THREE-DIMENSIONAL DEVICES TRANSPORT SIMULATION LIFETIME AND RELAXATION SEMICONDUCTOR

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Abstract:- Our objectif consists in creating a 3D three-dimensional simulator conceived for the study of components with low geometry of conception, allows determining in the volume of a structure, the distributions of potential and the densities of free carries according to a given polarization, by resolution of Poisson 's equation as well as both equations of continuity.
The initial version can simulate components based on lifetime semiconductor.
Our work consists in making a comparison between lifetime and relaxation semiconductors in the conduction mode, with the aim of creating a more developed simulator.
We consider the case corresponding to two values very different from diffusion lifetime τ_0 which is a measure of the life expectancy in diet of transport, corresponding to two different semiconductor, lifetime and relaxationSC.
The method of resolution consists of a linearization of the equations of transport by the method of a finite-difference. The algorithm adapted to the resolution of the not linear equations and strongly coupled ensuing from the physical model is the one of Newton Raphson, However to allow better one convergence and consequently an improvement in the weather of 3D calculation often prohibitive, a combined method, integrating at the same time the algorithm of Newton and that of Gummel was finalized.
The tests of simulation for the validation of the model are made on the long diodes of type PIN.

Key words: Lifetime semiconductor, relaxation semiconductor, three-dimensional Simulation, Newton algorithm, Gummel algorithm

1 Introduction

With the aim of improving the software 3D SIM developed within our laboratory, we created a more general tool allowing calculating the distributions of potential and the concentrations of the free carriers, by a digital resolution of the equations of transport for semiconductors III-V.
For a value τ_0 very upper in the time of dielectric relaxation τ_{rd}($\tau_{rd} << \tau_{0)}$ **[1]** the obtained results can be analyzed by using of simple injection and by supposing a common lifetime of the carriers in excess wich is constant for electrons and holes through the region ν this type of semiconductor will be called a life semiconductor according to Van Roosbroeck's terminology.
Should the opposite occur or τ_0 is very lower in the time of Dielectric relaxation τ_{rd} ($\tau_{rd} >> \tau_0$), the effects of load of space is very important by everything and the life expectancies of the carriers in excess vary a great deal of a point to another one along the structure.This type of semiconductor will be called relaxation semiconductor. It is the case of GaAs.
The algorithm best in compliance with the resolution of the not linear equations in the differences partial ensuing from the physical established model is the one of Newton, this method however converges quickly only if the
introduced values are suitably chosen, we thus adapted a combined method, which gathers at the same time the method of Gummel and that of the Newton, so creating

a relay between both algorithms, allowing at the end a decrease of calculation time and a better convergence. We are going to be interested to do the calculation of the potential, the density of electrons and free holes for the semiconductor with life expectancy and with relaxation in the balance thermodynamics and under polarization for different tensions.
We present in the order the adapted mathematical model, as well as the used physical model, the digital model followed by the results of modeling and their interpretation

2 Three-Dimensional Representation Of The Physical Equations [2]-[3]

In the stationary case and for the analysis of a homogeneous structure in three dimensions, the Basic (Fish and continuity) equations take the following form [4]-[5]

$$\begin{cases} \dfrac{\partial^2\psi}{\partial x^2}+\dfrac{\partial^2\psi}{\partial y^2}+\dfrac{\partial^2\psi}{\partial z^2}=\dfrac{q}{\varepsilon}.\left(n-p+N_D^+-N_A^--n_r\right) \\ \dfrac{1}{q}.\left(\dfrac{\partial j_n}{\partial x}+\dfrac{\partial j_n}{\partial y}+\dfrac{\partial j_n}{\partial z}\right)=U \\ \dfrac{1}{q}.\left(\dfrac{\partial j_p}{\partial x}+\dfrac{\partial j_p}{\partial y}+\dfrac{\partial j_p}{\partial z}\right)=-U \end{cases} \quad (1)$$

With

$$U=U_n=U_p=\frac{n.p-n_1.p_1}{\tau_{pe}.(n+n_1)+\tau_{ne}.(p+p_1)}$$

$$j_n=q.n.\mu_n.\left(\frac{\partial\psi}{\partial x}+\frac{\partial\psi}{\partial y}+\frac{\partial\psi}{\partial z}\right)+q.D_n.\left(\frac{\partial n}{\partial x}+\frac{\partial n}{\partial y}+\frac{\partial n}{\partial z}\right)$$

$$j_p=q.p.\mu_p.\left(\frac{\partial\psi}{\partial x}+\frac{\partial\psi}{\partial y}+\frac{\partial\psi}{\partial z}\right)-q.D_p.\left(\frac{\partial p}{\partial x}+\frac{\partial p}{\partial y}+\frac{\partial p}{\partial z}\right) \quad (2)$$

With

$\varepsilon=\varepsilon_o.\varepsilon_r$ The dielectric permittivity of the semiconductor
ε_o : The permittivity of vacuum
ε_r : Relative to the semiconductor permittivity
ψ: Electrostatique potentiel
q: elementary charge $=1.6.10^{-19}$ C
p et n : free holes and electrons densities
N_D^+ et N_A^- : donors and acceptors ionized densities
n_r: The charge trapped on a deep centre. Where there are n deep centers be replaced nr by

$$\sum_{i=1}^{n} n_{ri}$$

$j_n$et j_p : vector current densities of electrons and holes
μ_n et μ_p : mobilities of electrons and holes. D_n et D_p: Diffusion of électrons and holes constants

$$\frac{D_n}{\mu_n}=\frac{K.T}{q} \qquad et \qquad \frac{D_p}{\mu_p}=\frac{K.T}{q} \quad (3)$$

With
K : BOLTZMANN constant
T : absolue temperature.
μ_n et μ_p : mobilities of electrons and holes

We shall study the transport of loads in a material having a low density N_R of combining center, the space charge-trapped – (enr) is low compared with the space charge of the free carriers and the donors or the ionized acceptors. The recombination plays an important role, it depends on values of the parameters τ_{ne} and τ_{pe}, the time of dielectric relaxation τ_{rd} and the diffusion lifetime τ_o are important for analyzing the behavior, under conditions of not balance of a given semiconductor.

$$\tau_{rd}=\frac{\varepsilon}{\sigma_e}=\frac{\varepsilon}{e\left(n_e\mu_n+p_e\mu_p\right)} \quad (4)$$

$$\tau_o=\frac{\tau_{ne}(p_e+p_t)+\tau_{pe}(n_e+n_t)}{(n_e+p_e)} \quad (5)$$

These two characteristic times allow defining both categories of semiconductors:
Lifetime semi-conductor $\tau_{rd} \ll \tau_0$
Relaxation semiconductor $\tau_{rd} \ll \tau_0$

3. Numerical model [6]-[7]

First of all we were interested to realize a not uniform meshing which allows establishing from the application of a calculation based on a geometrical series of reason has a variable meshing. This type of meshing can be unrefined in neutral regions and squeezed in the nearby regions of the interface P+ν The calculation of the electric parameters in the equilibrium thermodynamics is deducted by the application of the method of Gummel called also method decoupled [8][9].
The method of Gummel consists of a successive resolution of three systems coupled of N equations in N unknowns. Every system of equation is dedicated to determine the value of a single type of unknown.For example Poisson's equation supplies the values of the potential ψ On the basis of the concentrations N and P.
The general principle of the method of Gummel is the following one:
From an estimated initial solution (ψ_0, N_0, P_0), the equation $F\psi(\psi,N,P)=0$ of the unknown ψ Is solved in the first one. The values of ψ so determined will be

postponed in the systems of equation Fn and Fp.
The equation F_n (ψ, N, P) 0 is so updated and solved in his turn for the unknown N. this process of update and resolution is repeated by alternation for F_ψ, F_n, F_p until complete convergence of the system.
Or:

$$\begin{cases} \dfrac{\partial^2\psi}{\partial x^2}+\dfrac{\partial^2\psi}{\partial y^2}+\dfrac{\partial^2\psi}{\partial z^2}-\dfrac{q}{\varepsilon}.\left(n-p+N_D^+-N_A^--n_r\right)=0= \\ \dfrac{1}{q}.\left(\dfrac{\partial j_n}{\partial x}+\dfrac{\partial j_n}{\partial y}+\dfrac{\partial j_n}{\partial z}\right)-U=0=f_n \\ \dfrac{1}{q}.\left(\dfrac{\partial j_p}{\partial x}+\dfrac{\partial j_p}{\partial y}+\dfrac{\partial j_p}{\partial z}\right)+U=0=f_p \end{cases} \quad (6)$$

Gummel algorithm is represented by the following flowchart:

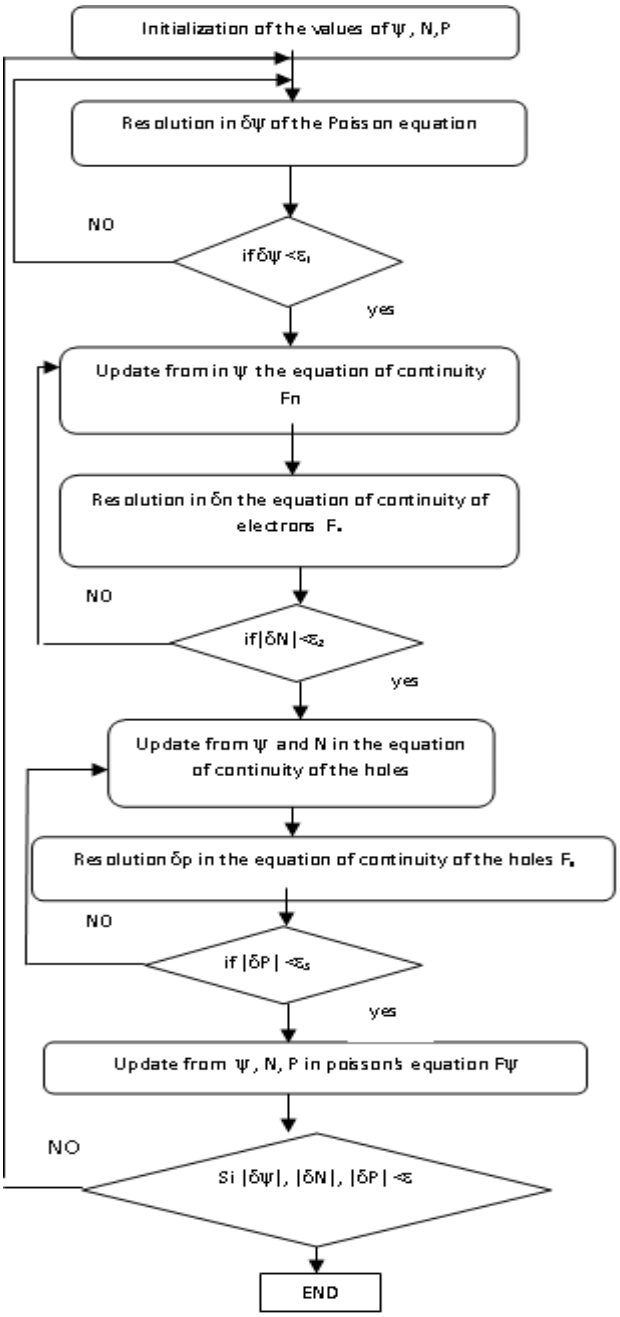

Fig.1. Resolution by the decoupled method chart

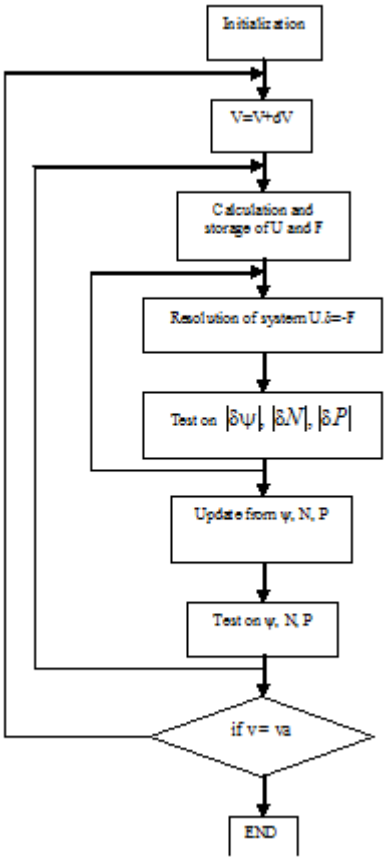

Fig.2. Organizational structure of resolution by the coupled method

Further to the calculations of the electric parameters in the Equilibrium thermodynamics, these values will be injected in Newton's algorithm so allowing to calculate the same parameters under polarization**[10][11][12],** one adding every time a step for the polarization of 1KT/q (Figure 2).

The application of Newton's in the digital simulation of plans leads to solve simultaneously F_ψ, F_n, F_p. It means calculating ψ N, P as solution in 3N equations, in every point of the network of three-dimensional discretization.

Three systems of equations discretized are grouped into a single system:

$$\begin{pmatrix} F_\psi(\Psi,N,P) \\ F_n(\Psi,N,P) \\ F_p(\Psi,N,P) \end{pmatrix}$$

The stage of linearization extended to three systems F_ψ , Fn, Fp leads to solve the following system:

$$\vec{u}.\vec{\delta} = -\vec{F},$$

where: $\vec{u}$: The complete Jacobian matrix of the system; $\vec{\delta}$: The correction vector

This method also called method coupled it to reduce considerably the time of calculation, the fix was to deal with three-dimensional matrices or each element of the matrix is a square matrix of dimension 3*3:

$$U = \begin{pmatrix} \frac{\partial F_\psi}{\partial \psi} & \frac{\partial F_\psi}{\partial N} & \frac{\partial F_\psi}{\partial P} \\ \frac{\partial F_n}{\partial \psi} & \frac{\partial F_n}{\partial N} & \frac{\partial F_n}{\partial P} \\ \frac{\partial F_p}{\partial \psi} & \frac{\partial F_p}{\partial N} & \frac{\partial F_p}{\partial P} \end{pmatrix} \qquad \delta = \begin{pmatrix} \delta_\psi \\ \delta_n \\ \delta_p \end{pmatrix}$$

So we created a new method receiver between the method of Gummel and Newton's method by using a not uniform meshing rather in the zones of loads of space and more unrefined in the neutral zones, with a considerable earnings in the run time which turns out long for the three-dimensional calculations.

4. Study of structure

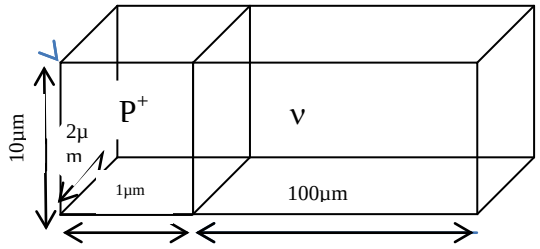

Fig.3. Structure used

The structure studied is a structure p ν The coat ν Is slightly of type N, and we handle the case of semiconductors with life expectancy and with relaxation, This opposite behavior is obtained by adjustment of the parameters τ_{ne} and τ_{pe}, we shall suppose that the conditions in the limits are such as the concentrations of carriers are fixed to their values in the equilibrium thermodynamics, and we are going sizes of the types of conditions of limits that of Dirichlet on the unknown plans.

5. Results and interpretation

Digital simulation software is written in C++, DEV C++. The study in the equilibrium thermodynamics is an essential stage for a first simulation of a structure of test. Besides, the sensibility of the method of Newton in the initial values will lead us to use the results obtained in the equilibrium thermodynamics, as initial values. Of more the case of equilibrium thermodynamics can give us a first vision of the

distributions of potential and free carriers through a junction [13]

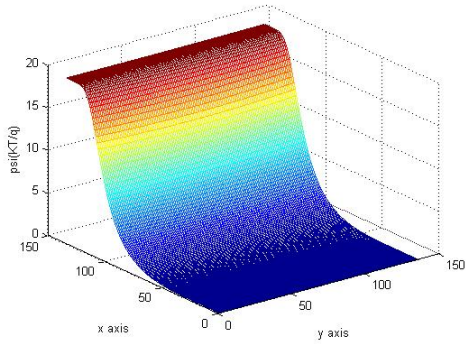

Fig.4. Profile potential distribution at thermodynamic equilibrium

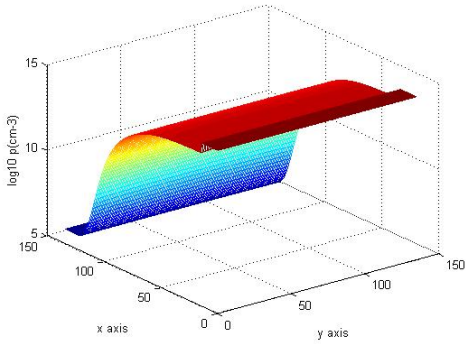

Fig.5. Profile holes distribution at thermodynamic equilibrium

The results of the simulation in the equilibrium thermodynamics are obtained by application of the algorithm of Gummel called also method decoupled, the results obtained for the lifetime SC represent the same for relaxation semiconductor and they are in accordance with the physical parameters given for the region p NA = 3.10^{14}cm^{-3} and the region ν Nd=$1.5.10^{11}$ cm $^{-3}$, to see better we are going to represent these results following the axis x only.

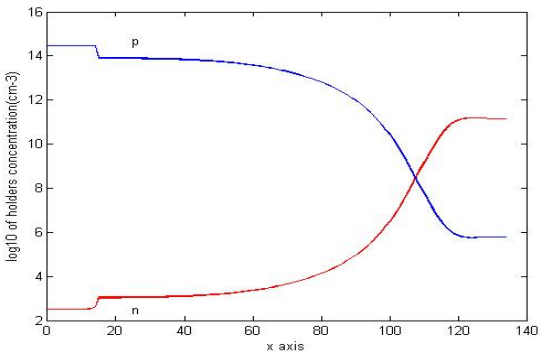

Fig.6. Profile holders distribution at thermodynamic equilibrium

It is visible that the zone of load of space extends essentially through the biggest structure through the least doped structure N. This has for consequence that the regime of conduction will be controlled by an effect of contact P ν, or the potential of distribution 20 KT\q in compliance with the analytical calculation.
Vd=log ((NA*Nd) / (ni*ni))**[13]**
By digital application we find:Vd =20.03 KT /q
The speeds of curves as well as the order of magnitude of the various concentrations determined by 3D calculation are physically correct.

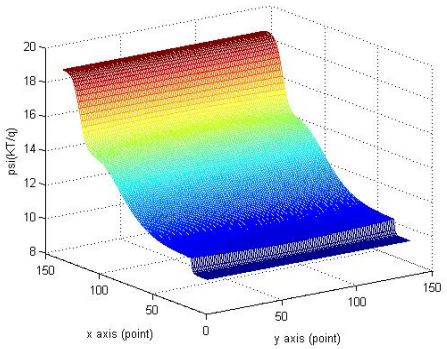

Fig.7. Profile of the distribution potential for a polarization of 10 KT\q for a lifetime SC

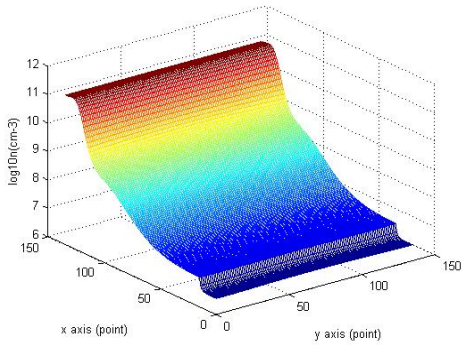

Fig.8. Profile of the density distribution of electrons for a polarization of 10 KT\q for a lifetime SC

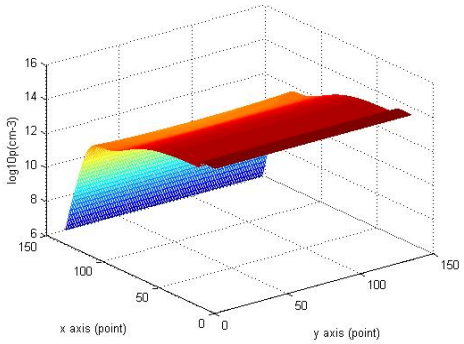

Fig. 9. Profile of the density distribution of the holes for a polarization of 10 KT\q for lifetime SC

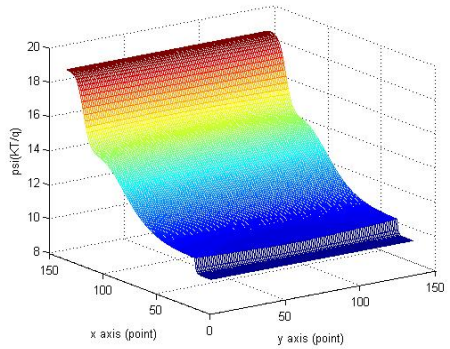

Fig.10.Profile of the density distribution of the electrons for a polarization of 10 KT\q for relaxation SC

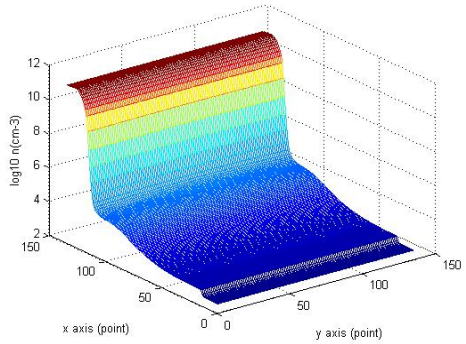

Fig. 11 Profile of the density distribution of electrons for a polarization of 10 KT\q

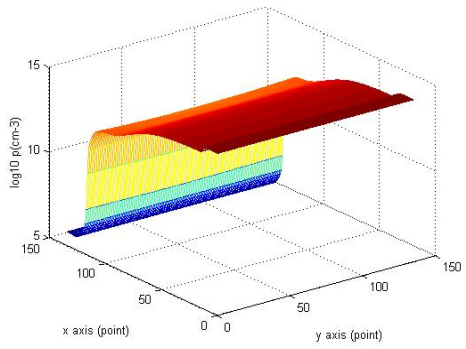

Fig.12. Profile of the density distribution for a relaxation of the holes for a polarization of 10 KT\q for a relaxation SC

Plots are given according to mesh point and not by length; the P^+ region is discretized on 15 points and region N on 135 points, thus allowing to better presenting the space charge zone. The plot are given according to mesh points and not by the length, P^+ region is discretized on 15 points and the N on 135 points, allowing better present area of space charge.
In the concern to be able to make a comparison enter various curved of distribution of free carriers under various polarizations and in the impossibility of tracer in the same graph, we chose tracer under the axis x

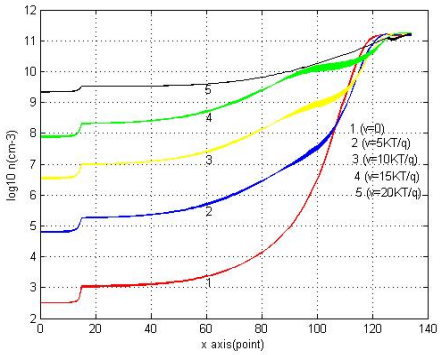

Fig.13. Profile of the density distribution of electrons for a lifetime SC

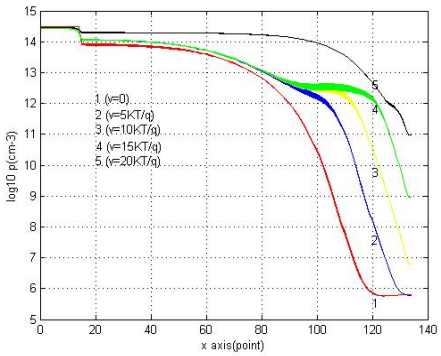

Fig.14.Profile of the density distribution of the holes for a lifetime SC

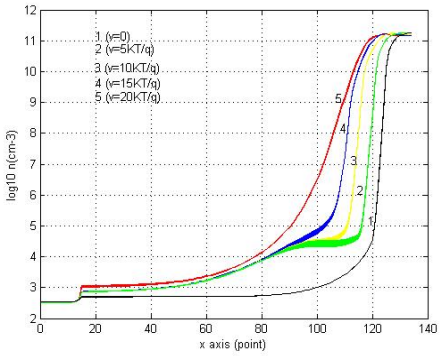

Fig.15. Profile of the density distribution of electrons for a relaxation

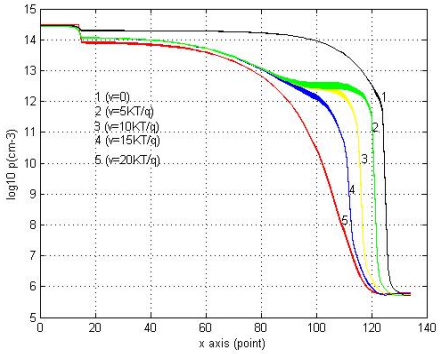

Fig.17. Profile of the density distribution of the holes for a relaxation SC

6. Interpretation of results

All the results found under polarization are obtained by application of the Newton's algorithm.

The structure is provided only with a single injections contract. For the SC with life expectancy under polarization we notice a decrease of the width of the zone of load of space with regard to the equilibrium thermodynamic's but widely more spread than that of the relaxation SC.

The contribution to the extension of the zone of load of space in the region ν results essentially from free carriers and from donors. Let us note that during the structure for a lifetime SC $\Delta n=\Delta p$, the trend is towards the neutralization of the load of space, the values of n and p in the neutral zones increase verifying the law.

$$n = n_0 \exp\left(\frac{ev}{KT}\right) \quad p = p_0 \exp\left(\frac{ev}{KT}\right)$$

For relaxation SC, the values of n and p in the neutral zones keep the same values as that of the equilibrium thermodynamics, For tensions more low than 20 KT\q the conduction is controlled by the effect of contact, as $\mu_n >> \mu_p$, The front of recombination occurs in the neighborhood of the contact P, in the right of the front of recombination we observe a depletion of hole. For the tension of 20 KT /q we affect practically the regime of flat bands, we notice the same remarks and an increase of the density of electrons and holes quoted P and quote ν respectively.

Contrary to the relaxation SC or we notice a closer front of recombination of the region P

7. Conclusion

The purpose of our study is the comparison of two semiconductors having the same electrical parameters except the relaxation time dielectric, for the lifetime semiconductor $\tau_{nt}=\tau_{pt}=10^{-8}$s and a relaxation semiconductor $\tau_{nt}=\tau_{pt}=10^{-11}$s with a $\tau_{rd}=4.810^{-9}$s. For the ν Zone this adjustment leads to a different behavior for the two semiconductors types. We also note a great difference between the semiconductor Relaxation and the insulators whose free-carrier concentration is negligible.

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