ELECTRONICS AND ELECTRICAL ENGINEERING

ISSN 1392 – 1215 *2009. Nr. 8(96)*

ELEKTRONIKA IR ELEKTROTECHNIKA

MICROELECTRONICS

T 171

MIKROELEKTRONIKA

Thermal Oxidation Process Influence to the Three-Dimensional Integrated Structures

D. Andriukaitis, R. Anilionis

Department of Electronics Engineering, Kaunas University of Technology,
Studentų st. 50, LT-51368 Kaunas, Lithuania, phone: +370 37 300503; e-mail: darius.andriukaitis@ktu.lt

Introduction

Twentieth century second half is characterized by the rapid development of electronics technologies, which have the effect seen in practically all industries and the global economy. In the twenty-first century nanoelectronics came together with very high integration of integrated circuits technology, the basis of which we have computers, mobile phones, electronics and computing devices and systems.

The first integrated circuit (IC) is designed and demonstrated in 1958 (Texas Instruments Inc.). The IC made modern day information processing and communications systems possible. It's basic functional element is the transistor, most commonly a silicon metaloxide semiconductor field-effect transistor (MOSFET). In MOS/CMOS structures regions between the active elements must be isolated [1].

Three-dimensional integrated circuit design and production brings a number of technical and economic problems in a very high integration technology. The most important problem – the design and production complexity is considered. This is why the imminent use of computer programs allowing design and make three-dimensional integrated circuits simulation and the various parameters and characteristics calculations.

The main aim of this paper is to analyze mathematical models of the thermal oxidation process and use them for three-dimensional mathematical structures simulation with mathematical software package, also to examine the selection of the three-dimensional integrated element in the three-dimensional integrated circuits.

Mathematical models

Thermally grown silicon oxide separates semiconductor elements. The area of element formation must be the same during all technological processes. Separation of MOS elements can be produced using local oxidation. *Si* reacts with oxygen in room-temperature and consists of 5-10 nm native SiO_2 layer [2]. Once an oxide forms, however, silicon atoms must travel through the oxide layer to react with the oxygen present at the surface of the wafer, or else – oxygen molecules must travel through the oxide to reach the silicon surface, where the reaction can occur. As a result, the chemical reaction occurs at the "SiO_2–Si" interface. The interface is produced by thermal oxidation [3–5].

Thermal oxidation process can be described in a system of partial differential equations in the mathematical point of view:

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 oxide;
3. the deformation of the entire structure to comply with the new geometry changes. SiO_2 layer deflection causes displacement of material and the stresses in materials.

A simulation is needed in order to calculate these displacements and stresses. Some mechanical models is used to describe stress analysis coupled with oxidation processes: elastic, viscous, visco-elastic mechanical models [6]. By the stress equilibrium relations (1)-(3)

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} = f_x . \quad (1)$$

$$\frac{\partial \sigma_{yx}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} = f_y . \quad (2)$$

$$\frac{\partial \sigma_{zx}}{\partial x} + \frac{\partial \sigma_{zy}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} = f_z . \quad (3)$$

During the course of chemical reactions, materials displacements are only exposed to the internal forces in thermal oxidation process $f_x = f_y = f_z = 0$.

Elastic model. The materials are treated as elastic solids bodies, defined by their Young modulus E and Poisson ratio v in this model. The stress tensor is calculated separately from the strain tensor which is calculated solving Navier Stokes equations, which describe the fluid flow processes.

From the Hook's law, the stress tensor $\tilde{\sigma}$ is given by

$$\tilde{\sigma} = D \cdot \left(\tilde{\varepsilon} - \tilde{\varepsilon}_0\right) + \tilde{\sigma}_0 , \quad (4)$$

here D – the material matrix; $\tilde{\varepsilon}$ – the strain tensor; $\tilde{\varepsilon}_0$ – the residual strain tensor; $\tilde{\sigma}_0$ – is the residual stress tensor.

The strain tensor can be described as follows

$$\tilde{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix}, \quad (5)$$

here ε_{ii} – the first derivatives; ($\varepsilon_{xx} = \frac{\partial u_x}{\partial x}, \varepsilon_{yy} = \frac{\partial u_y}{\partial y}, \varepsilon_{zz} = \frac{\partial u_z}{\partial z}$); ε_{ij} – the shear strain components.

In isotropic material is assumed, the strain tensor is symmetric due to $\varepsilon_{xy} = \varepsilon_{yx}$, $\varepsilon_{xz} = \varepsilon_{zx}$, $\varepsilon_{yz} = \varepsilon_{zy}$. Then in an isotropic material by small changes the stress tensor without residual stress, can be rewritten as follows

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{xy} \\ \sigma_{yz} \\ \sigma_{zx} \end{pmatrix} = \frac{E(1-v)}{(1+v)(1-2v)} \begin{pmatrix} 1 & \frac{v}{1-v} & \frac{v}{1-v} & 0 & 0 & 0 \\ \frac{v}{1-v} & 1 & \frac{v}{1-v} & 0 & 0 & 0 \\ \frac{v}{1-v} & \frac{v}{1-v} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2v}{2(1-v)} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2v}{2(1-v)} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2v}{2(1-v)} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} - \varepsilon_{0,xx} \\ \varepsilon_{yy} - \varepsilon_{0,yy} \\ \varepsilon_{zz} - \varepsilon_{0,zz} \\ \gamma_{xy} - \gamma_{0,xy} \\ \gamma_{yz} - \gamma_{0,yz} \\ \gamma_{zx} - \gamma_{0,zx} \end{pmatrix}, \quad (6)$$

here v – Poisson ratio; E – Young modulus, $\gamma_{ij} = 2\varepsilon_{ij}$.

Viscous model. Silicon oxide and nitride layers are treated as an incompressible viscous fluids in the viscous model. Solution is consistent with the oxidation process maintaining the widest possible connectivity. Viscous model allows the accurate calculation of the stresses, caused by thermal oxidation process in silicon oxide layer.

Visco–Elastic model. The material behavior of oxide and nitride are more realistically described with a visco–elastic model, especially with a Maxwell element (Fig. 1), which consists of a spring and a dashpot in series.

Fig. 1. Maxwell element: a spring and a dashpot in series

SiO_2 and Si_3N_4 layers are treated as a visco–elastic compressible fluid. In this case the stress is calculated estimating the strain and the strain rate. Then the Maxwell element is described mathematically as follows

$$\frac{d\varepsilon}{dt} - \left(\frac{d\sigma}{dt}\frac{1}{G} + \frac{\sigma}{\gamma_{kl}} \right) = 0, \quad (7)$$

here G – the shear modulus; γ_{kl} – the (shear) viscosity.

The evaluations of the stress expansion are the components associated with the volume expansion, compression and tolerance, which affects the form, then the stresses can be described as

$$\sigma(t) = \sigma_0 \cdot e^{-\frac{t-t_0}{\tau_\tau}} + \int_{t_0}^{t} G \cdot e^{-\frac{t-t_0}{\tau_\tau}} \frac{d\varepsilon}{dt} d\tau_\tau, \quad (8)$$

here σ_0 – the initial stress; τ_τ – the Maxwellian relaxation time constant ($\tau_\tau = \frac{\gamma_{kl}}{G}$).

Within a very short period of time Δt the shear rate is constant, therefore

$$\frac{d\varepsilon}{dt} = \frac{\varepsilon}{\Delta t}. \quad (9)$$

The initial stress relaxes exponentially with time, then we get

$$\sigma(t) = \int_{t_0}^{t} G \cdot e^{-\frac{t-t_0}{\tau_\tau}} \frac{d\varepsilon}{dt} d\tau_\tau = \tau_\tau G \left(1 - e^{-\frac{t-t_0}{\tau_\tau}} \right) \frac{\varepsilon}{\Delta t} = G_{eff} \cdot \varepsilon, \quad (10)$$

here G_{eff} – the effective shear modulus which is in the elastic case the same as the standard shear modulus, dependent on temporary discretization time interval Δt.

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, determined by molecules of *Si*, SiO_2 and oxidants. The method is widely applicable, because simulated structure can be presented both in two and three-dimensional space. It is seeked by this method to maintain the minimum transitional zone (usually the transition zone is limited by one element) [7].

Calculation accuracy depends on the number of grid nodes in finite element method. Increasing the number of nodes, receiving larger data arrays demands more computing memory and increases the calculation duration. Main lack of the finite element method – there is a need to update finite element mesh after each time step, since a new layer of SiO_2 is formed. It is quite difficult to preserve the quality of the grid during the oxidation process simulation. To facilitate this task the SiO_2 domains are regrouped after each time step [7, 8].

Simulation of mathematical structures

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 [9].

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). 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 shown in the Fig. 2.

Mathematical structures are created using the finite element method for local thermal oxidation process simulation (Fig. 3.). 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 (see Fig. 3., a).

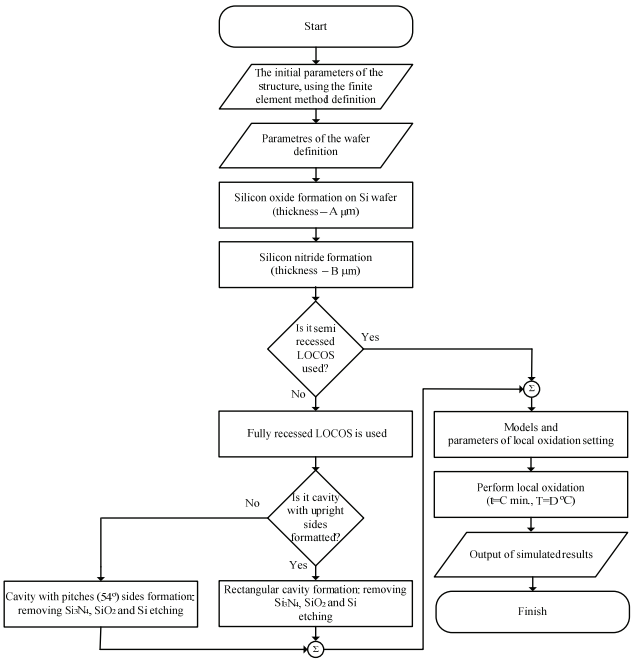


Fig. 2. The structure of the local oxidation model evaluation structure (A, B) and technology (C, D) parameters

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. 3., b).

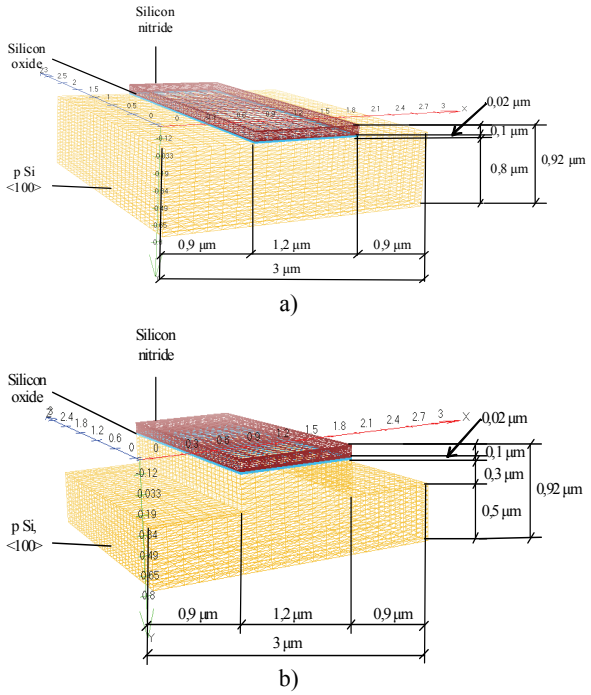


Fig. 3. Mathematical models: a – for semi-recessed LOCOS; b – for fully recessed LOCOS

It was found from the simulation results with program ATHENA that rational technology is semi-recessed LOCOS process in the three-dimensional integrated structures with rational parameters of the thermal process: t=90 min, T=1100 ºC, SiO_2=0,02 μm, Si_3N_4=0,1 μm, the region length – 1,8 μm, useful length 1,224 μm, L_{oks}=0,288 μm, H_{oks}=0,0209 μm, when projected IE length – 1,2 μm.

It is important to avoid distortion of integrated elements in the three dimensional integrated circuits. In this case mathematical model is created (three-dimensional field effect transistors (MOS)) (Fig. 4). It evaluates the variation of characteristics during local thermal oxidation process. The source and drain areas occupy 0.35 μm each, the channel length – 0,5 μm.

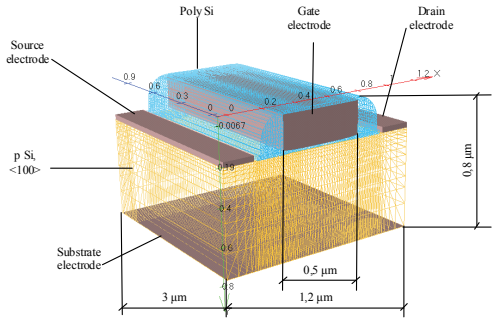


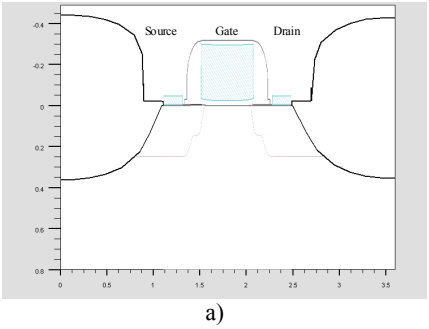
Fig. 4. MOS transistor mathematical model

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

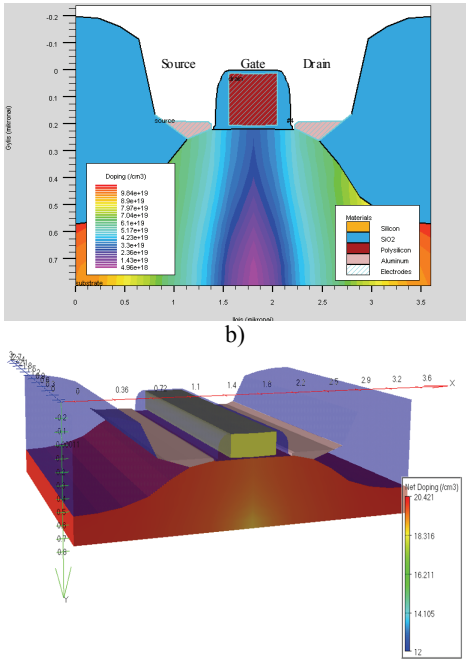
The parameters of three-dimensional integrated element and three-dimensional integrated structure change due to the thermal technology, which are difficult to identify and evaluate during the production. In this case the major human and material resources are required. That's why a mathematical simulation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

The simulation of three-dimensional structures conformation

The results of simulation have been carried out in the three-dimensional integrated structure simulation (Fig. 5), when transistor (Fig. 4) is simulated between local oxides. However, for large number of technological operations it is impossible to form an ideal structure, what the result of mathematical simulation using the finite element method of three-dimensional structure of is substantially strained.



a)



b)

c)

Fig. 5. Field-effect transistor in the integrated structure: a – expexted two-dimensional structure; b – simulated two-dimensional structure; b – simulated three-dimensional structure

Conclusion

1. The finite element method was used to create structures – the three-dimensional field-effect transistor, which estimates redistribution of impurities caused by thermal oxidation process in NMOS integrated three-dimensional structure.

2. In the case of impurity distribution and movement of pn areas it was received that the most impurities were redistributed after three-dimensional thermal oxide formation processes.

3. It was found out that during the thermal oxidation process impurities move into the lower doped layers in the three-dimensional integrated structures.

References

1. **Andriukaitis D., Anilionis R.** Investigation of Etching Process in Nano Structures // Electronics and Electrical Engineering. – Kaunas: Technologija, 2008. – No. 6(86). – P. 77–80.
2. **Štaras S.** Puslaidininkinės ir funkcinės schemos. Vilnius, 2002. – P. 621.
3. **Bhushan B.** Springer Handbook of Nanotechnology. Berlin: Springer, 2007. – ISBN: 978-3-540-35172-6. – P. 1916.
4. **Andriukaitis D., Anilionis R.** Oxidation Process and Different Crystallographic Plane Orientation Dependence Simulation in Micro and Nano Scale Structures. ITI 2007 Proceedings. 2007, Croatia, Cavtat. – P. 573–578.
5. **Mahalik N. P.** Micromanufacturing and Nanotechnology. Berlin: Springer, 2006. – ISBN: 978-3-540-25377-8. – P. 468.
6. **Andriukaitis D.** Thermal process simulation in three-dimensional integrated structures. Dissertation. Kaunas University of Technology, 2009. – 121 p.
7. **Causin P., Restelli M., Sacco R.** A simulation system based on mixed-hybrid finite elements for thermal oxidation in semiconductor technology. ComputerMethods in Applied Mechanics and Engineering. – 2004. – Vol. 193. – No.33-35. – P. 3687–3710.
8. **Noreika A., Tarvydas P.** Analysis of finite element mesh spacing influence on modeling results. // Electronics and Electrical Engineering. – Kaunas: Technologija, 2006. – No. 5(69). – P. 91–94.
9. Mathematical simulation program **ATHENA**. Official Website of SILVACO International. Internet. http://www.silvaco.com [2009 02 01].

Received 2009 06 19

D. Andriukaitis, R. Anilionis. Thermal Oxidation Process Influence to the Three-Dimensional Integrated Structures // Electronics and Electrical Engineering. – Kaunas: Technologija, 2009. – No. 8(96). – P. 81–84.

Problems of thermal oxidation process influence, related with MOS transistors separation was researched. Mechanical models are used to describe stress analysis coupled with oxidation processes: elastic, viscous, visco-elastic mechanical models. Three-dimensional integrated structures are formed using the finite element method for local thermal oxidation process simulation. Determinated, that parameters of three-dimensional integrated element and three-dimensional integrated structure change due to the thermal technology, which are difficult to identify and evaluate during the production. Redistribution of impurities in the thermal process is very important for the production of three dimensional integrated structures of increasingly higher integration degree, impurities move to other areas or redistribute because of the thermal process, error occurs in the formed areas. Ill. 5, bibl. 9 (in English; summaries in English, Russian and Lithuanian).

Д. Андрюкайтис, Р. Анилёнис. Влияние процесса термического окисления на трехмерные интегральные структуры // Электроника и электротехника. – Каунас: Технология, 2009. – № 8(96). – С. 81–84.

Исследовано влияние процесса термического окисления на разделение транзисторных МОП структур. Перемещение слоя SiO_2 вызывает натяжения в материалах, влияние которых определяется моделями эластичности и вязкости. Проведено моделирование интегральных структур применяя метод конечных элементов. Определено, что на параметры интегрального элемента и всей интегральной структуры влияют термические технологии, параметры которых довольно трудно определить при производстве. Перераспределения примесей после термических процессов наиболее важны при больших уровнях интеграции микросхем. Из-за этого возникают геометрические погрешности формируемых структур. Ил. 5, библ. 9 (на английском языке; рефераты на английском, русском и литовском яз).

D. Andriukaitis, R. Anilionis. Terminės oksidacijos proceso įtaka trimatėms integrinėms struktūroms // Elektronika ir elektrotechnika. – Kaunas: Technologija, 2009. – Nr. 8(96). – P. 81–84.

Išnagrinėta terminės oksidacijos proceso įtaka MOP tranzistorių atskyrimui. SiO_2 sluoksnio poslinkis sukelia medžiagų poslinkius ir įtempius, kuriems įvertinti taikomi elastingumo ir klampos modeliai. Atliktas trimačių integrinių struktūrų modeliavimas baigtinių elementų metodu. Baigtinių elementų metodo taikymas sąlygojamas oksidacijos procese vykstančių termodinaminių procesų, kurie sieja Si, SiO_2 ir oksidanto molekules. Nustatyta, kad trimačio integrinio elemento ir trimatės integrinės struktūros parametrų kaitą lemia terminės technologijos, kurių poveikį sunku nustatyti ir įvertinti gamybos metu. Priemaišų persiskirstymas po terminio proceso turi labai didelę reikšmę gaminant vis didesnio integracijos laipsnio trimačius integrinius grandynus, nes dėl terminių procesų priemaišos difunduoja, persiskirsto, atsiranda formuojamų sričių paklaidos. Il. 5, bibl. 9 (anglų kalba; santraukos anglų, rusų ir lietuvių k.).

DOI: 10.5755/j02.eie.9967