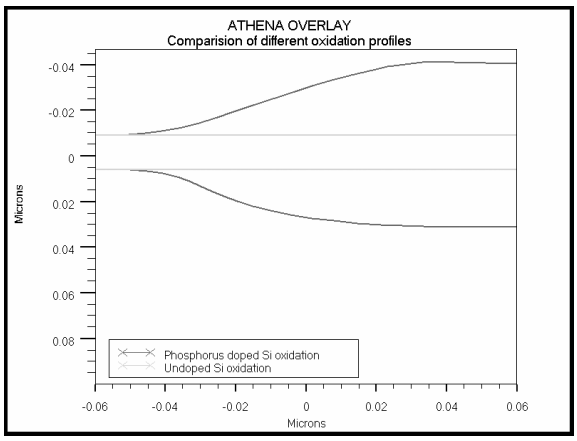


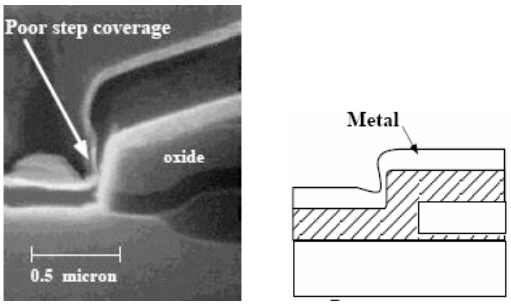
Fig. 6. Mathematical simulation results. Undoped and phosphorus doped Si oxidation results comparison

Oxidation of Si substrate with Si_3N_4 mask

Local oxidation of silicon (LOCOS) is using to isolate one integral element from another. By using Si_3N_4 mask LOCOS oxide is forming in the certain areas of Si substrate. In the course of Si oxidation oxygen molecules penetrate under the masking Si_3N_4 layer, therefore surface becomes uneven. Irregularities are rather high, up to 0.3-0.6 μm. Irregularities themselves do not increase metallization defects, however, they lift Si_3N_4 causing

cracks in it as well as impede the photolithography deposition process [5].

Inequalities of the surface getting very important in nano dimension scale because thickness of deposited layers is very small and in this case arising number of defects in the deposited layer (Fig. 7).



a) b)

Fig.7. Defect of metal deposition [6]

Simulation of oxidation technological process of Si substrate with Si_3N_4 mask it was performed by using mathematical simulation program ATHENA. In first of all it was performed undoped Si oxidation (Fig. 8) and then phosphorus doped Si oxidation (Fig. 10) to investigate the Si dopants influence to oxidation.

Ion implantation technology was used to dope Si by phosphorus (Fig. 9). Ion implantation dose is $3 \cdot 10^{15}$ C/cm^2, energy – 10 keV. The less ion implantation energy is using to form nano-structures.

Impurities diffuse from high-doped regions to adjacent layers then performing oxidation. Mathematical simulation results in figures 9 and 10 demonstrate that phosphorus diffuse in to adjacent areas of Si substrate. This effect is very important when need to form p-n junctions in the particular depth [7].

Mathematical simulation results of doped and undoped Si with Si_3N_4 layer oxidation (Fig. 11) demonstrate that dopants in the Si substrate accelerate SiO_2 forming process and also accelerate SiO_2 drift under the Si_3N_4 mask. Therefore growing SiO_2 form is changing markedly, surface becomes uneven. Irregularities of surface can reach ~ 40nm.

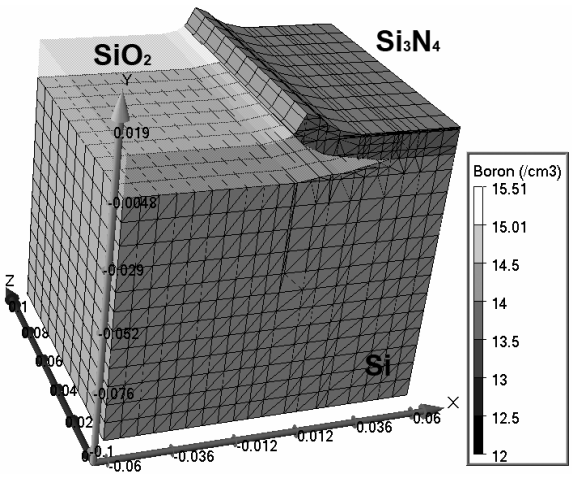


Fig. 8. Mathematical simulation results. Boron doped Si substrate oxidation with Si_3N_4 mask: oxidation time – 1min., temperature - 1000 ^oC, ambient – wet O_2

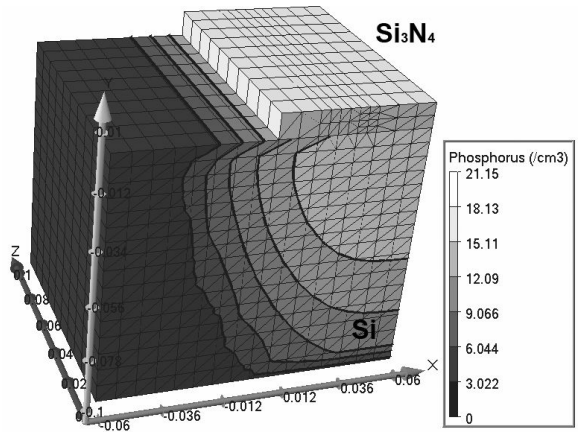


Fig. 9. Mathematical simulation results. Phosphorus implantation in to Si substrate: ion implantation dose – $3 \cdot 10^{15}$ C/cm^2, energy – 10 keV

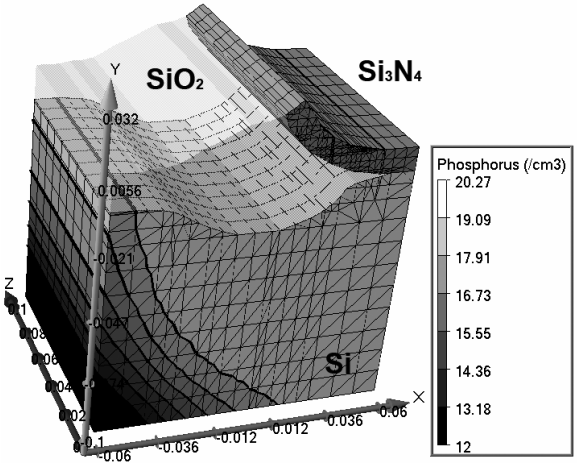


Fig. 10. Mathematical simulation results. Phosphorus doped Si oxidation with Si_3N_4 mask: oxidation time – 1min., temperature - 1000 ^oC, ambient – wet O_2

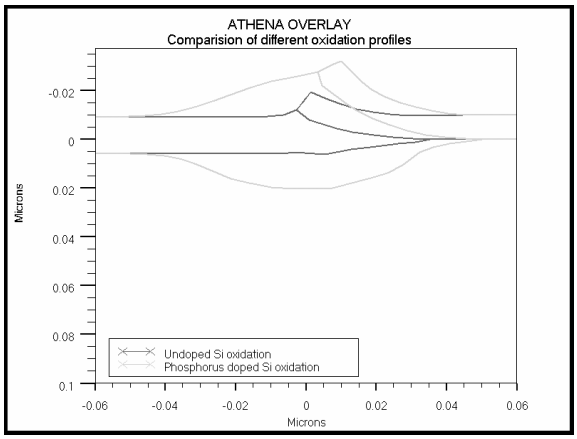


Fig.11. Mathematical simulation results. Undoped and phosphorus doped Si with Si_3N_4 mask oxidation results comparison

To prevent thermal diffusion of impurities it is purposeful in first of all to use thermal oxidation and then Si doping. In first of all Si substrate was oxidized in wet O_2 ambient 1 min at 1000 ^oC temperature. After that it was performed phosphorus doping by using ion implantation. Mathematical simulation results presented at Fig. 12.

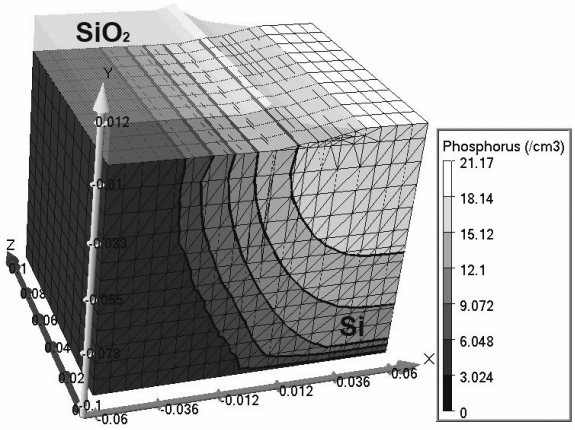


Fig. 12. Mathematical simulation results. Phosphorus doped regions forming in to oxidized Si substrate: ion implantation dose – $3 \cdot 10^{15}$ C/cm^2, energy – 10 keV

Comparison of simulation results in figures 8, 9, 10 and 14 demonstrate that more acceptable results obtaining then in first of all are using thermal oxidation and doping process after that. It is avoiding thermal diffusion of impurities and dopants influence to SiO_2 forming process. The surface of formed structure is smoother, therefore number of defects in deposited layer decreasing.

Conclusions

1. Inequalities of the surface are very important in nano dimension scale because thickness of deposited layers is very small and in this case arising number of defects in the deposited layer.
2. Dopant in Si substrate influent to SiO_2 growing form and to SiO_2 layer thickness – very important parameter. Dopants in the Si accelerate SiO_2 forming. After phosphorus doped Si oxidation process formed SiO_2 thickness is ~ 60nm bigger than oxidizing undoped Si. Surface of the structure becomes uneven and irregularities of surface can reach ~ 40nm.
3. To prevent dopants influence to SiO_2 growing and thermal diffusion of dopants it is purposeful in first of all to use thermal oxidation and then Si doping. The surface of formed structure obtaining smoother, therefore number of defects in deposited layer decreasing.

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The fabrication of microelectronic structures and devices vitally depends on the thermal oxidation. It is observed that thickness of SiO_2 layer getting uneven when oxidizing doped Si areas by various dopants. It was defined that dopants determinate SiO_2 formation in thermal oxidation technological process. Dimension is very important parameter in nano-technologies therefore doping dependent oxidation makes additional problems when forming nano-structures. By using mathematical simulation program ATHENA was performed mathematical simulation of Si thermal oxidation, and was evaluated the Si substrate doping dependent oxidation. Ill. 12, bibl. 7 (in English; summaries in English, Russian and Lithuanian).

Т. Кяршис, Р. Анилёнис, Д. Эйдукас. Моделирование окисление легированного кремния нано структур // Электроника и электротехника. – Каунас: Технология, 2008. – № 4(84). – С. 43–46.

В изготовлении полупроводниковых приборов чаще всего используется технологический процесс окисления кремния. Установлено что после процеса окисления легированного кремня полученный SiO_2 слой бывает неровный, что примеси кремния влияют на получение SiO_2. В легированных местах кремния SiO_2 получается толще. Это может вызывать дополнительныя затруднения в формировании наноструктур. Используя программу математического моделирования ATHENA, было произведено моделирование технологических процессов окисления кремния. Произведён анализ влияния примесей на процесс окисления кремния применяемого в производстве наноструктур. Ил. 12, библ. 7 (на английском языке; рефераты на английском, русском и литовском яз.).

T. Keršys, R. Anilionis, D. Eidukas. Legiruoto Si oksidavimo nanomatmenų lygmenyje matematinis modeliavimas // Elektronika ir elektrotechnika. – Kaunas: Technologija, 2008. – Nr. 4(84). – P. 43–46.

Si oksidacijos technologinis procesas plačiai taikomas integrinių grandynų gamybos technologijose. Pastebėta, kad oksiduojant legiruotas Si paviršiaus vietas susidarantis SiO_2 sluoksnio storis gaunamas nevienodas. Nustatyta, kad Si esančios priemaišos turi įtakos SiO_2 susidarymui. Oksiduojant legiruotas Si sritis susidariusio SiO_2 storis šiose vietose yra didesnis, o tai gali sukelti papildomų sunkumų formuojant nanostruktūras. Pasinaudojus matematinio modeliavimo programa ATHENA buvo atliktas oksidacijos technologinio proceso matematinis modeliavimas. Ištirta Si legiravimo priemaišomis įtaka oksidacijos technologiniam procesui, taikomam nanostruktūrų gamyboje. Il. 12, bibl. 7 (anglų k.; santraukos anglų, rusų ir lietuvių k.).