Analytical Surface Potential Model for Columnar Nanocrystalline Silicon Ultra-Thin Film Transistors

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***Abstract*—An analytical model to calculate the nano-crystalline silicon (nc-Si) ultra-thin film transistors (UTFT) surface potential is proposed. This pattern repose on an ultra-thin channel with a columnar morphology. Our approach is based on the charge trapping at the grain boundary, the well-defined charge distribution into the inversion layer, and the consideration of quantum size effects on dielectric constant and band gap. Results denote that, the surface potential is associated to the silicon crystallites size and geometry. The comparison of our results with existing research model shows a good agreement between the surface potential shapes, and an interesting difference in the surface potential variation, caused essentially by the morphology considered.**

Keywords—nanocrystalline silicon; thin film transistor; quantum size effects; columnar morphology; surface potential;

I. INTRODUCTION

The evolution in materials and process fabrication technologies is posing new challenges in large area nanoelectronics and optoelectronics. The driving force in this evolution is the silicon ultra-thin film technology.

The production of the nc-Si thin films have been under development since a few years ago. Nc-Si is a compromise solution between amorphous silicon (a-Si) and poly-crystalline silicon (poly-Si). The nc-Si films are promising material for the fabrication of Si based TFT [1-4], due to its better electrical stability and higher mobility when compared with its amorphous counterpart, which can be found in a variety of electronic applications [5, 6]. However, the nano-structural properties of nc-Si films are important issues for this technology. The consideration of nc-Si structure for circuit design and simulation is important for electrical and electronic behavior description of the device.

The research in this area is more condensed on the current-voltage relationships, so, several authors have made a considerable study concerning the surface potential for poly-Si TFTs [7-11]. However, a few researches has focused on the study of the nc-Si TFTs electrical characteristics. L.F. Mao [12] has studied the impact of quantum size effects on the dielectric constant and the band gap on the surface potential of nc-Si TFTs, without considering the channel morphology.

Experimental researches have been focused on ultra-thin silicon films in order to determine the crystallites shapes [13]. It has clearly found that the crystallites morphology is columnar, i.e. the columns were formed parallel to the growth direction.

The purpose of this work is to propose a new approach in order to define the surface potential analytical calculation, by considering a columnar crystallites structure, defined by an accurate crystallites size and geometry.

II. SURFACE POTENTIAL MODEL

We present in Fig. 1 an UTFT channel three-dimensional description with a columnar morphology characterized by nanometric crystallites sizes, i.e. crystallites diameter. We consider the silicon nanocrystallites as a set of grains, separated from each other's by an amorphous region (grain boundary).

We assume that in the inversion layer (represented by the dark region into the channel), the grain boundary adjacent electrons are trapped therein, which causes the depletion region formation. Then, by applying Gauss's theorem to the depletion region, the following equation can be derived from the quasi-2D Poisson's equation [14-18]:

$$\varepsilon_{Si}\int_0^{X_d}\frac{\partial\psi(x,y)}{\partial y}dx + C_{ox}\int_0^{y}\left[V_{gs}-V_{fb}-\psi(0,y)\right]dy = qN_aX_d y \qquad (1)$$

where $\psi(x,y)$ is the electrostatic potential, V_{gs} is the gate-source voltage, V_{fb} is the flatband voltage, N_a is the p-type channel doping concentration, X_d is the grain depletion charge depth, C_{ox} is the gate oxide capacitance (ε_{ox}/t_{ox}) where t_{ox} is the gate oxide thickness, and ε_{ox} and ε_{Si} are the permittivity of silicon-oxide and silicon, respectively. We assume that the electrostatic potential has a parabolic distribution with x-axis. Therefore:

$$\psi(x,y)=\psi(0,y)\left(1-\frac{x}{X_d}\right)^2. \qquad (2)$$

Replacing (2) into (1), differentiating both sides with respect to y, and with some algebraic manipulations, (1) becomes:

$$\frac{\partial^2 \psi(0,y)}{\partial y^2} - \left(\frac{3C_{ox}}{\varepsilon_{si} X_d}\right)\psi(0,y) = -\left(\frac{3C_{ox}}{\varepsilon_{Si} X_d}\right)\left(V_{gs} - V_{fb}\right) + \frac{3qN_a}{\varepsilon_{Si}}. \quad (3)$$

The grain depletion charge depth X_d, can be determined from the 1D Poisson's equation. It is expressed as:

$$X_d = \left(\frac{2\varepsilon_{Si}\psi_{S0}}{qN_a}\right)^{0.5} \quad (4)$$

where ψ_{S0} is the potential at (0,0), given by [14, 19]:

$$\psi_{S0} = \frac{kT}{q}\ln\left(\frac{N_a}{n_i}\right) + \frac{E_i - E_v - \chi_0}{q} \quad (5)$$

where E_i is the intrinsic level, E_v is the valence level, n_i is the intrinsic concentration and χ_0 is determined from the following expression:

$$\left[E_g - \chi_0 - \frac{q^2 N_a}{2\varepsilon_{Si}}\left(\frac{L_g}{2}\right)^2\right]N_D^D + N_D^T E_D^T \exp\left[-\frac{\chi_0}{E_D^T} - \frac{q^2 N_a}{2\varepsilon_{Si} E_D^T}\left(\frac{L_g}{2}\right)^2\right] = N_a L_g \quad (6)$$

where E_g is the band gap, N_D^D is the deep donors states density, E_D^T is the tail donors states level, N_D^T is the tail donors states density, and L_g represents the grain diameter.

Under the following boundaries conditions:

$$\psi(0,0) = \psi_{S0} \quad \text{and} \quad \left.\frac{\partial \psi(0,y)}{\partial y}\right|_{y=0} = 0$$

the solution of (3) represents the electrostatic potential at the grain boundary. It can be expressed as:

$$\psi(0,y) = V_{fb} - \frac{qN_a X_d}{C_{ox}} + \left(\psi_{S0} - V_{gs} + V_{fb} + \frac{qN_a X_d}{C_{ox}}\right)\cosh\left[\left(\frac{3C_{ox}}{\varepsilon_{Si} X_d}\right)^{0.5} y\right]. \quad (7)$$

We suppose that at the strong inversion and under the charge trapping at the grain boundary, we have a lateral depletion y_d along the y-axis as illustrated in Fig. 1. Then, (7) yields to:

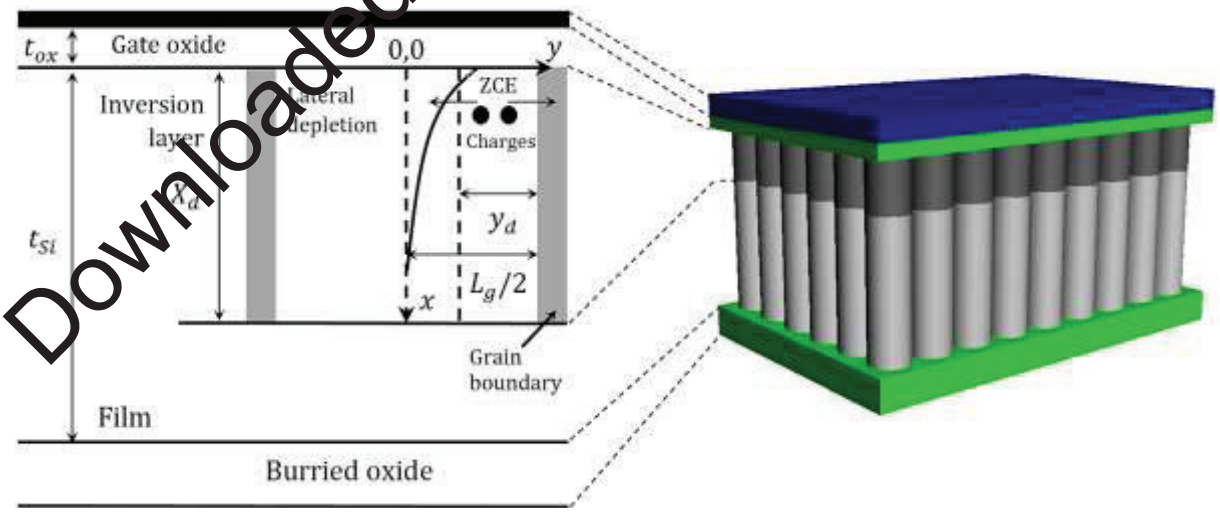


Figure 1. Right, nc-Si TFT ultra-thin channel columnar morphology. Left, channel grain cross section at the strong inversion..

$$\psi_S = V_{gs} - V_{fb} - \frac{qN_a X_d}{C_{ox}} + \left(\psi_{S0} - V_{gs} + V_{fb} + \frac{qN_a X_d}{C_{ox}} \right) \cosh\left[\left(\frac{3C_{ox}}{\varepsilon_{Si} X_d} \right)^{0.5} y_d \right]. \quad (8)$$

This equation shows the surface potential ψ_S at the grain boundary.

Because of the nanometric size of the silicon crystallites forming the channel, the quantum effect must be considered. In low scale, electron-hole pair is confined, this causes the apparition of quantum effects on dielectric constant, ε_{nc-Si}, given by [20, 21]:

$$\varepsilon_{nc-Si}(L_g) = 1 + \frac{10.4}{1 + \left(\frac{1.38}{10^9 L_g} \right)^{1.37}}. \quad (9)$$

The nano-electronic structures have an extremely dependence onto the crystallites size. They can be determined as a function of grain size as follows [22, 23]:

$$\Delta E_g(L_g) = \frac{3.4382}{\left(10^9 L_g\right)} + \frac{1.1483}{\left(10^9 L_g\right)^2}. \quad (10)$$

These both quantum effects, can be included into (8) through the potential ψ_{S0}. So, substituting (9) and (10) into (6), we get:

$$\chi_0 N_D^D - N_D^T E_D^T \exp\left(-\frac{\chi_0}{E_D^T} \right) = \left[E_g + \frac{3.4382}{\left(10^9 L_g\right)} + \frac{1.1483}{\left(10^9 L_g\right)^2} \right] N_D^D - \frac{q^2 N_a N_D^D}{2} \left[1 + \left(\frac{1.38}{10^9 L_g} \right)^{1.37} \right] \times \left[1 + \left(\frac{1.38}{10^9 L_g} \right)^{1.37} + 10.4 \right]^{-1} \left(\frac{L_g}{2} \right)^2 + N_D^T E_D^T \times \exp\left\{ -\frac{q^2 N_a}{2E_D^T} \left(\frac{L_g}{2} \right)^2 \left[1 + \left(\frac{1.38}{10^9 L_g} \right)^{1.37} \right] \right\} \left[1 + 10.4 + \left(\frac{1.38}{10^9 L_g} \right)^{1.37} \right]^{-1} \right\} - N_a L_g \quad (11)$$

χ_0 depends strongly on the both quantum effects on dielectric constant and band gap, it can be determined by solving (11).

It is obvious that there is no analytical solution for (11). To solve this equation, an iterative method has been used. The χ_0 solution can be substituted into (5). Considering (10), we obtain the new ψ_{S0} expression:

$$\psi_{S0} = \frac{kT}{q} \ln\left(\frac{N_a}{n_i} \right) + \frac{E_g}{2q} + \frac{3.4382}{2q\left(10^9 L_g\right)} + \frac{1.1483}{2q\left(10^9 L_g\right)^2} - \frac{\chi_0}{q}. \quad (12)$$

Finally, by replacing (12) into (8), and for $y_d = L_g / 2$ we obtain:

$$\psi_S = V_{gs} - V_{fb} - \frac{qN_a X_d}{C_{ox}} + \left[\frac{kT}{q} \ln\left(\frac{N_a}{n_i} \right) + \frac{E_g}{2q} + \frac{3.4382}{2q\left(10^9 L_g\right)} + \frac{1.1483}{2q\left(10^9 L_g\right)^2} - \frac{\chi_0}{q} - V_{gs} + V_{fb} + \frac{qN_a X_d}{C_{ox}} \right] \cosh\left\{ \left(\frac{3C_{ox}}{4X_d} \right)^{0.5} \left[1 + \left(\frac{1.38}{10^9 L_g} \right)^{1.37} \right]^{0.5} \times \left[1 + \left(\frac{1.38}{10^9 L_g} \right)^{1.37} + 10.4 \right]^{-0.5} L_g \right\}. \quad (13)$$

This final expression shows a new analytical surface potential as a function of the grain diameter, i.e. the surface potential for an UTFT with a nanocrystalline silicon structure described as a range of columnar nanocrystals, separated by amorphous grain boundaries regions. Note that X_d mentioned into (13) becomes:

$$X_d = \frac{1}{q}\left\{\frac{2}{N_a}\left[1+\left(\frac{1.38}{10^9 L_g}\right)^{1.37}\right]^{-1}\left[1+10.4+\left(\frac{1.38}{10^9 L_g}\right)^{1.37}\right]\right\}^{0.5}\left[kT\ln\left(\frac{N_a}{n_i}\right)+\frac{E_g}{2}+\frac{3.4382}{2\left(10^9 L_g\right)}+\frac{1.1483}{2\left(10^9 L_g\right)^2}-\chi_0\right]^{0.5} \quad (14)$$

III. Results and Discussions

We present in Fig. 2 the surface potential variation versus crystallites sizes. The surface potential increases rapidly with a linear form from a crystallite size ~1 nm and reaches a maximum value at ~1 V for a crystallite size ~7 nm. From this crystallite size, the surface potential decreases exponentially and tends to stabilize from a crystallite size ~40 nm.

The evolution of the numerical solution χ_0 of (11) (Fig. 2) shows a strong decay from 5.5 eV to 0.3 eV, when the crystallites size increases in the range of ~1 nm to ~7 nm, due to the influence of the quantum effects on dielectric constant and band gap [20-23]. From a crystallite size of ~7 nm (quantum effects disappearance), χ_0 tends to take a quasi-constant values.

According to Fig. 3, the solutions χ_0 of (11) depend clearly on the both quantum effects on dielectric constant and band gap, since these quantum effects have the same strong variation in the crystallites sizes ranging from 1 nm to 7 nm. i.e. a large decrease for the quantum effect on band gap, from 5.5 eV to 1.5 eV, and large increase for the quantum effect on dielectric constant, from 5.1 to 10.7. For crystallite sizes larger than 7 nm, both quantum effects on dielectric constant and band bap reach to stabilize at ~11.2 and ~1.2 eV respectively. Therefore, we have a quasi-constant values attributed to both effects for the crystallite sizes larger than ~7 nm.

The influence of the both quantum size effects for the crystallite sizes less than ~7 nm is very important. This influence affects significantly the surface potential.

For crystallite sizes larger than ~7 nm, the surface potential values decrease slightly into an exponential. Indeed, the term $\cosh\left(\sqrt{3C_{ox}/4\varepsilon_{nc-Si}X_d}L_g\right)$ in the surface potential expression, becomes dominant.

We compare in Fig. 4(a) our model results with those obtained by L.F. Mao [12]. The model described by L.F. Mao repose onto the consideration of the quantum size effects for a nc-Si TFT, but do not specify the channel morphology, it gives a vague description concerning the channel structure, which is mentioned to be silicon nanocrystals separated by the very thin amorphous grain boundaries.

We present into Fig. 4(b) our model with respect to Mao model with different surface potential axes in order to show the shape comparison. For crystallite sizes ranging from 1 nm to 7 nm, we have a clear difference of ~0.6 V for a crystallite size of 1 nm, which tends to a maximum surface potential difference of ~1.18 V at the peak value corresponding to a crys-

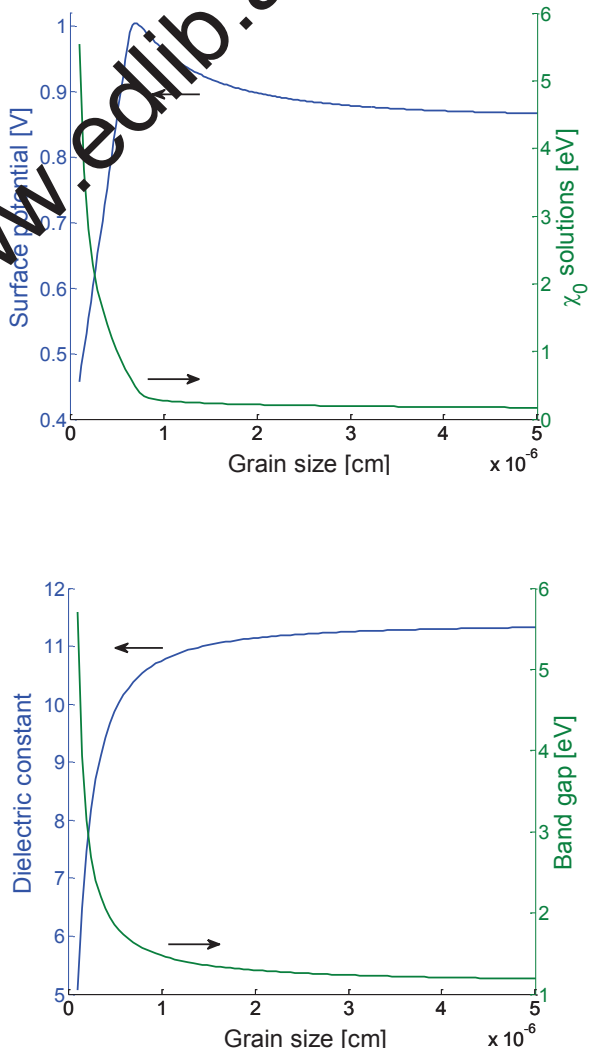
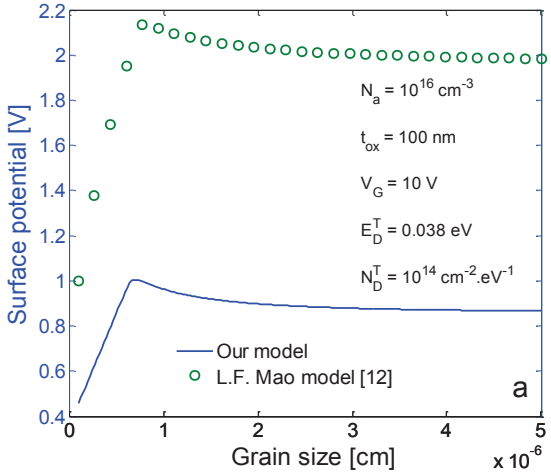


Figure 2. Surface potential and χ_0 solution as function grain size.



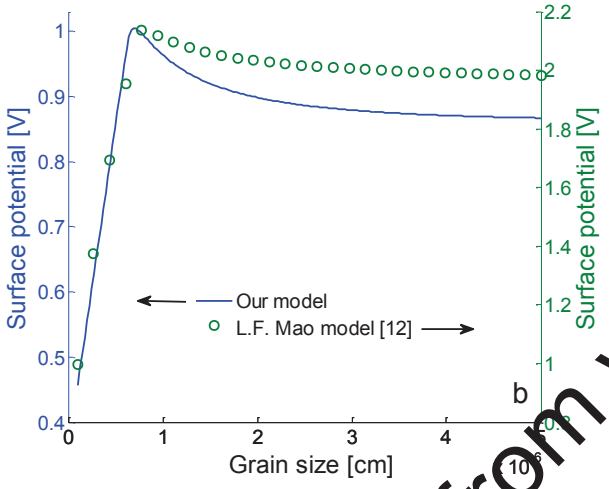


Figure 3. Both quantum size effects on dielectric constant and band gap.

Figure 4. Surface potential versus grain size comparison with L.F. Mao model, (a) same axis and (b) different axis.

tallites size of ~7 nm. A slight difference in the slope is noted in the same range, due to the quantum effects combined with the solutions χ_0 and the hyperbolic cosine. From the crystallites size larger than ~7 nm, we obtain via our model a light exponential decay with respect to the surface potential variation range. This difference highlights the impact of the channel morphology on the surface potential expressed by the term $\cosh\left(\sqrt{3C_{ox}/4\varepsilon_{nc-Si}X_d}\,L_g\right)$, and shows clearly that the channel morphology strongly affects the nc-Si UTFT surface potential.

Basing on these results, we can confirm that our model, which repose on a well-defined channel structure, presents an advantage with respect to L.F. Mao model.

IV. Conclusion

In this work, we have presented an analytical method to calculate the nc-Si UTFT surface potential, by assuming a well-defined channel morphology with a nanometer crystallites size and a columnar crystallites geometry. Results show the effect of the crystallinity in terms of crystallites size and shape on the surface potential. Thus, the quantum effects have a considerable impact on the surface potential especially for small crystallites size. The effect of the crystallites geometry on the surface potential variation has been clearly highlighted, especially for silicon crystallites larger than ~7 nm.

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