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Theoretical analysis of the charge collection at a nano-Schottky contact

Abdelillah El Hdiy

LRN (EA4682), bât. 6, case n°15, UFR SEN, Moulin de la Housse, URCA, BP 1039, 51687 Reims cedex 2, France

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ABSTRACT

A theoretical analysis of the current collected in semiconductors in the electron beam induced current technique in the case of a nano-Schottky contact is given. The electron beam is in normal incidence and the surface recombination velocity is taken to be equal to zero. The analysis is based on the use of new boundary conditions imposed by the nano-scale size and shape of the electrode. Different expressions of the induced current are obtained from the diffusion equation as a function of polar coordinates, and their reliability are analyzed for the purpose of describing the induced current profiles which can be used for the determination of the minority carrier diffusion length. All expressions of the current depend on the nano-contact size, which has a great importance in the charge collection process, but not on nano-contact area.

1. Introduction

The electron beam induced current (EBIC) technique of the scanning electron microscope has been largely used to characterize semiconductor structures [1–7]. Its performance was usually used to determine different physical parameters like as the minority carrier diffusion length [1,2,4,5,7], their life time [8–11] and the surface recombination velocity [1,5,12]. It was also used to analyze electronic circuits [13]. However, as technology improves with time, image processing has become an important element in the analysis of microscopic images. Combined to complicated techniques, the EBIC method had to be improved. Since a decade, a powerful experimental technique method using a nano-contact to collect EBIC was used to study *p-n* silicon junction [14] and structures containing at their surfaces quantum dots [15], or nanocrystals [16]. This system was labeled nano-EBIC technique.

However, at our knowledge no theoretical analysis was proposed up to now for this nano-EBIC technique to analyze the data contrary to the standard EBIC technique [17–19]. This is the reason why we try in the present paper to give analysis of the charge collection in this particular configuration. The surface recombination velocity is taken to be equal to zero. The collecting contact geometry and its size complicate the analysis. So, the solution of the minority carrier diffusion equation is not easy to find. This study is an attempt for giving an acceptable and physical solution which will describe the induced current profiles.

2. Theoretical analysis and discussions

To take into account of the experimental arrangement in the nano-EBIC technique, we choose the configuration of which the electron beam (e-beam) is incident normal to the plane of the collecting metal - semiconductor (MS) nano-contact. In the present study, the semiconductor is supposed to be *n*-doped. In this case, it is well known that if the surface of a metal with a work function W_M is in contact with a *n*-doped semiconductor with work function W_S, two cases of electrical contact can be considered; *(i)* if $W_M - W_S < 0$, the contact has ohmic properties, *(ii)* but if $W_M - W_S > 0$, the contact has Schottky properties with a barrier height $\phi_{MS} = W_M - \chi$, where χ is the electron affinity of the semiconductor. But this expression is only valid for macroscopic MS contacts for which some effects are neglected. Remind that in the case of a nano-Schottky diode, the barrier height is affected by the force image and by the enhancement of the local electric field at the interface which is attributed to the reduction of the depletion layer size and to the limited metal contact region where the transferred minority carriers from the semiconductor into the metal is confined to a small surface area. Indeed, it was recently shown that for MS nano-contacts the barrier height decreases with the depletion size decreasing [20,21]. In the case of a nano-Schottky diode, a local electric field is created through the depletion zone by the Fermi levels alignment. In this regard, a simple calculation of the local electric field by means of the resolution of the Poisson's equation in radial coordinate shows that this filed increases when the depletion layer size decreases. This suggests that the MS nano-contact size will be considered as a significant parameter in the following of this study. So, we are focusing our efforts on the resolution of the excess minority carrier diffusion equation for which the nano-contact size will control the boundary conditions. The calculation is processed in the presence of the depletion zone which was usually neglected in standard studies because of the macroscopic

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E-mail address: abdelillah.elhdiy@univ-reims.fr.

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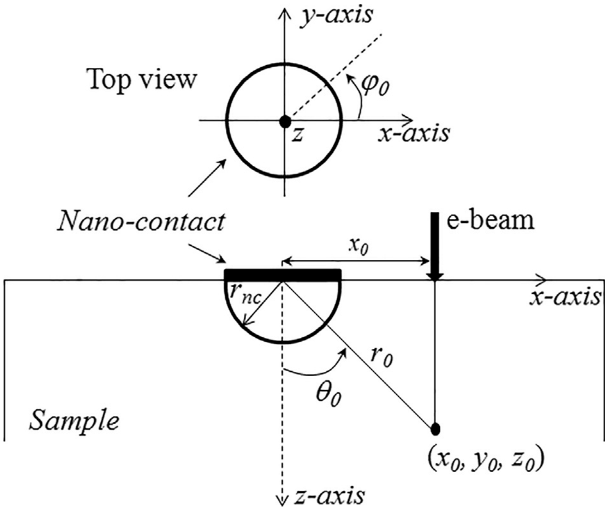

Fig. 1. Schematic representation of the charge collection analysis in the case of a nano-Schottky barrier. Spherical coordinates (r, θ, φ) are used to localize the generation unit point source and created minority carriers.

dimension of the metallic electrode [19]. In the present case, the depletion zone is considered to have a hemispherical shape with a radius r_{nc} of order of few nanometers [22]. Let us notice that the notion of spherical shape of the depletion layer underlines the fact that this zone is generated by a circular nano-contact between a metallic nano-electrode and the semiconductor surface. There is no spherical shape of the depletion layer, or at least neglected, in the case of a macroscopic electrode. This case of a Schottky nano-contact can be an interesting study since MS nano-contacts are intended for use in a wide range of prospective applications of nanotechnology.

The schematic representation used in the theoretical calculation is illustrated in Fig. 1. The Schottky nano-contact is represented by a disc of radius r_{nc} at the semiconductor surface, and with a hemispherical depletion nano-zone with the same size in the semiconductor. The diffusion equation governing the density of excess minority carriers $p(x, y, z)$ generated by a point source at coordinates (x_0, y_0, z_0) inside the semiconductor is:

$$\frac{\partial^2 p}{\partial x^2}+\frac{\partial^2 p}{\partial y^2}+\frac{\partial^2 p}{\partial z^2}-\frac{p}{L^2}=-\frac{G}{D}\delta(x-x_0)\delta(y-y_0)\delta(z-z_0) \tag{1}$$

where, G and D, are respectively the minority carrier generation rate ($\mathrm{cm}^{-3}\,\mathrm{s}^{-1}$) at the coordinates (x_0, y_0, z_0) and the diffusion coefficient ($\mathrm{cm}^2\,\mathrm{s}^{-1}$). And δ is the Dirac delta function which represents a unit point source ($G = 1\,\mathrm{cm}^{-3}\,\mathrm{s}^{-1}$). The parameter L represents the excess minority carrier diffusion length.

The symmetrical geometry leads to limit the resolution to the $x \geq 0$ part. Moreover, the equiprobable distribution of charges with respect to the x-axis suggests to restrict the resolution to the (x, z) plan with $x \geq 0$ and $z \geq 0$. In this case, Eq. (1) becomes:

$$\frac{\partial^2 p}{\partial x^2}+\frac{\partial^2 p}{\partial z^2}-\frac{p}{L^2}=-\frac{1}{D}\delta(x-x_0)\delta(z-z_0) \tag{2}$$

This equation will be used to describe the excess minority carrier distribution in the sample which will lead to determination of the collected current.

In the case of a Schottky nano-contact with a surface recombination velocity $v_s = 0$, the boundary conditions are:

$$p(x, z)=0, \quad for \quad \sqrt{x^2+z^2} \leqslant r_{nc} \tag{3a}$$

$$\left.\frac{\partial p(x, z)}{\partial z}\right|_{z=0}=0, \quad for \quad x > r_{nc} \tag{3b}$$

where r_{nc} is the radius of the hemispherical nano-contact as quoted in Fig. 1. Eq. (3a) indicates that the minority carriers are rapidly removed to the external circuit across the depletion nano-layer by the local electric field established in the nano-contact. Eq. (3b) represents the fact that the surface recombination velocity $v_s = 0$ at the free surface (outside the nano-contact).

Instead of Cartesian coordinates (x, z), we use polar coordinates (r, θ) where $0 \leq r < \infty$ and $0 \leq \theta \leq \pi/2$, with $z = r \times \cos(\theta)$ and $x = r \times \sin(\theta)$, to obtain:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial p}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 p}{\partial \theta^2}-\frac{p}{L^2}=-\frac{1}{Dr}\delta(r-r_0)\delta(\theta-\theta_0) \tag{4}$$

With the new boundary conditions:

$$p(r, \theta)=0, \quad for \quad r < r_{nc} \tag{5a}$$

$$\frac{\partial p(r, \pi/2)}{\partial \theta}=0, \quad for \quad r > r_{nc} \tag{5b}$$

Eq. (4) is similar to that used by Donolato to analyze the charge collection in the case of a macroscopic nano-Schottky diode [19]. The difference is given by the boundary conditions taking into account of the nano-metric contact size and shape. The equation is physically acceptable for all polar coordinates (r, θ) except for r_0 and θ_0; the position of the unit point source. In the basis of a general technique ([23, p. 825]), and taking into account of the boundary conditions (5a) & (5b), we suggest using the following expression:

$$p(r, \theta)=\sum_{n=0}^{+\infty} u_n(r)\sin[(2n+1)\theta] \text{ for } r > r_{nc}\, p(r, \theta)=0 \text{ for } r < r_{nc} \tag{6}$$

where $u_n(r)$ represents the Fourier coefficients of $p(r, \theta)$ which is solution of the inhomogeneous Eq. (4). The factor $(2n + 1)$ inside the sine function helps to justify the boundary condition given in Eq. (5b). The choice of this expression and not others like as those quoted in [19] is imposed by the boundaries conditions.

Eq. (6) must verify Eq. (4) in order to identify the elementary solutions $u_n(r)$. Introducing expression of $p(r, \theta)$ into (4), this becomes:

$$\sum_{n=0}^{+\infty}\left[\frac{1}{r}\frac{d}{dr}\left(r\frac{du_n(r)}{dr}\right)-\frac{(2n+1)^2u_n(r)}{r^2}-\frac{u_n(r)}{L^2}\right]\sin[(2n+1)\theta] \\ =-\frac{1}{Dr}\delta(r-r_0)\delta(\theta-\theta_0) \tag{7}$$

Multiplying both sides of this equation by $\sin[(2m + 1)\theta]$ and integrating over θ from 0 to $\pi/2$, and taking into account that the integration on the left-hand side involves the orthogonal properties of the $\sin[(2m + 1)\theta] \times sin[(2n + 1)\theta]$, the equation becomes:

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{du_m(r)}{dr}\right)-\left(\frac{1}{L^2}+\frac{(2m+1)^2}{r^2}\right)u_m(r) \\ =-\frac{4}{\pi Dr}\delta(r-r_0)\sin[(2m+1)\theta_0] \tag{8}$$

The factor $\sin[(2m + 1)\theta_0]$ in the right-hand side of Eq. (8) results from integration of the product $\sin[(2m + 1)\theta] \times \delta(\theta - \theta_0)$ for $0 \leq \theta_0 \leq \pi/2$.

It is well known that the solutions of the homogeneous equation are called modified Bessel functions $I_{(2m+1)}(r/L)$ and $K_{(2m+1)}(r/L)$ of the first and second kind, respectively. So, in the basis of ([19]; [24, p. 116]; [23, p. 827]), the elementary solutions $u_m(r)$ are given by (see Appendix A):

$$u_m(r)=\frac{4}{\pi D}\sin[(2m+1)\theta_0]I_{(2m+1)}(r_</L)K_{(2m+1)}(r_>/L) \tag{9}$$

where $r_</L$ ($r_>/L$) is the smaller (larger) of r/L and r_0/L. So, the solution $p(r, \theta)$ is given by: