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Spatio-temporal Simulation of a Microjunction

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Abstract: The goal of the simulation of electronic transport is to obtain, starting from the geometrical and physical description of a device, behaviours in static or dynamic mode of the charge carriers (electrons and holes), according to the boundary conditions (polarizations applied, currents injected, emission of light). One of the results usually used is for example the characteristic current-voltage of the component, which makes it possible to extract a great number of information on its performances. The physical model generally retained for the simulation of electronic transport corresponds to a strongly nonlinear system of equations and posing very many problems in terms of stability and quality of convergence. Moreover, the simulation of the devices, with heterojunctions, introduced new problems, unknown in micro-electronics of the devices, such as the appearance of discontinuities of material in the structure, which make the case still much more delicate to solve. The solutions adopted to be able to free it self from these difficulties now also found besides applications in the simulation of silicon- silicon polycrystalline junctions. The present study, explains in detail the physical and numerical models used in our study of a p-n silicon microjunction.

Key words: Microjunction, silicon, transport characteristics, Gummel and Scharfetter model, simulation

INTRODUCTION

Optoelectronics industry unceasingly directing towards a miniaturization increasingly more pushed size of the electronic devices, problems of scale arise: with low dimensionality the properties of materials are changeable. The search for materials having the good properties and making it possible to preserve the chains of industrial production to integrate them in the circuits is essential. In industry, the interest of the semiconductors (in particular silicon) is multiple: contrary to metals, they lead better and better when their temperature increases and they have a better conductivity than metals. Moreover, one can manufacture "perfect" semiconductors, quasi-crystalline; by controlling doping one very precisely controls the number of carriers and thus the electronic properties. The use of P/N junctions (a semiconductor doped P and one doped N) is very much used for all the devices of the diode type (lets pass the current only in one direction); this kind of junction also reveals interesting optical properties (electroluminescent, laser diodes with semiconductors...). The world of electronics could not thus occur without these invaluable semiconductors, which are at the base of the majority of the devices.

The study of p-n junction is important for the electronic applications and comprehension of the operation of semiconductor's components. The most important characteristic of these junctions is the modulation of the direction of the current, the switchage and other operations in the electronic circuits. This junction constitutes the base of manufacture of the thyristors and the bipolar transistors, like for JFETs and MOSFETs. Exposed to luminous radiations, the p-n junction can function like a microwave or a photonic device (Sze, 1985). Various models can be used to study the properties of the junction theoretically: abrupt, exponential, gradual junction (Schockley, 1952; Filoche, 1992; Marshak, 1987). We consider a monocrystal of semiconductor, in which the concentrations of the additives, N_a and N_d, are variable of a point to another. If on the assumption that all the additives are ionized at the ambient temperature, there is a surface which we will suppose generally plane, on which $N_a = N_d$, one says that it is a junction. The difference of the densities of donors and acceptors ($N_d - N_a$) passes from a negative value in the area of the type p to a positive value in the area of the type n. The law of variation of this size depends primarily on the technique of manufacture. We will limit present study of the p-n junction if the crystal is a silicon semiconductor bar, the concentrations N_a and N_d depending only on one direction, x, direction length of the bar. Obtaining a junction can be attaining only by special techniques: alloy, diffusion, epitaxy, ionic implantation (Sze, 1985).

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PHYSICAL MODEL OF A P-N JUNCTION

The model of the abrupt junction gives results in very good agreement with the behaviour of the microjunction. It is the model which we will develop. The basic equations used in the simulation of any semiconductor's device are the equations of continuity of the electrons and holes according to the density of the charge carriers' j and the rate of generation recombination G of the carriers in agreement with Snowden (1988), Mathieu (1996) and De *et al.* (1994).

$$\frac{\partial n}{\partial t} = \frac{1}{q}\vec{\nabla}.\vec{j}_n - qG \tag{1}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\vec{\nabla}.\vec{j}_p - qG \tag{2}$$

The electric field E and the potential V are related with the charge q in material by the Poisson's equation:

$$\vec{\nabla}.\vec{E} = -\nabla^2 V = \frac{q}{\varepsilon_0 \varepsilon_r}\left(N_D - N_A + p - n\right) \tag{3}$$

NUMERICAL MODEL

The numerical solution of any system of equations requires that the domain of simulation chosen to represent the geometry of the component must be partitioned in a number of discrete areas, which make it possible the numerical method to complete the desired precision. The partial differential equations which constitute the equations characterizing a semiconductor are approximated in each area by a whole of equations which describe the variables at specific points of the field. This operation is called the discretization and gives a whole of nonlinear equations (Snowden, 1988). Numerical techniques are then employed to solve this whole of equations. Among these methods the most used to solve these equations are the finite differences and of the finite element's methods. In what follows we treat the method of finite differences in which the method of Gummel and Scharfetter evolves in agreement with Mohammad (1992), Lin *et al.* (1992), Liou (1992), Singh *et al.* (1996), Vecchi and Reyna (1994), Kobeissi *et al.* (1993), Akcasu (1984), Yoshi *et al.* (1987).

Presentation of the model: The space-time evolution of the carrier's densities and the electric potential is obtained by the integration of the equations of continuity and transport equations for the densities of charged particles and of the Poisson's equation for the potential. We present in what follows the model used to integrate these equations in space-time. This model was developed for problems of charge transport in the semiconductors by Kurata (1982). The three basic variables are: the electronic density n, the density of the holes p and the potential V, which they depend on position x and time t.

Equations used: The system of equations to be solved includes:

Equations of continuity (1) and (2), but by replacing this time the density of current j by the flow of the charge carriers $\Phi = j/q$:

$$\frac{\partial n}{\partial t} + \frac{\partial \Phi_n}{\partial x} = G_n \tag{4}$$

$$\frac{\partial p}{\partial t} + \frac{\partial \Phi_p}{\partial x} = G_p \tag{5}$$

The terms source G_n and G_p represent the rates of recombination generation of the electrons and holes, respectively. Flows Φ_n and Φ_p are given by the transport equations:

$$\Phi_n = n\mu_n E - D_n \frac{\partial n}{\partial x} \tag{6}$$

$$\Phi_p = p\mu_p E - D_p \frac{\partial p}{\partial x} \tag{7}$$

$$E = -\frac{\partial V}{\partial x}$$

Poisson equation with $N_D = N_A$:

$$\nabla^2 V = \frac{q}{\varepsilon_0 \varepsilon_r}\left(n - p\right) \tag{8}$$

Integration in time-iteration of newton: The general principle of integration in the time used in this model rests on the following principle: Let us suppose that the space variations of n, p and V are known at the moment t^0: n^0, p^0, V^0. At the moment $t = t^0 + \Delta t$, these sizes becomes: $n_t = n^0 + \delta n$, $p_t = p^0 + \delta p$ and $V_t = V^0 + \delta V$. A change of variables in the system of equations makes it possible to express this one according to the increments δn, δp and δV. The values of n_t, p_t and V_t are then obtained by an iterative method, said method of Newton (Benaissa, 2001).

Discretization of the equations

Discretization in space: The space of the junction is represented by a grid of nx+1 points: The position of the

point x = 0 corresponds to i = 1, the position of the point x = xmax corresponds to i = nx + 1. The fundamental variables (ϕ_n, ϕ_p, E...) are defined in the medium of the meshes (points i+1/2). One supposes in the continuation that the grid is uniform $\Delta x = \Delta x_i = \Delta x_{i+1}$.

Discretization in time: The successive moments are subscripted t^k, t^{k+1}...the interval of time between two successive moments is Δt, such as $t^{k+1} = t^k + \Delta t$. The resolution of the equations is done at initial moment t_0 (= $t^{k=1}$), to the final moment t_f, by increments of Δt. After discretization, the equations become:

$$\frac{n_i^{k+1} - n_i^k}{\Delta t} + \frac{1}{2}\left[\left(\frac{\partial \Phi_n}{\partial x}\right)_i^{k+1} + \left(\frac{\partial \Phi_n}{\partial x}\right)_i^{k}\right] = \frac{1}{2}\left(G_{ni}^{k+1} + G_{ni}^{k}\right),$$

i = 1, nx (9)

$$\frac{p_i^{k+1} - p_i^k}{\Delta t} + \frac{1}{2}\left[\left(\frac{\partial \Phi p}{\partial x}\right)_i^{k+1} + \left(\frac{\partial \Phi p}{\partial x}\right)_i^{k}\right] = \frac{1}{2}\left(G_{ni}^{k+1} + G_{ni}^{k}\right),$$

i = 1, nx (10)

$$\frac{V_{i-1}^{k+1} - 2V_i^{k+1} + V_{i+1}^{k+1}}{\Delta x^2} + \frac{e}{\varepsilon_0}\left(p_i^{k+1} - n_i^{k+1}\right) = 0\,,$$

i = 1, nx (11)

Linearization of flows: As one already mentioned higher, the variables n, p and V will be replaced in the system by their increments δn, δp and δV. The terms

$$\left(\frac{\partial \Phi_n}{\partial x}\right)_i^{k+1}$$

must be transformed to be also expressed according to these increments.

$$\left(\frac{\partial \Phi_n}{\partial x}\right)_i^{k+1} = \left(\frac{\partial \Phi_n}{\partial x}\right)_i^{0} + \left(\frac{\partial(\delta\Phi_n)}{\partial x}\right)_i$$

and $$\left(\frac{\partial(\delta\Phi_n)}{\partial x}\right)_i = \frac{\delta\Phi_{ni+1/2} - \delta\Phi_{ni-1/2}}{\Delta x_i}$$

A development in Taylor series to order 1 of $\delta\Phi_{ni+1/2}$ gives:

$$\delta\Phi_{ni+1/2} = \frac{\partial\Phi_{ni+1/2}}{\partial n_i}\delta n_i + \frac{\partial\Phi_{ni+1/2}}{\partial V_i}\delta V_i + \frac{\partial\Phi_{ni+1/2}}{\partial V_{i+1}}\delta V_{i+1}$$

To carry out a change of variables, one replaces n^{k+1}, p^{k+1} and V^{k+1} by $n^0+\delta n$, $p^0+\delta p$ and $V^0+\delta V$.

Writing in matrix form: The change of variables carried out, each equation is transformed into nx equations since i vary from 1 to nx. One thus defines the matrix δX, made of nx elements δX_i and each element δX_i is a vector of the form:

$$\delta X_i \;:\begin{pmatrix}\delta n_i\\ \delta p_i\\ \delta V_i\end{pmatrix}$$

The system can then be written:

$$A_i\delta X_{i-1} + B_i\delta X_i + C_i\delta X_{i+1} = D_i \qquad (i = 1, nx) \qquad (12)$$

The resolution of the system (12) is summarized with the inversion of a tridiagonale matrix per blocks.

Discretization of flows: The diagram of Scharfetter and Gummel (1969) is used to obtain the expression of Φ (Φ_n or Φ_p) at the points i+1/2. The final form of Φ is obtained by supposing that the mobility and the coefficient of diffusion are constant between two items i and i+1 and by integrating the Eq. (6) between these two points. The expression obtained is:

$$\Phi_{i+1/2} = \frac{1}{e^z - 1}\frac{z}{\Delta x}\left(n_i D_i e^z - n_{i+1}D_{i+1}\right)$$

$$z = -\frac{\mu_{i+1/2}}{D_{i+1/2}}\left(V_{i+1} - V_i\right)$$

Or:

$$\Phi_{i+1/2} = \frac{1}{\Delta x}\left(n_i D_i a_i - n_{i+1}D_{i+1}b_i\right)$$

$$a_i = \frac{ze^z}{e^z - 1} \quad \text{and} \quad b_i = \frac{z}{e^z - 1}$$

*The expressions of derived from flows compared to the densities are obtained directly:

$$\frac{\partial\Phi_{i+1/2}}{\partial n_i} = \frac{1}{\Delta x}D_i a_i$$

$$\frac{\partial\Phi_{i+1/2}}{\partial n_{i+1}} = -\frac{1}{\Delta x}D_{i+1}b_i$$

$$\frac{\partial\Phi_{i-1/2}}{\partial n_{i-1}} = \frac{1}{\Delta x}D_{i-1}a_{i-1}$$

$$\frac{\partial\Phi_{i-1/2}}{\partial n_i} = -\frac{1}{\Delta x}D_i b_{i-1}$$

Table 1: Data (Zommiti, 1982) used in the study of silicon p-n microjunction at T = 300°K

Parameters	Values
Intrinsic concentration of silicon n_i (cm^{-3})	1.4×10^{10}
Length of the junction x_d (μm)	10-100
Biasing (V)	0-1
Electrons lifetime τ_n (s)	8.4×10^{-10}
Holes lifetime τ_p (s)	3×10^{-10}

CONDITIONS AND PARAMETERS OF CALCULATION

Table 1 collects data (Zommiti, 1982) used in the study of a p-n microjunction of silicon at T = 300°K by the method of Gummel and Scharfetter.

RESULTS AND DISCUSSION

Evolution of the characteristics of a nonpolarized abrupt P-N junction: The space evolution of the holes and electrons charge carriers, if the junction is not polarized, is represented on the Fig. 1a. At thermal equilibrium, the majority carriers' densities of electrons and holes within dimensions N and P, respectively are primarily equal to the completely ionized concentrations of doping N_D and N_A (symmetrical p-n junction). The interface considered as the zone depopulated by the majority free carriers but occupied mainly by the negative and positive ions, extends from x = 0.002 to 0.003 cm on the figure. On the level of this interface precisely exists an electric field due to the ions whose evolution is represented on the Fig. 1b, the density of free carriers in this area is negligible. Moreover the borders between the depopulated zone and the neutral zones of the junction are very abrupt. The presence of the electric field involves a d.d.p which is the potential of diffusion V_d between the neutral areas P and N of the p-n junction (Fig. 1c). This potential barrier and

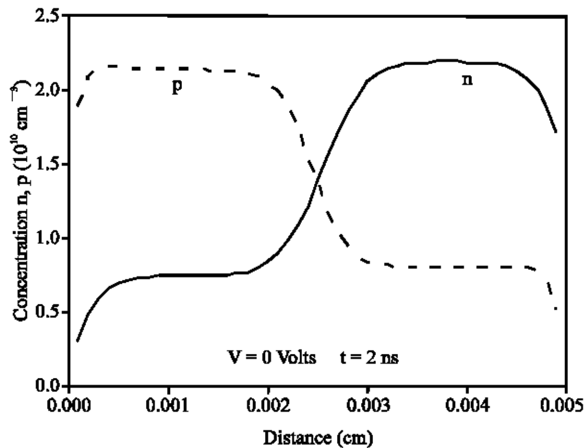

Fig. 1a: Space evolution of n and p concentrations at time t = 2 ns

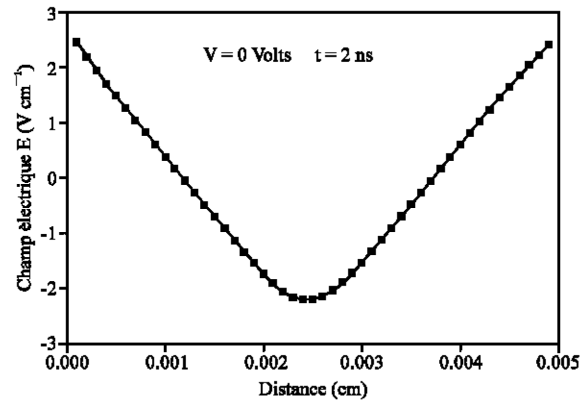

Fig. 1b: Space evolution of the electric field at time t = 2 ns

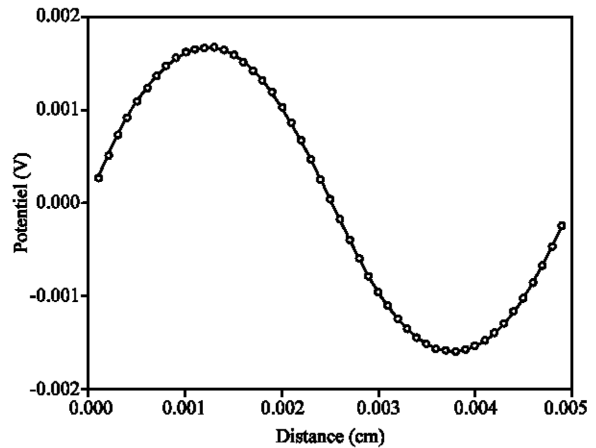

Fig. 1c: Space evolution of the electric potential at time t = 2 ns

the electric field which accompanies it directed N towards P, is opposed in the passing majority carriers from one area to another. This opposition however isn't total because one knows that at T ≠ 0°K, there exist always electrons and holes which have important energies, but their number decrease exponentially with energy considered. It results from it that the tension of diffusion limit, but does not completely prevent the passage of the holes of P towards N, nor that of the electrons of N towards P. Near N and P junction dimensions, the concentrations of the charge carriers reach constant levels, as indicated in Benaïssa (2001) thesis. The space evolution of the carriers' densities which we studied corresponds perfectly to the profile of the carriers envisaged by the model of Shockley (1952) and Zommiti (1982).

Evolution of the characteristics of a polarized P-N junction: When one polarizes the junction with a positive tension V, one modifies the potential barrier and

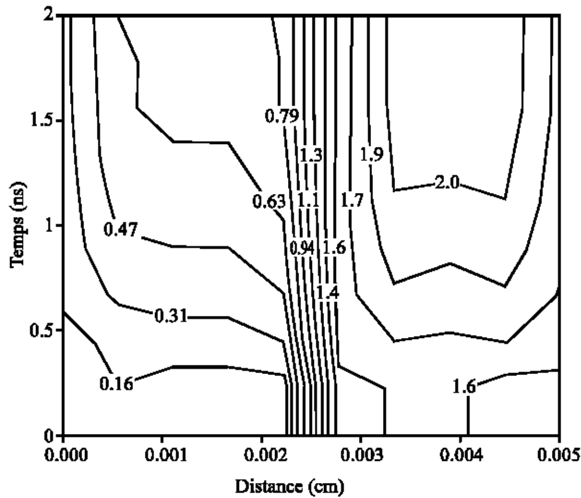

Fig. 2a: Space-time evolution of the electrons concentration in level lines for V = 0.4 V

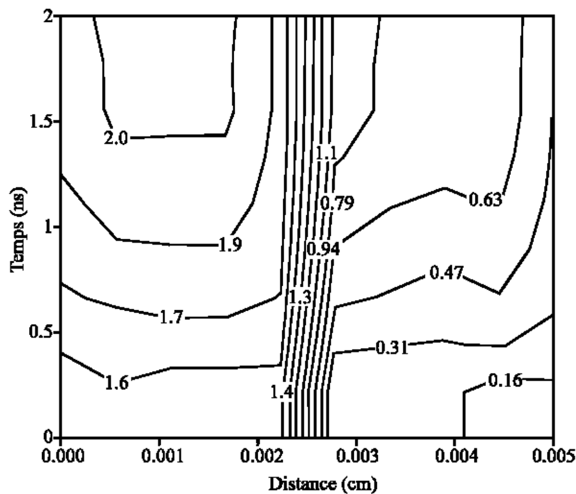

Fig. 2b: Space-time evolution of the holes concentration in level lines for V = 0.4 V

consequently the diffusion of the carriers of an area towards the other (Fig. 2g). The height potential barrier $q(V_d\text{-}V)$ is not sufficient any more to stop the diffusion of the carriers; the electrons diffuse area N towards the area P and the holes of the area P towards area N. The junction is polarized in the direct direction; the forward current circulates of the area P towards area N. The tension applied is not sufficient to create an important concentration of carriers. The carriers' charge density in the junction practically did not change, because we placed ourselves on the assumption of low level of injection. i.e., those in each area, the majority carriers at thermodynamic equilibrium remain majority when the junction is polarized. In other words we suppose that the

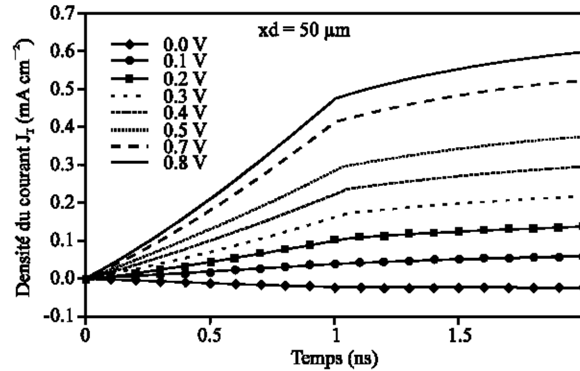

Fig. 2c: Temporal evolution of the total current density for xd = 50 μm and several polarizations V

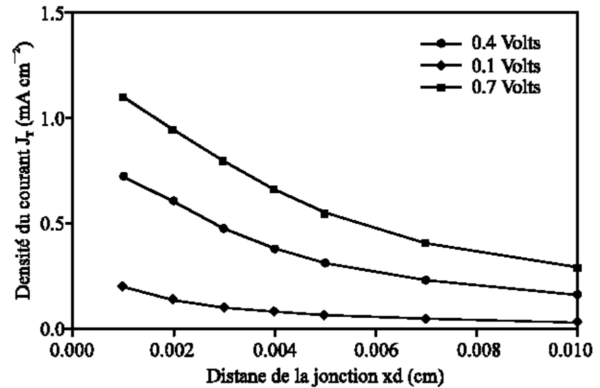

Fig. 2d: Space evolution of the total current density for polarizations of 0.1, 0.4 and 0.7 V

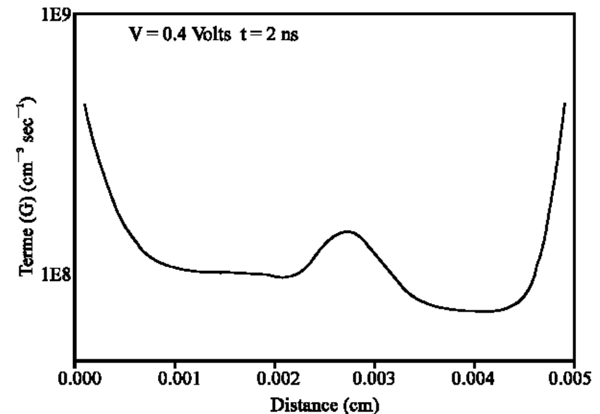

Fig. 2e: Space evolution of the recombination generation rate for a polarization V = 0.4 V at time t = 2 ns

majority carriers' density in each area is not affected by polarization (Fig. 2a, b). The p-n junction is the seat of thermal generations and recombinations. At the interface, the carriers' density is low because of the recombinations which are important and prevalent in this case of direct polarization and the conditions of weak injection. Thus,

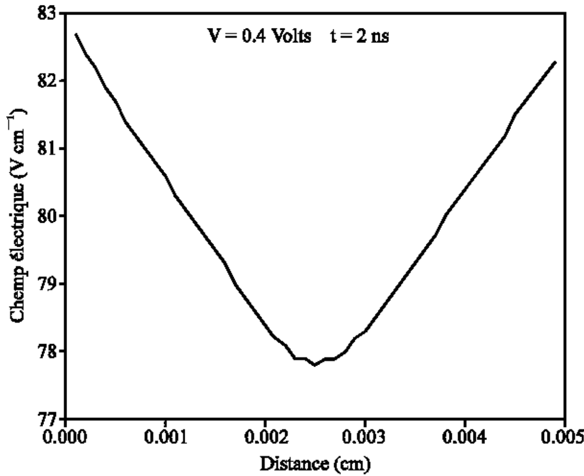

Fig. 2f: Space evolution of the electric field for a polarization V = 0.4 V at time t = 2 ns

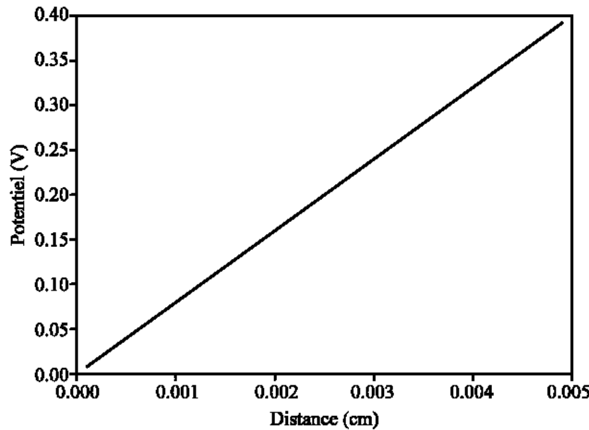

Fig. 2g: Space evolution of the electric potential for a polarization V = 0.4 V at time t = 2 ns

because of the phenomena of recombination generation, the currents of the electrons and the holes are not constant with the crossing of the interface of the junction in x = xj, but are modified by creations due to impact moreover of carriers recombinations. This is precisely justified by the rate of g-r G of the Fig. 2e, which differs from area N to area P of the direct polarized junction. This rate of recombination generation which is governed by the lifetime of the minority carriers, evolves with dimension x_d of the polarized p-n junction. When the junction is not polarized, the rate G is due mainly to the rate of thermal g-r $G_{thermiq}$. By polarizing the junction, the impact of the ions takes part more in this phenomenon of g-r and this G_{impact} rate contributes more to the total rate of g-r G. The rate G is important at the edges of the junction where the density of majority carriers is maximum and where the ionic impact is important. A direct tension

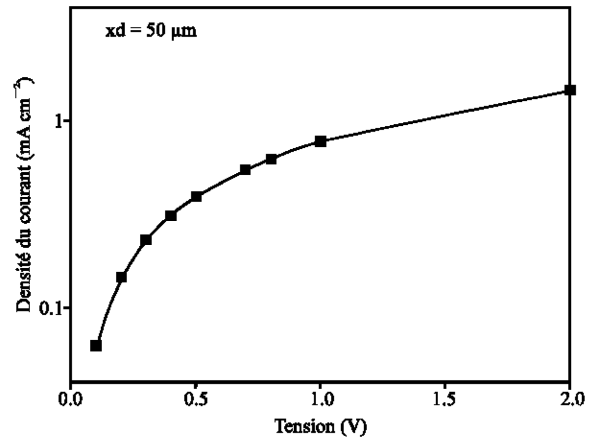

Fig. 2h: The characteristic current-voltage of the abrupt p-n microjunction at t = 2 ns for xd = 50 µm

applied to the junction decreases the height of the potential barrier. The own junction resistance decreases what implies that the total current density junction increases and grows with the applied tensions 0.1, 0.4 and 0.7 V in time and decreases with the dimension of the sample (Fig. c-g). On the Fig. 2h we notice that starting from V = 1V, the current density tends towards a certain constant value, because generally in the p-n junctions the value of the direct tension is lower than 1V in order to avoid the breakdown tension of the junction, in agreement with Sze (1985).

CONCLUSIONS

The simulation method of Gummel and Scharfetter enable us to calculate various important parameters in the abrupt microjunction, like the carriers' charge densities, current densities, electric field and potential, according to the time or to the junction polarity. The characteristic current-voltage calculated in direct polarization of the abrupt junction, gave satisfactory results in agreement with the physical properties of a p-n junction (Snowden, 1988). The simulation method used for the model of the abrupt p-n junction thus allows the calculation and the study of any physical junction parameter with an impressive and satisfactory exactitude at the same time. Gummel's and Scharfetter simulation method is a method which proved already reliable and brought solutions in the resolution of physical problems in much of systems, where analytical calculations or did not make it possible to lead to the possible results, or although they were too extravagant and tortuous, provides important results as for the evolution of the characteristics and properties of a p-n microjunction.

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