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Rational Parameters Selection Influence to the Adequate Selection Algorithm by Estimating Local Oxide Influence

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Introduction

The production process is a sequence of operations in order to obtain the implementation of the elements or integrated structures with the necessary performance characteristics of the very large scale integration or ultra large scale integration. The characteristics of the element during the formation of integrated elements of integrated structure intended to not impair. In this case the manufacture of integrated circuits focuses on the area where the integrated element is being formed. It is essential that the area dimensions at the beginning of the technological processes must be kept the same during the whole technological process. The main aim is to maintain unchanged characteristics of the three-dimensional structure using local oxidation technology for isolation of integrated elements and to verify if the three-dimensional integrated element fits into the integrated circuits.

The main objective of this series of papers is to examine and evaluate the adequate selection of the three-dimensional integrated element in the three-dimensional integrated circuits, modeling of the thermal oxidation using mathematical models.

The main aim of this paper is to define rational parameters of local oxidation process in the three-dimensional structures.

Finite element method in the simulation of the process of local oxidation of silicon

Application of finite element method is conditioned by thermodynamic processes of oxidation, which are connected by Si, SiO_2 and oxidants molecules [1–4].

For the definition of the model consider Fig. 1 as computation domain Ω which consists of a pure silicon dioxide range Ω_1, an interface range Ω_2 with a mixture of silicon and silicon dioxide, a pure silicon range Ω_3 and a nitride mask Ω_4 that is defined on a separate mesh and is connected to Ω_1 via boundary Γ_4 to transmit mechanical displacements [4, 5].

For the nitride mask an elastic model is used to calculate its stress-strain contribution. To describe the different phases of oxygen within the domain $\Omega_1 \cup \Omega_2 \cup \Omega_3$ a generation/recombination rate of oxygen

$$R_{O_2} = k_x \left(1 - \eta(x,t)\right) \cdot C_{O_2}, \tag{1}$$

here C_{O_2} – oxygen concentration at./cm^2; k_x – oxygen recombination rate constant; η – function of a normalized silicon dioxide concentration related to the C_{SiO_2} concentration of silicon in pure crystal

$$\eta = j\left(\frac{C_{SiO_2}(x,t)}{C_{Si_0}}\right), \tag{2}$$

here C_{Si_0} – silicon concentraton in the crystal; C_{SiO_2} – concentration of silicon oxide, at./cm^2. η varies between one (pure silicon dioxide) and zero (pure silicon). The level function describes a jump in the material in case of a huge parameter ac:

$$f(ac, x) = 0{,}5 + \frac{\operatorname{atan}(ac \cdot x)}{\pi} \quad \text{with } ac \to \infty. \tag{3}$$

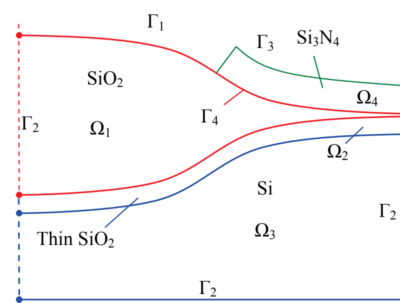


Fig. 1. Domain and boundary location [3]

In contrast to previous approaches the transition zone can now be calculated as an immediate jump from zero to

one within one element. The accuracy of mathematical simulation method depending from finite element meshes spacing and form correct description of imputing parameters such as mechanical and physical materials characteristic used in the model.

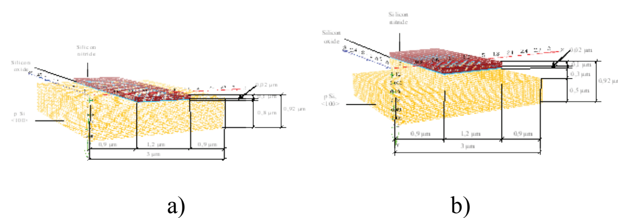
The main problem in the thermal silicon oxidation process – diffusion impurities in the lower doped layers, leading to redistribution of diffuse areas and characteristics of the three-dimensional integrated structures.

To ensure minimum impact on three-dimensional integrated element the local thermal oxidation must take place under conditions which allow the minimum deviation of characteristics of the integrated structures from the designed ones. Rational conditions of thermal oxidation process can be achieved with sustainable technological and structural parameters, such as oxidation time, temperature, thickness of silicon nitride mask and SiO_2 (P_{O2}=1 atm).

ATHENA program of mathematical simulation software package TCAD is used for mathematical structures simulation. It is adapted to the specific case of simulation using subprograms.

Local oxide profile is influenced by time and temperature of the process, the thickness of nitride mask and SiO_2 leading to the specific parameters of the integrated elements. Each of these parameters affects the type of LOCOS formation, stress distribution, lift-up nitride mask, lateral oxide under the silicon nitride mask, thin oxide form in the three-dimensional structures. Simulation was carried out in accordance with the model structure.

Mathematical structures are created using the finite element method for local thermal oxidation process simulation. Mathematical structures consist of a silicon substrate (thickness – 0,8 µm), crystallographic plane orientation <100>, a silicon oxide (thickness – 0,02 µm) and silicon nitride (thickness – 0,1 µm). The area (1,2 µm) committed for the three-dimensional integrated element and areas for thermal oxide are formed (Fig. 2., a). Another mathematical structure is created for the fully recessed local thermal oxidation process with etched 0,3 µm deep cavity (length – 0,9 mm). The area (1,2 µm) committed for the three-dimensional integrated element is formed (Fig. 2., b).



a) b)

Fig. 2. Mathematical models: a – for semi-recessed LOCOS; b – for fully recessed LOCOS

The parameters of three-dimensional integrated element and three-dimensional integrated structure changes due the thermal technology, whose are difficult to identify and evaluate during the production. In this case the major human and material resources required, that's why a mathematical simulation of technological processes adapting methods is used.

The assessment of alternation parameters of three-dimensional structures using the thermal local oxidation process

The assessment of time. Thermal local oxidation may last from 30 min. up to several hours and takes place under the [800–1100] °C temperature range in the three-dimensional structures. Modeling was carried out in accordance with the model structure shown in the [3, 5].

LOCOS parameter dependence on the local oxidation process time was simulated, when the oxidation temperature was T=1000 °C. Three-dimensional structures were simulated using thermal oxidation in 85-200 min. range. The most important parameter is the length of the area between locos oxides, which directly affects the formation of integrated element (IE). The concept are introduced – "the region length" (a parameter before the thermal oxidation) and "a useful length" – a parameter after the oxidation.

Maximum silicon oxide imbalances were identified at the oxidation time t=85 min., when the time interval of simulation was [85–200 min.] (Fig. 3). The increase of the thermal process duration increases stress zone and the deformation rate, which reached a maximum of t=120 min. in the three-dimensional structures, minimum – t=90 min. The stresses formed in the latter case are not as widely distributed in the local oxide in the three-dimensional integrated structures. In the case of very strong constant stresses the defects or dislocations are formed which completely destroy the structure. This is a consequence of the decline in a useful length.

At t=85 min. shaped local oxide thickness is 0,508 µm, at t=200 min. – 0,799 µm, the growth rate of ~ 2,53 nm/min. Examination of the LOCOS oxide growth dependence on time indicates that the three-dimensional structure of the simulation is least affected by extraneous factors at time t=90 min.

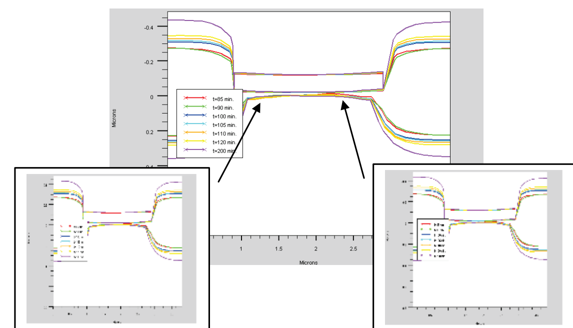


Fig. 3. Local oxide profile dependence on the local oxidation process duration (T=1000 ºC, SiO_2=0,02 µm, Si_3N_4=0,1 µm, a region length=2 µm)

It was found, that the extraneous parameter – the lateral length (L_{ox}) has linear dependence [85–100 min.] transforming to the exponential dependence in the range of [100–200 min.]. Lifting force affects silicon nitride uniformly over time and always keeps exponential dependence [85–200 min.].

The assessment of temperature. Temperature is a significant LOCOS technological parameter of oxide formation process in the three-dimensional structures. The

oxide growth rate increases at the higher temperature, because the oxygen atoms or oxygen–containing molecules move deep down through the oxide and the reaction speed depends on oxygen diffusion rate.

Three-dimensional local oxide parameters dependence on the local oxidation process temperature was simulated when the oxidation time t=90 min., temperature range from 900 ºC to 1250 °C. Simulated three-dimensional structures are presented which reflect the thermal oxidation process impact most.

After the evaluation of stress distribution the lowest degree of deformation in the structure has been achieved after thermal process at 900 ºC (Fig. 4) temperature, but the useful length is only 0,584 µm – area for IE formation is deformed, the lateral oxide and lift-up of the silicon nitride is the largest from the investigated cases: L_{ox}=0,708 µm, H_{ox}=0,0568 µm.

Three-dimensional local oxide thickness is recommended of 0,3 µm up to 1 µm. Thickness of local oxide formed at thermal process temperature 900 ºC is 0,209 µm, in this case it is needed to increase the temperature of the thermal process, otherwise impurities redistribute in the source and drain regions and significantly increase the parasitic capacitance between source and drain regions in the three-dimensional structure.

According to the simulation results the minimum lateral oxide and lift-up of the silicon nitride masks (L_{ox}=0,301 µm, H_{ox}=0,024 µm) is characteristic to the structure simulated at the oxidation temperature of 1100 ºC. Local oxide thickness – 0,763 µm, useful length – 1,398 µm. Growth rate variation (from 900ºC to 1100 ºC) ~ 2.77 nm/°C.

In the process of local oxidation the lateral oxide length has no linear dependence in the range [900–1100 °C], as opposed in the [1100–1250 °C] temperature range. Silicon nitride is acting lifting-up force and uniformly always keeps exponentially decreasing function over time dependence on simulating [900–1050 °C] the range, and in [1050–1250 °C] temperature range of growing unevenly.

The assessment of thin silicon oxide thickness. The exchange of variable "A" [3] of the silicon oxide thickness formed before the oxidation process, effects for LOCOS were simulated in three-dimensional structures.

It was found from the simulation results that the silicon oxide formed before the oxidation process practically does not affect local oxide thickness (Fig. 4): at 0,01 µm – the thickness of LOCOS 0,488 µm, when 0,03 µm – 0,493 µm i.e. 1% increase in local oxide thickness. If silicon oxide is thinner before oxidation, the higher deformation forces affect the LOCOS oxide after oxidation. Silicon oxide thickness (formed before oxidation) increase of 0,01 µm and lateral oxide length increased by 14% reduces the useful length by 28%, because the oxygen diffusion through the oxide also formed lateral oxide under Si_3N_4 mask. Plastic deformation begins (Fig. 4) and stresses are greater below the oxide edge resulting in a destroyed three-dimensional integrated structures. The longest useful length 1,294 µm was obtained when SiO_2=0,01 µm. If SiO_2 thickness change by 0,01 µm, useful region length shorten from 1,294 µm (SiO_2=0,01 µm) to 0,97 µm (SiO_2=0,03 µm), i.e. 25%.

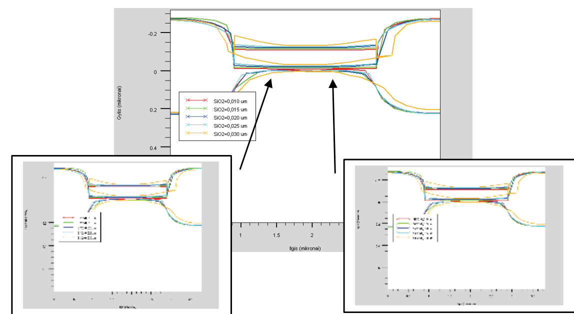


Fig. 4. Local oxide profiles dependence on the silicon oxide thickness, formed before the oxidation process (t=90 min, T=1000 ºC, Si_3N_4=0,1 µm, region length=2 µm)

For three-dimensional integrated structure and its three-dimensional elements (if it's the field-effect transistor) the assessment of a silicon oxide thickness could be impacted by the mathematically calculated output characteristics (Fig. 5).

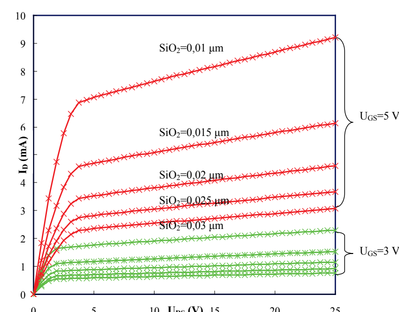


Fig. 5. MOS transistor output characteristics (L=0,5 µm, B=3 µm, U_{GD}=(3V, 5V), U_{DS}=25V, U_{tr}=1V) dependence on the silicon oxide thickness, formed before the oxidation process (SiO_2 [0,01÷0,03] µm, t=90 min, T=1000ºC, Si_3N_4=0,1 µm, region length=2 µm)

It was found that the output current is reduced three times if the oxide thickness is increased from 0,01 to 0,03 µm.

Since the gate voltage increases the the electron concentration in the channel increases also, when the thickness of the silicon oxide is 0,01 µm the output current is 6.97 mA. If the voltage $U_{GD} = U_{GS} - U_{DS}$ falls below the threshold voltage, the inversion layer disappears near the drain, but current flow through the transistor continues: channel drifting electrons reach the end of the channel layer and the output current reaches 9,207 mA, when U_{DS} = 25V i.e. increase of 25%.

The assessment of silicon nitride mask thickness. There are important technological and structural parameters during the production processes in the three-dimensional integrated structures. It is necessary to evaluate silicon nitride layer influence on LOCOS formation.

It is difficult to prevent oxygen diffusion through the oxide and lateral oxide under Si_3N_4 mask is formed during the thermal oxidation. Thicker silicon nitride layer is formed by the thermal processes which make the lower potential to nitridation process. The formation of thinner silicon nitride mask creates greater opportunities to formation of lateral oxide, i.e., to greated lift-up of the

silicon nitride mask edge. Formed stress reaches ~ $3{,}25 \cdot 10^8$ Pa throughout the area, a useful length – 0,994 μm (L_{ox}=0,503 μm, H_{ox}=0,0492 μm) (Fig. 6).

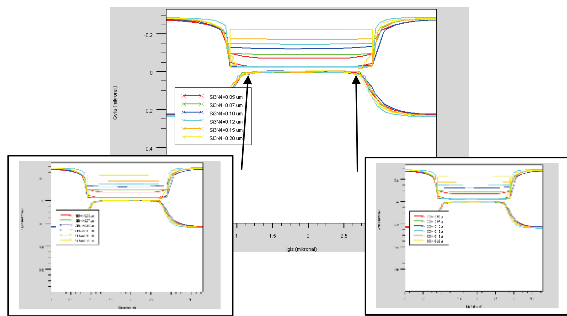


Fig. 6. Three-dimensional local oxide parameters dependence on the silicon nitride thickness (t=90 min, T=1000 ºC, SiO_2=0,02 μm, region length=2 μm)

It was received that minimal stresses (10^8 Pa) act when nitride thickness is at 0,10 and 0,12 μm; here the opposite polarity stresses strongly dominate.

It was found that a region length is 2 μm before oxidation and the maximum useful area length – 1,184 μm was met with nitride mask thickness of 0,1 μm; minimum – 0,806 μm in the nitride mask thickness of 0,12 μm. L_{ox} parameter does not have exponentially decreasing dependence of H_{ox} parameters in the three-dimensional integrated structures. Theoretically two exponential curves are expected, but such dependence can be eliminated in simulation results by lateral oxidation and strong structural deformation.

It was found during the modeling using program ATHENA that rational parameters of the thermal process creating the LOCOS in the three-dimensional integrated structures are t=90 min, T=1100 ºC, SiO_2=0,02 μm, Si_3N_4=0,1 μm. They allow to increase the integration degree, quick-action, reduce parasitic capacitances, the stresses, create maximum useful length in the three-dimensional integrated structures.

Conclusion

1. The finite element method was used to create structures – the three-dimensional MOS and V-MOS transistors, which estimates redistribution of impurities caused by thermal oxidation process in integrated three-dimensional structure.
2. Redistribution of impurities in the thermal process is very important for the production of three dimensional integrated structures of increasingly higher integration degree.
3. It was found during the modeling that rational parameters of the thermal process creating the LOCOS in the three-dimensional integrated structures are t=90 min, T=1100 ºC, SiO_2=0,02 μm, Si_3N_4=0,1 μm.

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The production process is a sequence of operations in order to obtain the implementation of the elements or integrated structures with the necessary performance characteristics of the very large scale integration. In this case the manufacture of integrated circuits focuses on the area where the integrated element is being formed. It is essential that the area dimensions at the beginning of the technological processes must be kept the same during the whole technological process. Rational parameters are defined of the thermal process simulation, creating the LOCOS, where the t=90 min, T=1100 ºC, SiO_2=0,02 μm, Si_3N_4=0,1 μm (P_{O2}=1 atm) in the three-dimensional integrated structures. Ill. 6, bibl. 5 (in English; summaries in English, Russian and Lithuanian).

Д. Андрюкайтис. Влияние рациональных параметров к адекватному алгоритму по оценке влияния термического оксида // Электроника и электротехника. – Каунас: Технология, 2010. – № 3(99). – С. 27–30.

Технологический процесс производства – это реализация отдельных операций с целью получить интегральные элементы микросхем. При производстве микросхем особое внимание уделяется области подложки, в которой и формируется интегральный элемент. Необходимо, чтобы эта область сохраняла свои параметры во всем технологическом процессе производства. При моделировании процесса оксидирования (LOCOS) установлен рациональный режим, который содержит такие условия: t=90 мин, T=1100 ºC, SiO_2=0,02 мкм, Si_3N_4=0,1 мкм. Ил. 6, библ. 5 (на английском языке; рефераты на английском, русском и литовском яз).

D. Andriukaitis. Racionalių parametrų įtaka atitikties algoritmui įvertinant terminio lokaliojo oksido poveikį // Elektronika ir elektrotechnika. – Kaunas: Technologija, 2010. – Nr. 3(99). – P. 27–30.

Gamybos technologinis procesas yra atskirų operacijų atlikimas, siekiant gauti reikiamų parametrų integrinių grandynų elementus. Todėl gaminant integrinius grandynus daug dėmesio skiriama sričiai, kur formuojamas integrinis elementas. Būtina, kad technologinių procesų pradžioje palikta atitinkamų matmenų sritis išlaikytų savo parametrus viso technologinio proceso metu. Modeliuojant nustatyti terminės oksidacijos proceso (LOCOS) racionaliausi parametrai: t=90 min, T=1100 ºC, SiO_2=0,02 μm, Si_3N_4=0,1 μm (P_{O2}=1 atm). Il. 6, bibl. 5 (anglų kalba; santraukos anglų, rusų ir lietuvių k.).

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