

A 2-D MODELING OF THE FIELD EFFECT IN A METAL-OXIDE-SMALL GRAIN POLYSILICON STRUCTURE

O. BONNAUD, Y. COLIN, H. LHERMITE

Groupe de Microélectronique . Université de RENNES
Campus de BEAULIEU . F-35042 RENNES CEDEX

SUMMARY

The two-dimension integration of POISSON's equation is applied to the study of the field effect in a metal-oxide-small grain polycrystalline silicon structure . Both grain boundaries perpendicular or parallel to the Si/SiO₂ interface are considered . We show the particular role of the first parallel grain boundary on the electrostatic potential variations induced by the gate voltage. It impedes these variations drastically and limits them to the first grain.

INTRODUCTION

In the prospect of three-dimension devices and flat panel displays of large area, which combine both the driver circuit and the liquid crystal display, deposition of silicon on amorphous or vitreous substrates is studied. Due to the low temperature process imposed by the nature of the substrate, silicon is polycrystalline or amorphous. Some displays elaborated with amorphous silicon have been manufactured (LE CONTELLEC, 1985), but the poor qualities of these devices (high response time, low mobility...) increase the need of a specific study of polycrystalline silicon in either a technological or a theoretical way.

This paper deals with the modeling of the field effect within a polycrystalline silicon layer. The complete modeling of the field effect needs to account, on one hand, for the electrostatic phenomena by solving the POISSON's equation and on the other hand, for electrical conduction phenomena by solving the two equations of continuity, (GUERRERI, 1986). We choose to pay a particular attention to the only POISSON's equation to study, in a first approach, the electrostatic potential variations induced by a gate voltage in a polysilicon MOS capacitor. The only way is the numerical integration of this equation with a proper choice for the geometrical modeling of the polycrystalline silicon layer. We firstly detail the numerical method we use to solve the POISSON's equation, then we specify the

simulation domain and finally, we present and discuss the results of the simulation.

THE POISSON EQUATION

POISSON's equation is considered in it's general form:

$$(1) \quad \text{div}(k \times \text{grad}(\bar{\phi})) = q \times (n(\bar{\phi}) - p(\bar{\phi}) - N_d^+ + N_a^- + \Sigma(N_{t,d}^-(\bar{\phi}) - N_{t,d}^+(\bar{\phi})))$$

where k is the permittivity, $\bar{\phi}$ the electrostatic potential, n and p electron and hole concentrations, N_d^+ et N_a^- impurity concentration (donor or acceptor), $N_{t,d}^+$ and $N_{t,d}^-$ ionized trap densities (donor or acceptor) at grain boundaries whose energy level $E_{t,d}^+$ or $E_{t,d}^-$ is located in the energy gap.

Electron and hole concentrations are calculated by MAXWELL BOLTZMANN's statistics .

$$(2) \quad n(\bar{\phi}) = N_c \exp \frac{q\bar{\phi} - q\bar{\phi}_{e,n} + kh_e}{kT}$$

$$(3) \quad p(\bar{\phi}) = N_v \exp - \frac{q\bar{\phi} - q\bar{\phi}_{e,p} + kh_h + E_g}{kT}$$

where N_c et N_v are the effective densities of states in the conduction and valence band edges, $\bar{\phi}_{e,n}$ et $\bar{\phi}_{e,p}$ electrochemical potentials for electrons and holes, kh_e electron affinity and E_g the band gap.

As long as thermodynamical equilibrium is concerned, the electrochemical potentials are identical and constant throughout the complete structure. Impurities are assumed ionized at room temperature, $T = 300$ K. Ionized traps densities are given by the SHOCKLEY, READ and HALL model, (S.R.H), (SHOCKLEY, 1952) :

$$(4) \quad N_{t,d}^- = \frac{C_{n,j} \cdot n + C_{p,j} \cdot p_i}{C_{n,j} \cdot (n + n_{1,j}) + C_{p,j} \cdot (p + p_{1,j})}$$

$$(5) \quad N_{t,d}^+ = \frac{C_{p,j} \cdot p + C_{n,j} \cdot n_{1,j}}{C_{n,j} \cdot (n + n_{1,j}) + C_{p,j} \cdot (p + p_{1,j})}$$

C_n , et C_p , are the capture coefficients for electrons and holes, but only their ratio is needed. In the lack of precise values for C_n and C_p , we assume $C_n = C_p$. In a previous work, we have shown that the exact value has no

significant importance on numerical results at least at room temperature (LHERMITE, 1988a).

Parameters $n_{i,j}$ et $p_{i,j}$ are calculated in the MAXWELL-BOLTZMANN statistics by the following expressions :

$$(6) \quad n_{i,j} = N_c \exp \frac{E_{i,j} - E_c}{kT}$$

$$(7) \quad p_{i,j} = N_v \exp \frac{E_v - E_{i,j}}{kT}$$

In its general form, POISSON's equation is an elliptic second-order non linear differential equation and therefore has no analytical solution. So it is necessary to solve it by means of a numerical method. The method we choose, is a finite difference method whose main points are hereafter detailed.

NUMERICAL METHOD

Due to the exponential terms in the free carrier concentrations expressions, POISSON's equation is strongly non linear.

First, we linearize this equation by setting:

$$(8) \quad \tilde{\phi} = \tilde{\phi}^0 + \delta\tilde{\phi}$$

$\tilde{\phi}^0$ is an initial estimate for electrostatic potential which satisfies the boundary conditions, and $\delta\tilde{\phi}$ becomes the new unknown parameter.

All densities are linearized in this way :

$$(9) \quad n(\tilde{\phi}) = n(\tilde{\phi}^0) + \frac{d(n(\tilde{\phi}))}{d\tilde{\phi}} \cdot \delta\tilde{\phi}$$

$$(10) \quad p(\tilde{\phi}) = p(\tilde{\phi}^0) + \frac{d(p(\tilde{\phi}))}{d\tilde{\phi}} \cdot \delta\tilde{\phi}$$

$$(11) \quad N_{t_{a,j}}^-(\tilde{\phi}) = N_{t_{a,j}}^-(\tilde{\phi}^0) + \frac{d(N_{t_{a,j}}^-(\tilde{\phi}))}{d\tilde{\phi}} \cdot \delta\tilde{\phi}$$

$$(12) \quad N_{t_{a,j}}^+(\tilde{\phi}) = N_{t_{a,j}}^+(\tilde{\phi}^0) + \frac{d(N_{t_{a,j}}^+(\tilde{\phi}))}{d\tilde{\phi}} \cdot \delta\tilde{\phi}$$

The linearized POISSON's equation is written as follows :

$$(13) \quad \text{div}(k \text{ grad}(\delta\bar{\phi})) - q \frac{d(n(\bar{\phi}) - p(\bar{\phi}) + \Sigma(N_{e,ij}^-(\bar{\phi}) - N_{e,ij}^+(\bar{\phi})))}{d\bar{\phi}} =$$

$$-\text{div}(k \text{ grad}(\bar{\phi})) + q(n(\bar{\phi}) - p(\bar{\phi}) - N_{e,i}^+ + N_{e,i}^- + \Sigma(N_{e,ij}^-(\bar{\phi}) - N_{e,ij}^+(\bar{\phi})))$$

Besides, we have to discretize the divergence and gradient terms by means of a classical five points scheme (SELBEHERR, 1984).

The discretized POISSON's equation is written in its matricial form :

$$(14) \quad B_{i,j} \times \delta\bar{\phi}_{i-1,j} + H_{i,j} \times \delta\bar{\phi}_{i+1,j} + G_{i,j} \times \delta\bar{\phi}_{i,j-1} + D_{i,j} \times \delta\bar{\phi}_{i,j+1} - T_{i,j} \times \delta\bar{\phi}_{i,j} = V_{i,j}$$

where the $\delta\bar{\phi}$ value at point (i,j) is now given by the four neighbouring values. The B, H, G, D, T and V factors are matrix elements. To obtain the $\delta\bar{\phi}_{i,j}$, it may be necessary to inverse the matrix, but it is a time consuming and rather critical procedure if we want a good accuracy for $\bar{\phi}_{i,j}$.

So, we have solved the POISSON's equation by an indirect method, line after line, then column after column. The matrix of the system has now a tridiagonal form and the solution is reached by means of a gaussian algorithm, (GERALD, 1978).

Using relation (8), $\bar{\phi}_{i,j}$ is deduced from the $\delta\bar{\phi}_{i,j}$ value ; $\bar{\phi}_{i,j}$ becomes a better approximation of the electrostatic potential than $\bar{\phi}_{i,j}^*$. This iterative scheme is repeated as long as the maximum of $\delta\bar{\phi}_{i,j}$ is greater than an arbitrary value which sets the required precision we want for the electrostatic potential.

This method, derived from the GUMMEL method, (GUMMEL, 1962), has the disadvantage to under-evaluate $\delta\bar{\phi}_{i,j}$. In the first iterations, $\delta\bar{\phi}_{i,j}$ can be close to, and even greater than the $\bar{\phi}_{i,j}$ values. The linearization of the concentrations in expressions 9-12 is only valid if $\delta\bar{\phi}_{i,j}$ is small compared to $\bar{\phi}_{i,j}$. If not, a dumping method is needed to calculate the $\delta\bar{\phi}_{i,j}$. The method we used was firstly proposed by J.E. VIALLET and S. MOTTET (1985).

As long as the maximum of the $\delta\bar{\phi}_{i,j}$ is greater than $kT/2q$, we used the following relaxation :

$$(15) \quad \delta\bar{\phi}_{i,j} = \frac{|\delta\bar{\phi}_{i,j}|}{\delta\bar{\phi}_{i,j}} \times \frac{kT}{q} \times \text{Ln} \left(1 + \frac{q|\delta\bar{\phi}_{i,j}|}{kT} \right)$$

This method gives the opportunity of reaching the maximum accuracy for the calculated $\bar{\Phi}_i$, : 1×10^{-16} in double precision. Nevertheless, to minimize the computation time, we assigned 1×10^{-6} to this precision.

SIMULATION DOMAIN

The simulation domain shown in Fig.1 consists of two regions : the first one relative to oxide, the second to polycrystalline layer.

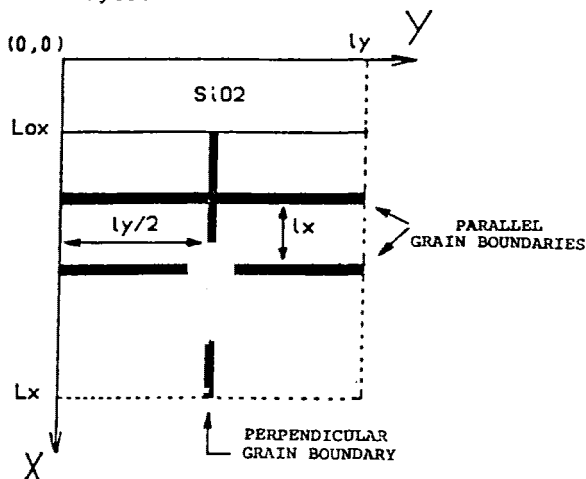


FIG.1 Simulation domain.

The oxide, 100 nm thick, is assumed ideal, and then does not contain any fixed charges ; in the same way its interface with the polycrystalline layer is assumed ideal.

The polycrystalline layer consists of several crystallites separated by grain boundaries. Crystallites are made of monocrystalline silicon, and have the classical properties generally attributed to this material.

The small grain polycrystalline silicon have grain boundaries randomly distributed in the entire polycrystalline layer . A quite simple way to this layer is to consider grain boundaries perpendicular and parallel to the Si/SiO₂ interface. As far as we are concerned, we assume a perpendicular grain boundary and two parallel grain boundaries distant of 100 nm. Furthermore, we assume that grain boundary has a finite width. The method we use to solve the POISSON's equation makes this assumption necessary. Moreover, this assumption gives the convenience to consider

the grain boundary as a material with its own properties. We consider that grain boundary is 1 nm thick. The surface densities are converted into bulk concentrations uniformly distributed in the grain boundary region. So, the minimum value 1 nm is assigned at grain boundary and is increased by means of a geometrical series on both sides of the grain boundary.

The simulation domain is $L_y=600$ nm wide and $L_x=1$ μm long.

MODELING PARAMETERS.

a- Constants (SZE, 1985).

The physical parameters of the oxide are those of a thermally grown oxide from a monocrystalline silicon substrate. So, we get the following values for the permittivity and the electron affinity :

$$k_{h_{i.o.}} = 4.1 \text{ eV} ; k_{o.} = 3.9$$

The crystallites made of monocrystalline silicon, have the following physical values :

$$N_c = 2.82 \cdot 10^{19} \text{ cm}^{-3} ; N_v = 1.02 \cdot 10^{19} \text{ cm}^{-3} \\ E_g = 1.12 \text{ eV} ; k_i = 4.04 \text{ eV} ; k_{s,i} = 11.7$$

b-Simulation parameter.

The electron concentration in the n-doped polysilicon layer is $1 \times 10^{14} \text{ cm}^{-3}$. Doping is assumed evenly distributed, as generally admitted.

The main problem with a numerical simulation within a polycrystalline layer is the modeling of the grain boundary. We take into account here the trapping carrier model firstly proposed by SETO, (1975). Because of the high crystallographic disorder inside the grain boundary, this region is the centre of high traps densities whose energy levels are possibly distributed over the entire band gap.

The real distribution of the trap levels is quite problematic because it varies from a sample to an other and strongly depends on the measurement methods. To account for the electric phenomena inside the polycrystalline silicon either n type or p type doped, it is necessary to consider both kind of traps, acceptor traps and donor traps. The reason put forward is the existence, at the interface between two crystallites, of dangling bounds which introduce one acceptor level and one donor level symmetrically located from midgap (LANNOO, 1981). This well explains the relative position of the fermi level at midgap

over a large range of concentrations (SEAGER, 1978). A previous work has shown that one acceptor level and one donor level both at midgap with the same densities, allows to account for the electrostatic phenomena within a polycrystalline layer (LHERMITE, 1988b). So, we used the following values :

$$N_{t,a} = N_{t,d} = 10^{12} \text{ cm}^{-2} ; E_{t,a} - E_c = E_{t,d} - E_c = -E_g/2$$

BOUNDARY CONDITIONS

Boundary conditions are assigned at each limit of the simulation domain.

i) a DIRICHLET condition at the oxide surface where the electrostatic potential is fixed by the gate voltage.

ii) a NEUMANN condition at the other limits where we assumed that the electrostatic potential no longer varies.

The perpendicular grain boundary in the simulation domain shown figure 1 is a symmetrical plane. Nevertheless, to avoid an elliptic condition, we consider the entire domain (instead of the half one) because the DIRICHLET and NEUMANN condition are quite easy to satisfy.

NUMERICAL RESULTS

Figure 2 shows the band bending inside the polycrystalline layer when a -3-Volts-gate voltage is applied. At the interface, far from the perpendicular grain boundary, the layer is inverted because the gate bias is enough sufficient to induce hole concentration higher than the electron concentration. At the intersection of the perpendicular grain boundary and the interface, we see a band bending due to the trapping of holes by donor traps. Along the interface, in the inverted layer, a depleted layer is localized near the grain boundary. From the interface, the induced hole concentration decreases and the ionized donor trap rate decreases ; the electron concentration increases and consequently the ionized acceptor trap rate increases. Combining both these phenomena leads to a complete depletion between the two grain boundaries parallel to the interface : bands are flat in this region. Far from the last parallel grain boundary, the neutral bulk is reached : a band bending appears near the perpendicular grain boundary because the electrons ionize acceptor traps ; consequently, an electron depleted region exists near the grain boundary. This barrier height has opposite sign than the interface one.

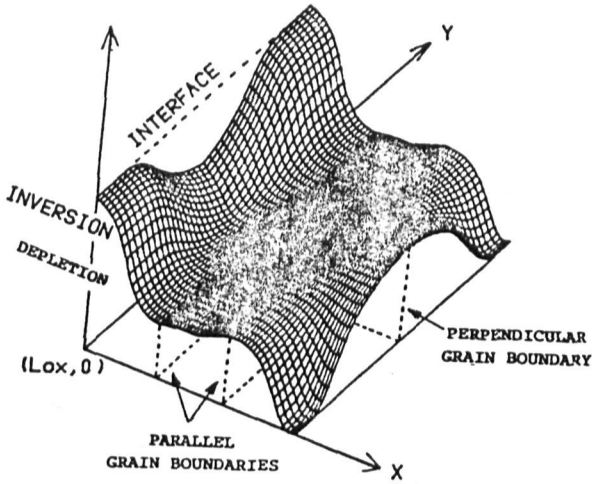


FIG.2 2D-representation of the electrostatic potential in the simulated layer.

The outstanding result of this simulation is that the field effect is limited by the first parallel grain boundary. To give evidence of that, we plotted the variation of the electrostatic potential versus the gate voltage in a plane parallel to the Oy axis.

Figure 3 shows this variation in the plane $x = 0$. We note that, whatever the gate voltage is, the electrostatic potential variation induced by the voltage is limited by the first parallel grain boundary. Moreover, the region behind the last parallel grain boundary presents the classical variation of the electrostatic potential in the vicinity of a grain boundary : these variations would be the same in the absence of a field effect.

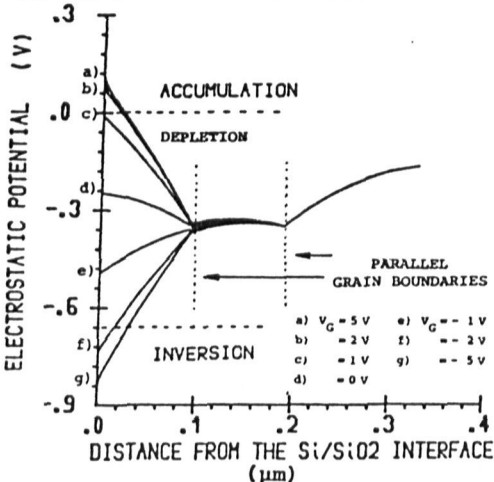


FIG.3 Electrostatic potential variations versus the gate bias in the plane $x = 1_y/7$.

Figure 4 shows a section in the plane $x = L_y/2$. We see similar but more pronounced results because the traps are close to the interface.

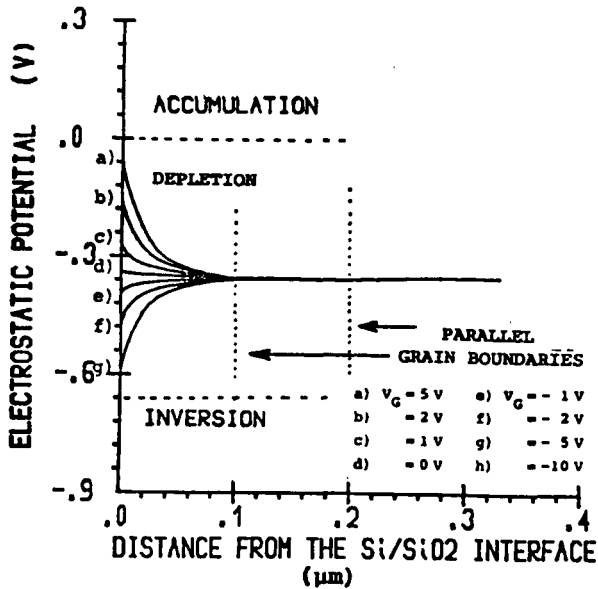


FIG.4 Electrostatic potential variations versus the gate bias in the plane $x=0$.

CONCLUSIONS

We have shown the particular role of a parallel grain boundary. It drastically impedes the variation of the electrostatic potential induced by a gate voltage. Furthermore, we note that the variation of the so-called deserted layer is limited by the position of this grain boundary; that is of great importance in the quasi static variation of the C-V characteristic of a capacitor elaborate with polycrystalline silicon. Furthermore the parallel grain boundary plays a relative important role compared to the perpendicular grain boundary. That explains why one can obtain a suitable modeling of the quasi static behavior of a metal-oxide-small grain polysilicon capacitor by using a one dimension geometrical model (LHERMITE, 1986a)

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