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Simulation of the Conduction Mechanisms in Polycrystalline Silicon Thin Film Transistors

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Abstract

A simulator for the design of polycrystalline silicon thin film transistors, used for the command of flat panel liquid crystal display pixels, is discribed. This simulator is based on the plolycrystalline silicon specific physical equations. It permits to describe both passing and blocking operating modes.

1. Introduction

Polycrystalline silicon thin film transistors are being used for the command of flat panel liquid crystal display pixels [1]. A major point is to determine their blocking capability. Therefore the simulation needs to describe both passing and blocking characteristics. The transistors are made of a thin undoped polycrystalline silicon film deposited on a glass substrate (figure 1). The film thickness is about 500 Å. The monocrystalline grain thickness is the layer thickness. The grain size, in the film plane, is about 3000 Å. The drain and source contacts are made of n+ polycrystalline silicon.

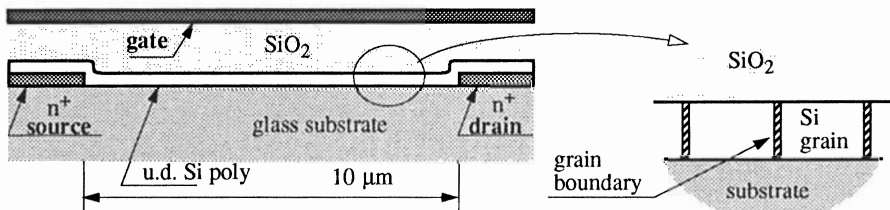

Figure 1 : Polycrystalline Silicon Thin Film Transistor structure, and detail of the grains.

The grain surface has a major influence on the conduction properties of the thin film. The surface lattice defect implies silicon dangling bonds and band tail densities which govern the surface charge density and the recombination-generation mechanisms. The grain boundary medium is a disordered material (amorphous) with a large band gap, comparable to an oxide one. The conduction through the grain boundary (about 10 Å thick) is governed by tunnel effect. The monocrystalline silicon grains are supposed to have the same energy band structure as bulk silicon,

except at the surface where dangling bonds and band tails are added.

2. Physical model

The modelling of the layer supposes parallelepipedic monocrystalline grains. The physical model describing the steady state conduction in semiconductor material is composed of Poisson's equation $\nabla (\varepsilon \cdot \nabla \bullet \varphi) = -\rho$ (1)

and electron and hole balance equations $-\frac{1}{q} \cdot \nabla \bullet J_n = -U \; ; \; \frac{1}{q} \cdot \nabla \bullet J_p = -U$ (2)

2.1 Grain material

In the grains (bulk silicon), the carrier densities are expressed within Maxwell-Boltzmann statistics $n = N_c \cdot exp(-\frac{E_c - E_{Fn}}{k \cdot T}) \; ; p = N_v \cdot exp(\frac{E_v - E_{Fp}}{k \cdot T})$ (3)

and the charge density is $\rho = -q \cdot (n - p - dop)$ (4)

where dop is the residual doping density.

The drift-diffusion model is used for the electron and hole current densities (including a mobility law to take into account the high field velocity saturation) :

$$J_n = n \cdot \mu_n \cdot \nabla E_{Fn} \qquad J_p = p \cdot \mu_p \cdot \nabla E_{Fp} \quad \text{with } \mu_{n,p} = \frac{\mu_{0n,p}}{1 + \frac{\mu_{0n,p}}{v_{Sn,p}} \cdot \left|\frac{1}{q} \cdot \nabla E_{Fn,p}\right|} \quad (5)$$

The recombination-generation is governed by the Shockley-Hall-Read mechanism:

$$U_{SHR} = \frac{n \cdot p - n_i^2}{\tau_p \cdot (n + n_i) + \tau_n \cdot (p + n_i)} \quad (6)$$

In the blocking mode (hole accumulation), high fields appear in the space charge region close to the drain contact due to the reverse diode biased effect (figures 2, 3).

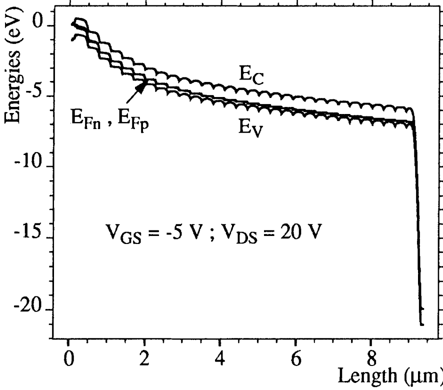

Figure 2: Band diagram along the channel in blocking mode showing both serial resistance effect and diode voltage drop on drain side.

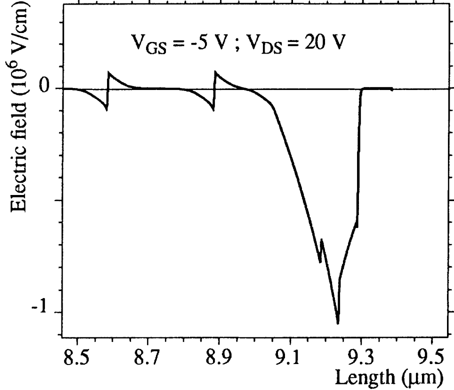

Figure 3: Enhancement of the near drain region showing the very high electric field values (blocking mode).

This induces electron and hole generation by impact ionisation :

$$G_{In,p} = \frac{1}{q} \cdot \alpha_{n,p} \cdot |J_{n,p}| \text{ with } \alpha_{n,p} = \alpha_{0n,p} \cdot exp\left(-\frac{E_{n,p}}{\left|\frac{1}{q} \cdot \nabla E_{Fn,p}\right|}\right) \quad (7)$$

So that the total recombination-generation term is $U = U_{SHR} - G_{In} - G_{lp}$ (8)

2.2 Grain surface and grain boundary

Band tails and ionised dangling bonds densities govern the equilibrium of the grain surface. The carrier surfacic densities in the band tails are :

$$n_s = \int_{-\infty}^{E_c} \frac{N_{0c} \cdot exp\left(-\frac{E_c - E}{E_{0c}}\right)}{1 + exp\left(\frac{E - E_{Fn}}{k \cdot T}\right)} \cdot dE \; ; \quad p_s = \int_{E_v}^{\infty} \frac{N_{0v} \cdot exp\left(\frac{E_v - E}{E_{0v}}\right)}{1 + exp\left(\frac{E_{Fp} - E}{k \cdot T}\right)} \cdot dE \quad (9)$$

where N_{0c} and N_{0v} are the effective state densities in the conduction and valence band tails ;. E_{0c} and E_{0v} are the respective energy extrema of the band tails. The dangling bonds of the silicon atoms make appear two deep energy levels E_{lp1} and E_{lp2}. The total dangling bond surfacic charge density is summation of the two ionised states of this amphoteric defect [2].

$$N_{lp}^- = N_{lp} \cdot \frac{n_s + p_{s1}}{(n_s + n_{s1}) + (p_s + p_{s1})} \; ; \; N_{lp}^+ = N_{lp} \cdot \frac{n_{s2} + p_s}{(n_s + n_{s2}) + (p_s + p_{s2})} \quad (10)$$

where $n_{s(1,2)} = n_s \cdot exp\left(\frac{E_{lp(1,2)} - E_{Fn}}{k \cdot T}\right) \quad p_{s(1,2)} = p_s \cdot exp\left(\frac{E_{Fp} - E_{lp(1,2)}}{k \cdot T}\right)$

the charge density is then $\rho_s = -q \cdot (n_s - p_s + N_{lp}^- - N_{lp}^+)$ (11)

The surfacic recombination is governed by the capture emission process between band tails and dangling bonds :

$$U_{lp} = N_{lp} \cdot C_{lp} \cdot \left(\frac{n_s \cdot p_s \cdot \left(1 - exp\left(\frac{E_{Fn} - E_{Fp}}{k \cdot T}\right)\right)}{(n_s + n_{s1}) + (p_s + p_{s1})} + \frac{n_s \cdot p_s \cdot \left(1 - exp\left(\frac{E_{Fn} - E_{Fp}}{k \cdot T}\right)\right)}{(n_s + n_{s2}) + (p_s + p_{s2})} \right) \quad (12)$$

The conduction through the grain boundaries is described by electron and hole tunnel effects.

$$J_n = -q \cdot v_n \cdot \Pi \cdot n \cdot \left(1 - exp\left(\frac{\Delta E_{Fn}}{k \cdot T}\right)\right) \text{ and } J_p = q \cdot v_p \cdot \Pi \cdot p \cdot \left(1 - exp\left(\frac{\Delta E_{Fp}}{k \cdot T}\right)\right) \quad (13)$$

where ΔE_{Fn} and ΔE_{Fp} are the variations of the imref at the grain boundary ; n, p are the carrier concentrations at the surface of the grain. Π is the transmission factor of the intergrain medium and $v_{n,p}$ is the thermionic emission velocity [3].

The interband tunnel effect (Zener) which appears on the top of the drain contact for large gate biases in blocking mode is added to these mechanisms [4]. This mechanism depends directly on the electric field induced by the gate on the top of the n+ material.

3. Numerical method

The numerical model is composed of the equations 1 to 13 describing the different mechanisms. The discretisation scheme is a Box Method [5] type which allows to describe easily the surfacic terms. The internal behaviour of each grain and grain boundary has to be described. A full 2D simulation leads to a prohibitive number of nodes. In order to minimize the number of nodes the discretisation is simplified so as to have a 2D description of Poisson equation and a 1D description of the balance equations (see figure 4). So that the total equation set can be solved within a 1D direct coupled method.

4. Application

Figure 5 shows the characteristics of the structure described in figure 1. This figure shows both the passing and blocking characteristics. This classical device exhibits an excess of current under blocking operation which may penalize its use in flat liquid crystal display applications. The origin of the excess current is both impact ionisation and Zener effects. These mechanisms which increase rapidly with the fields are presently limited by the grain surface recombinations on the dangling bonds. No breakdown can be observed in the blocking characteristics because of this very efficient limiting mechanism. A new offset-gate structure has been optimized by means of the simulator [6]. This type of device does not exhibit any excess current. The study permitted to verify the quality of the simulator to predict the behaviour of new devices

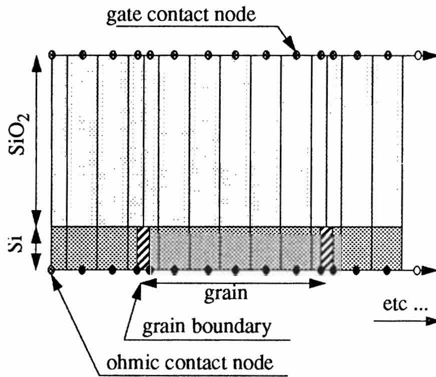

Figure 4 : Box method discretisation scheme used to simulate the transistor structure, including the grain boundaries. The unknown nodes are black dots.

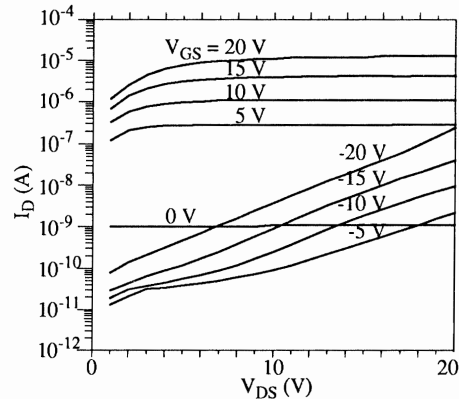

Figure 5 : Simulation showing the dynamics between blocking ($V_{GS} < 0$) and passing ($V_{GS} > 0$) characteristics.

References :

[1] B. Loisel, L. Haji, P. Joubert and M. Guendouz, "Crystallized silicon films for actives devices", Springer Proceedings in Physics 35, pp. 283-288 (1988)

[2] J. Hubin, A.V. Shah and E. Sauvin,"Effects of dangling bonds on the recombination function in amorphous semiconductors," Philosophical Magazine Letters, Vol. 66, No. 3, pp. 115-125, (1992)

[3] S. Mottet and J.E. Viallet, "Thermionic emission in semiconductors," SISDEP, Vol.3, Ed. G. Baccarani, M. Rudan - Bologna (Italy), pp. 97-108, (1988)

[4] A. Schenk, "Rigorous theory and simplified model of the band to band tunneling in silicon," Solid-State Electronics, Vol. 36, No. 1, pp. 19-34, (1993)

[5] C. Simon, S. Mottet and J.E. Viallet, "Autoadaptative Mesh Refinement", SISDEP, Vol. 4, Ed. W. Fichner, D. Aemmer (Hartung-Gorre), pp. 225-233,(1991)

[6] M. Bonnel, N. Duhamel, M. Kandouci, B.Loisel and Y. Pelous, "Si Poly TFT's with low off-current for flat panel displays," Proceedings of EURODISPLAY' 93, Strasbourg (F), sept (1993)