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Thermal Oxidation in LOCOS, PBL and SWAMI Micro and Nano Structures

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Introduction

Bipolar technology has been used in a wide range of processing and communications area. However, low cost of CMOS technology has replaced bipolar technology. CMOS technology was started off by complementing bipolar technology in the entry and mid-range systems. CMOS technology uses only energy when signals change, thus reducing operating and cooling requirements by more than 50% compared with conventional bipolar technology. Lower power consumption means less cost. Neighboring element isolation is significant point of cumulative integration degree in CMOS technology [1].

Thermal oxidation is one of various methods used for neighboring element isolation. During thermal oxidation silicon forms a perfect oxide – SiO_2. Silicon dioxide [2] is a high-quality electrical insulator and can be used as a barrier material during impurity implants or diffusion, for electrical isolation of semiconductor device technology, as a component in MOS/CMOS structures, or as an interlayer dielectric in multilevel metallization structures such as multichip modules [3].

In MOS/CMOS structures regions between the active elements must be isolated [4]. LOCOS *(Local Oxidation of Silicon)*, PBL *(Poly-Buffered LOCOS)*, SWAMI *(Side Wall Masked Isolation)* technologies are composite isolation methods, which are formed using thermal oxidation [5].

The main purpose of this paper is to analyze stress, which appears during thermal oxidation in mentioned above micro and nano scales technologies. Using thermal oxidation conversion of micro scale into nano scale isn't the same as reducing structures dimensions and technological parameters N times if integration degree of integrated circuit (IC) is N in these technologies.

Thermal oxidation

The formation of SiO_2 on a silicon surface is most often accomplished through a process called thermal oxidation. Thermal oxidation is a technique that uses extremely high temperatures (usually between 700 – 1300 ºC) to promote the growth rate of oxide layers.

The oxide thickness is an important parameter for the oxidation process. Oxide growth rate is affected by time, temperature, and pressure. Oxide growth is accelerated by an increase in oxidation time, oxidation temperature or oxidation pressure. Other factors that affect thermal oxidation growth rate for SiO_2 are: the wafer's doping level, the presence of halogen impurities in the gas phase, the presence of plasma during growth and the presence of a photon flux during growth, the crystallographic orientation of the wafer.

There are two types of the thermal oxidation of SiO_2. This type depends on which oxidant type is used (O_2 or H_2O):

1. Dry oxidation (the oxidant is O_2):

$$Si_2(solid) + O_2(vapor) = SiO_2(solid). \quad (1)$$

2. Wet oxidation (the oxidant is H_2O):

$$Si_2(solid) + 2H_2O(vapor) = SiO_2(solid) + 2H_2. \quad (2)$$

Due to the relationships in these reactions and the difference between the densities of silicon and silicon oxide, approximately 44% of the silicon surface is "consumed" during oxidation [6]. For every 100 nm of SiO_2 growth, about 44 nm of silicon is "consumed" (Fig. 1), (3).

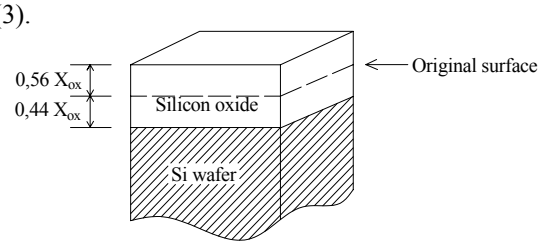

Fig. 1. Thermal oxidation

$$\frac{Thickness\ of\ Si}{Thickness\ of\ SiO_2} = \frac{Molar\ volume\ (Si)}{Molar\ volume\ (SiO_2)} =$$

$$= \frac{\dfrac{Molecular\ weight\ (Si)}{Density\ (Si)}}{\dfrac{Molecular\ weight\ (SiO_2)}{Density\ (SiO_2)}} = \frac{\dfrac{28{,}9\ g/mol}{2{,}33\ g/cm^3}}{\dfrac{60{,}08\ g/mol}{2{,}21\ g/cm^3}} = 0{,}44. \quad (3)$$

The growth of silicon oxide is the reaction of surface only – after the SiO_2 thickness begins to build up, the arriving oxygen molecules must diffuse through the growing silicon dioxide layer to get to the silicon surface in order to react. As a result, the chemical reaction occurs at the Si – SiO_2 surface.

Silicon thermal oxidation process consists of:

1. the diffusion of oxidant species through the silicon dioxide;
2. the reaction of Si and O_2 at the Si/SiO_2 interface that consumes silicon and generates new silicon dioxide;
3. the deformation of the entire structure to comply with the new geometry changes.

The Deal-Grove model

The Deal-Grove model of oxidation is used for the oxide growth kinetics. This model is generally valid for temperatures between 700 ºC and 1300 ºC, partial pressures between 0,2 and 1,0 atmospheres, and oxide thicknesses between 25 and 2000 nm for both wet and dry oxidation. Oxides thicker than 1000 nm require long exposures to very high temperatures and this will lead to dopant diffusion in the wafer that is often undesired.

In general case the growing silicon oxide thickness has following curve form (Fig. 2).

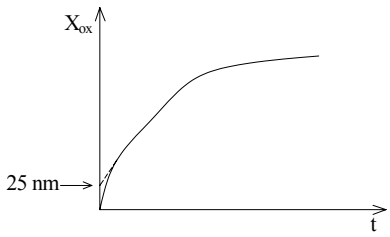

Fig. 2. Silicon oxide thickness dependence on time

The reaction of Si surface effectively stops and the oxide will not get much thicker than 2,5 nm at room temperature. The silicon wafer must be heated in the presence of an oxidizing ambient to occur an uninterrupted reaction. If the ambient is O_2, then the growth rate at the Si – SiO_2 interface is R [4]:

$$R = \frac{Hk_s P_g}{N_i(1 + \frac{k_s}{h} + \frac{k_s t_{ox}}{D})}, \quad (4)$$

where H – Henry's gas constant; k_s – the constant of proportionality; P_g – the ideal gas constant; t_{ox} – time of oxidation; D – diffusivity; N_i – the half the number density of oxygen atoms in SiO_2 ($2{,}2 \cdot 10^{22}$ cm^{-3}); $h = h_g / HkT$, h_g – mass transport coefficient; k – Boltzmann's constant; T – absolute temperature.

The Deal-Grove model exactly predicts that the oxidation rate slows as the oxide thickens.

For oxidation processes have very long durations, the rate of oxide formation may be modeled by the Parabolic Growth law:

$$X_0^2 = Bt_{ox}, \quad (5)$$

where X_0 – the thickness of the growing oxide; B – the parabolic rate constant, t_{ox} – the oxidation time.

This formula shows that the oxide thickness grown is proportional to the square root of the oxidizing time, which means that the oxide growth is disturbed as the oxide thickness increase. This is because the oxidizing fractions have to travel a greater distance to the Si – SiO_2 interface as the oxide layer thickens.

If oxidation processes have very short durations then it maybe modeled by the Linear Growth law:

$$X_0 = C(t_{ox} + \tau), \quad (6)$$

where X_0 – the thickness of the growing oxide; C – the linear rate constant; t_{ox} – the oxidation time; τ – the initial time displacement to account for the formation of the initial oxide layer at the start of the oxidation process.

Process simulation

Thermal oxidation process is simulated with ATHENA. ATHENA is a simulator that provides general capabilities for numerical, physically – based, two – dimensional simulation of semiconductor processing. Oxidation takes place when there is an interface between silicon (or polysilicon) and silicon dioxide or a silicon (polysilicon) surface is exposed to an oxidizing ambient. ATHENA simulates polysilicon oxidation in a very similar manner as silicon (almost all oxidation parameters for polysilicon are the same as for silicon). ATHENA also allows oxidation completely through a silicon (polysilicon) layer. This is a very important in processes (e.g., PBL) where polysilicon regions are completely consumed during oxidation. Exposed silicon surfaces usually have a thin native oxide layer, that's why ATHENA automatically deposits a thin native oxide layer on all exposed silicon (polysilicon) surfaces at the beginning of oxidation steps [7].

Oxide and nitride is as viscous flow. Oxidation process is running in water steam. Thermal oxidation process in ATHENA is based on the linear-parabolic theory of Deal and Grove model. In micro scale simulated structures are shown in Fig. 3 – 5.

Lateral oxidation can take place in LOCOS structure during thermal oxidation. In this way lateral encroachment (bird's beak) is created. Stress and dislocations less or more are created in all structures during oxidation. As see in Fig. 3 stress and defects is situated in silicon nitride, only small area of silicon oxide is defected. The main problem of this structure is that defects are situated in gate zone, where impurity and defects form voltage puncture, dielectric permittivity and others instabilities [1]. Push and pull forces are created in simulated structures:

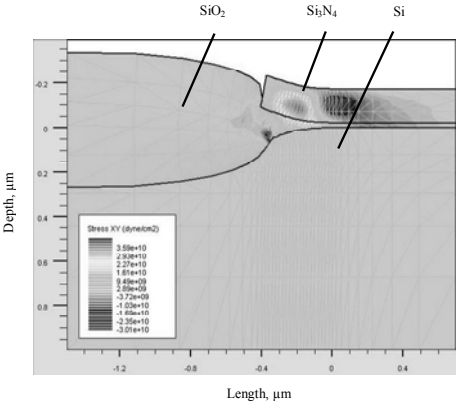

Fig. 3. Stress XY in Local Oxidation of Silicon in micro scale (t=120 min., T=1000 ºC, SiO_2=20 nm, Si_3N_4=150 nm, σ_{xy_max} – $3{,}59\cdot10^{10}$ dyne/cm^2, σ_{xy_struct} – $2{,}89\cdot10^{9}$ dyne/cm^2)

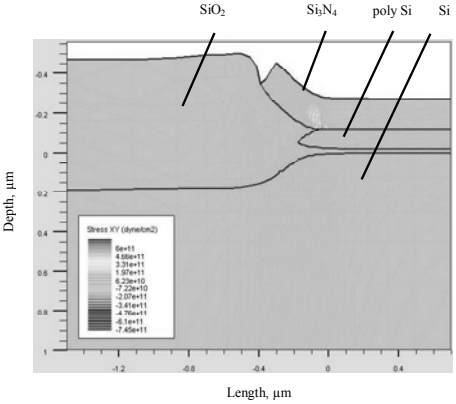

Fig. 4. Stress XY in Poly-Buffered Local Oxidation of Silicon in micro scale (t=120 min., T=1000 ºC, SiO_2=20 nm, poly Si=100 nm, Si_3N_4=150 nm, σ_{xy_max} – $6{,}05\cdot10^{11}$ dyne/cm^2, σ_{xy_struct} – $1{,}97\cdot10^{11}$ dyne/cm^2)

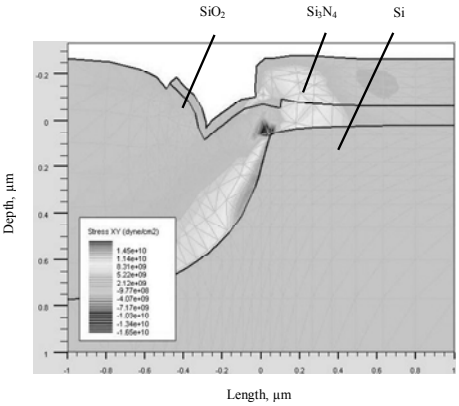

Fig. 5. Stress XY in Side Wall Masked Isolation in micro scale (t_1=4 min., t_2=500 min., T=1000 ºC, SiO_2=40 nm, Si_3N_4 (1st)=160 nm, Si_3N_4 (2nd)=40 nm, σ_{xy_max} – $1{,}45\cdot10^{10}$ dyne/cm^2, σ_{xy_struct} – (-$9{,}77\cdot10^{8}$) dyne/cm^2)

Thermally grown SiO_2 is under compressive stress and as a result reduces the substrate forces exerted by the patterned Si_3N_4 film. In addition, significant stress relaxation occurs in the LOCOS structure due to the viscoelastic properties of the oxide, σ_{xy_max} – $3{,}59\cdot10^{10}$ dyne/cm^2, σ_{xy_struct} – $2{,}89\cdot10^{9}$ dyne/cm^2. In PBL picture (Fig. 4) a polysilicon layer is inserted between the pad oxide and the Si_3N_4 layer. In this case the purpose of the polysilicon is to provide relief of the stress that builds up during the oxidation. During thermal oxidation (Fig. 4) the stress zone is very small (σ_{xy_max} – $1{,}45\cdot10^{10}$ dyne/cm^2, σ_{xy_struct} – -$9{,}77\cdot10^{8}$ dyne/cm^2), the gate zone is not modified. But the deposition conditions of the polysilicon play a very important role in the stress-relief process and lead to extensive defect formation. PBL structure is prone to substrate pitting during polysilicon removal and these two effects can cause severe gate-oxide reliability problems. That's why the Side Wall Masked Isolation is created. Lots of problems can be alleviated by using the SWAMI isolation structure. After thermal oxidation a low substrate defect density is created. In this structure σ_{xy_max} – $1{,}45\cdot10^{10}$ dyne/cm^2, σ_{xy_struct} – -$9{,}77\cdot10^{8}$ dyne/cm^2. There is no polysilicon, which cause gate-oxide reliability. Structure stress created in SWAMI is smaller than in PBL and LOCOS. Maximum stress XY created in LOCOS is greater than in SWAMI, but less than PBL.

Integration degree of IC is important in electronics technologies. Using thermal oxidation micro scale into nano scale conversion aren't the same as reduce structures dimensions and technological parameters N times if integration degree of IC is N. What happens if we reduce all dimensions and technological parameters 10 times? Results are shown in Fig. 6 – 8.

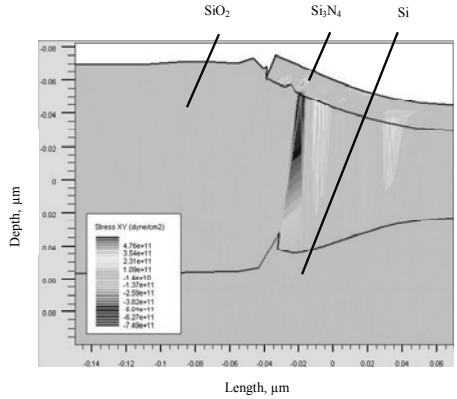

Fig. 6. Stress XY in Local Oxidation of Silicon in nano scale (t=12 min., T=1000 ºC, SiO_2=2 nm, Si_3N_4=15 nm, σ_{xy_max} – $1{,}44\cdot10^{11}$ dyne/cm^2, σ_{xy_struct} – (-$7{,}09\cdot10^{09}$) dyne/cm^2)

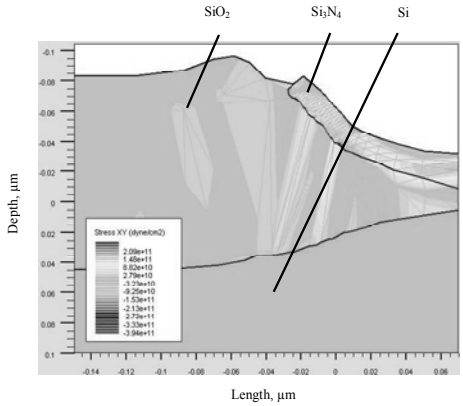

Fig. 7. Stress XY in Poly-Buffered Local Oxidation of Silicon in nano scale (t=12 min., T=1000 ºC, SiO_2=2 nm, poly Si=10 nm, Si_3N_4=15) nm, σ_{xy_max} – $2{,}09\cdot10^{11}$ dyne/cm^2, σ_{xy_struct} – $2{,}79\cdot10^{10}$ dyne/cm^2)

In LOCOS structure grown silicon oxide doesn't have isolation oxide form with attributes, gate zone is modified. The main plus is that silicon nitride is without of stress and defects (compare Fig. 3 and Fig. 6). Stress XY value is σ_{xy_max} – $1{,}44\cdot10^{11}$ dyne/cm^2, σ_{xy_struct} – -$7{,}09\cdot10^{9}$ dyne/cm^2. Grown silicon oxide has more stress and defects

(compare Fig. 4 and Fig. 7) and in this structure polysilicon has gone in deep gate zone during thermal oxidation in PBL structure (σ_{xy_max} – $2{,}09\cdot10^{11}$ dyne/cm^2, σ_{xy_struct} – $2{,}79\cdot10^{10}$ dyne/cm^2).

As mentioned above polysilicon removal can cause severe gate-oxide reliability problems. The best results are achieved with SWAMI technology, where best form and less stress (σ_{xy_max} – $7{,}26\cdot10^{10}$ dyne/cm^2, σ_{xy_struct} – $4{,}59\cdot10^{9}$ dyne/cm^2) and defects appear according to micro scale structure. In this case silicon nitride is modified a little and stress in silicon oxide appeared only in one line (Fig. 8). Structure stress created in SWAMI is smaller than in PBL and LOCOS. Maximum stress XY created in LOCOS is greater than in SWAMI, but less than PBL in nano scale structures.

When compared different structures in scale level, in nano scale all structures have greater stress than in micro scale.

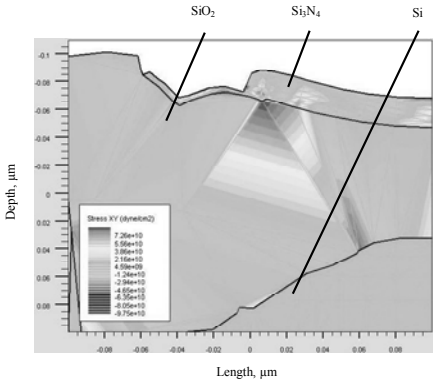

Fig. 8. Stress XY in Side Wall Masked Isolation in nano scale (t_1=0,4 min., t_2=50 min., T=1000 ºC, SiO_2=4 nm, Si_3N_4 (1st)=16 nm, Si_3N_4 (2nd)=4 nm, σ_{xy_max} – $7{,}26\cdot10^{10}$ dyne/cm^2, σ_{xy_struct} – $4{,}59\cdot10^{9}$ dyne/cm^2)

Conclusions

1. Stress depends on technologies type (LOCOS, PBL, SWAMI) in thermal oxidation.

2. The Deal-Grove model is used for the oxide growth kinetics and the oxidation rate slows as the oxide thickens.

3. Both in micro and nano scale structures stress created in SWAMI is smaller than in PBL and LOCOS. σ_{xy_max} created in LOCOS is greater than in SWAMI, but less than PBL.

4. Using thermal oxidation in nano scale created stresses (e.g. in SWAMI – σ_{xy_struct} – $4{,}59\cdot10^{9}$ dyne/cm^2) is greater than in micro scale structures (e.g. in SWAMI – σ_{xy_struct} – $-9{,}77\cdot10^{8}$ dyne/cm^2).

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Problems of thermal oxidation, related with LOCOS, PBL and SWAMI technologies wyky researched. The stresses, which appear during thermal oxidation are analysed in micro and nano scales levels in mentioned technologies. Thermal oxidation process is simulated with ATHENA. The Deal-Grove model is used for the oxide growth kinetics. Both in micro and nano scale structures stress created in SWAMI is less than in PBL and LOCOS. Maximum stress created in LOCOS is greater than in SWAMI, but less than PBL. Using thermal oxidation in nano scale created stresses are greater than in micro scale structures. Ill. 8, bibl. 7 (in English; summaries in English, Russian and Lithuanian).

Д. Андрюкайтис, Р. Анилёнис. Термическое окисление в LOCOS, PBL и SWAMI структурах при микро- и наноуровнях // Электроника и электротехника. – Каунас: Технология, 2007. – № 3(75). С. 23-26

Исследованы проблемы термического окисления возникающие в LOCOS, PBL и SWAMI технологиях. Напряжения, возникающие при окислении, изучены на уровне микро- и наноизмерений. При увеличении степени интеграции увеличиваются напряжения. Для моделирования процесса термического окисления применена программа ATHENA и модель Дила-Грау. Напряжения в структурах, изготовленных по технологии SWAMI, получены меньше чем в PBL и LOCOS. При переходе на меньшие размеры напряжения в структурах увеличиваются. Ил. 8, библ. 7 (на английском языке; рефераты на английском, русском и литовском яз.).

D. Andriukaitis, R. Anilionis. Terminė oksidacija LOCOS, PBL ir SWAMI mikro ir nano matmenų technologijose // Elektronika ir elektrotechnika. – Kaunas: Technologija, 2007. – Nr. 3(75). – P. 23-26.

Išnagrinėtos terminės oksidacijos problemos LOCOS, PBL ir SWAMI technologijose. Terminės oksidacijos metu atsirandantys įtempiai išanalizuoti mikro- ir nanomatmenų lygiais. Didėjant integracijos laipsniui ir pereinant iš mikro- į nanomatmenų lygį, keičiasi struktūrų įtempimai. Terminės oksidacijos modeliavimo procesas atliktas su programa ATHENA. Oksido augimui modeliuoti naudojamas Dilo-Grau modelis. SWAMI technologijoje gauti struktūros įtempiai yra mažesni nei PBL ir LOCOS technologijose tiek mikro- tiek nanomatmenų lygiu. Maksimalūs įtempiai gauti terminės oksidacijos metu LOCOS yra didesni nei SWAMI, bet mažesni nei PBL. Visose technologijose pereinant iš mikro- į nanomatmenų lygį įtempiai didėja. Il. 8, bibl. 7 (anglų kalba; santraukos anglų, rusų ir lietuvių k.).