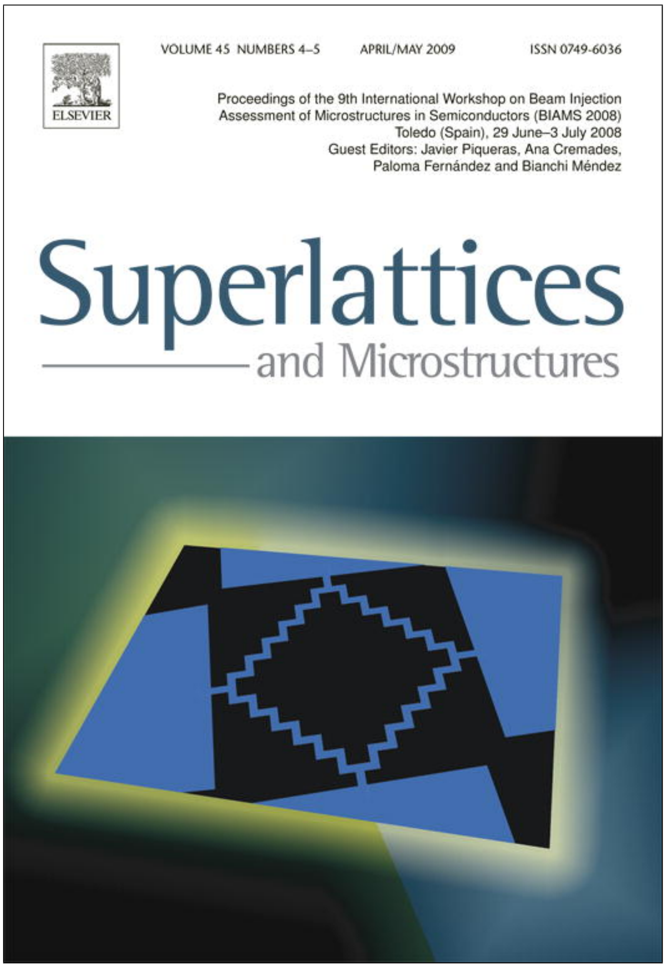
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Monte Carlo simulation of the EBIC collection efficiency of a Schottky nanocontact

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ABSTRACT

We have used a Monte Carlo (MC) algorithm to simulate the Electron Beam Induced Current (EBIC) collection efficiency of a nano-sized Schottky contact of radius r_c perpendicular to the incident electron beam. The surface area around the metallic contact was assumed to be an infinite recombination velocity. The results show that, at low beam energies, the EBIC collection efficiency increases rapidly as the radius of the contact (r_c) increases, and converges to a constant value as r_c becomes comparable to the carrier diffusion length. At higher beam energies, the variation of the EBIC signal with r_c is much slower because of the larger lateral extension of the generation volume. It is also shown that the maximum collection efficiency increases with the increase of the carrier diffusion length, and decreases as the incident beam energy increases, regardless of the size of the contact.

1. Introduction

The scanning electron microscope (SEM) in the charge-collection mode EBIC has been extensively used to characterize the electrical properties of semiconductors. The lifetime, diffusion length and surface recombination velocity of minority carriers can be measured and the electrical activity of defects such as grain boundaries and dislocations can be imaged using this technique. An old but good review on the subject has been published [1]. The development of nanotechnology has given rise to the

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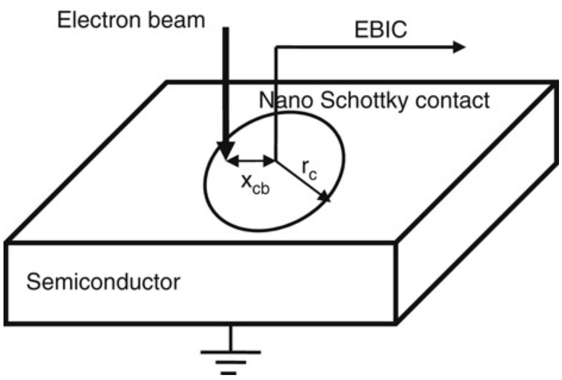

Fig. 1. Schematic diagram of the EBIC analysis of a nano Schottky contact.

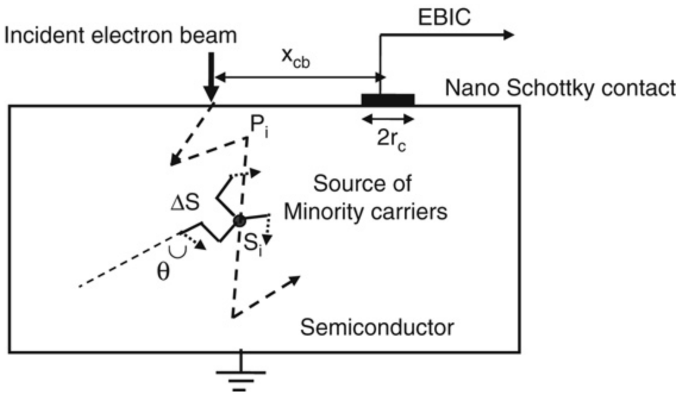

Fig. 2. Schematic diagram of the random diffusion of minority carriers in the semiconductor.

need for a good modeling of the EBIC signal measured in nano-size devices. Theoretical models have been developed to analyze the current induced at a Schottky contact [2,3]. In these models, analytical expressions of the collected current were derived for a Schottky contact of infinite radius. In this study, we have used a Monte Carlo algorithm to simulate the carrier collection at a Schottky contact of finite size, surrounded by an area of infinite surface recombination velocity.

2. Monte Carlo simulation algorithm

The Schottky contact is described as a disc of radius r_c perpendicular to the incident electron beam (Fig. 1). The surface area around the metallic contact was assumed to be an infinite recombination velocity.

In the instance, our algorithm simulates the generation function of the excess minority carriers as in references [4,5]. This was achieved by simulating the primary electron trajectories and the energy loss in the sample. The generation function was obtained in the form of a three dimensional distribution of point-like sources S_i localized at the middle of the path between two successive primary electron collisions (Fig. 2). The number of minority carriers generated at the source S_i whose coordinates are x_i, y_i, z_i, is given by:

$$N_{gi} = \frac{\Delta E_i}{\varepsilon_{e-h}} \tag{1}$$

ΔE_i is the energy loss at the source S_i and ε_{e-h} is the formation energy of the electron–hole in the semiconductor.

In the second step, we simulate the random diffusion and collection of the minority carriers that originate from S_i. The random diffusion of the minority carriers emitted from each point-like source S_i was simulated by considering successive small steps of constant duration Δt. The time interval Δt

was taken as a small fraction of the minority carrier lifetime τ:

$$\Delta t = \frac{\tau}{N} \tag{2}$$

where N was given typical value ranging from 100 to 10000 without significant impact on the simulated current. During the time Δt, the carrier crosses a distance ΔS given:

$$\Delta S = \sqrt{D \cdot \Delta t} \tag{3}$$

D is the diffusion constant of the minority carrier.

The scattering direction can be characterized using spherical coordinates by two angles θ and ϕ. The angle θ is the angle between the scattering direction and that of the carrier before collision (Fig. 2). The angle ϕ (not shown on Fig. 2) has the usual meaning in spherical coordinates. For a given value of θ, ϕ needs to be varied from 0 to 2π to cover all possible scattering directions making the angle θ with the carrier direction before scattering. θ and φ are calculated randomly as follows:

$$\varphi = 2\pi \cdot R_1 \tag{4}$$

$$\cos\theta = 1 - 2 \cdot R_2 \tag{5}$$

R_1 and R_2 are two random numbers between 0 and 1.

A minority carrier was considered as collected if, during its random diffusion, it reaches the metal/semiconductor interface. It was considered as recombined if it reaches the free surface surrounding the nano Schottky contact or remains in the bulk after a large number of steps.

For each position x_{cb} of incident primary electron beam, the EBIC collection efficiency $\eta^{mcs}(x_{cb})$ was calculated as follows:

$$\eta^{mcs}\,(x_{cb}) = \frac{\sum_{i=1}^{N_S} N_{ci}}{\sum_{i=1}^{N_S} N_{gi}} \tag{6}$$

N_{ci} and N_{gi} are respectively the number of collected and generated minority carriers for each source S_i. N_S is the total number of sources S_i.

As in [6], the diffusion/recombination process is simulated for a maximum number N_t of steps ΔS. N_t is adjusted by carrying successive simulations of the EBIC collection efficiency η_∞^{mcs} of an infinite Schottky contact, perpendicular to the electron beam, until it coincides with the theoretical value given by :

$$\eta_\infty^{SS} = \frac{\sum_{i=1}^{N_S} N_g\,(z_i) \cdot \exp\left(-\frac{z_i}{L}\right)}{\sum_{i=1}^{N_S} N_g\,(z_i)} \tag{7}$$

$N_g(z_i) = N_{gi}$ is the number of minority carriers that are generated at the depth zi and $\exp(-z_i/L)$ is the collection probability.

3. Results

All computations were carried out for a GaAs sample. Fig. 3 shows the EBIC efficiency profile $\eta^{mcs}(x_{cb})$ for a contact radius $r_c = 100$ nm, carrier diffusion length $L = 100$ nm and an incident beam energy $E_0 = 5$ keV. This figure shows a symmetrical profile, as expected, the maximum of the efficiency being localized at the nano contact center. We also observe that the value of the full-width-at-half maximum (FWHM) is approximately equal to the diameter of the contact (200 nm).

We have carried out computations to study the effect of the diffusion length L on the EBIC collection efficiency profile. The results are reported on the Fig. 4. This figure shows that the EBIC efficiency

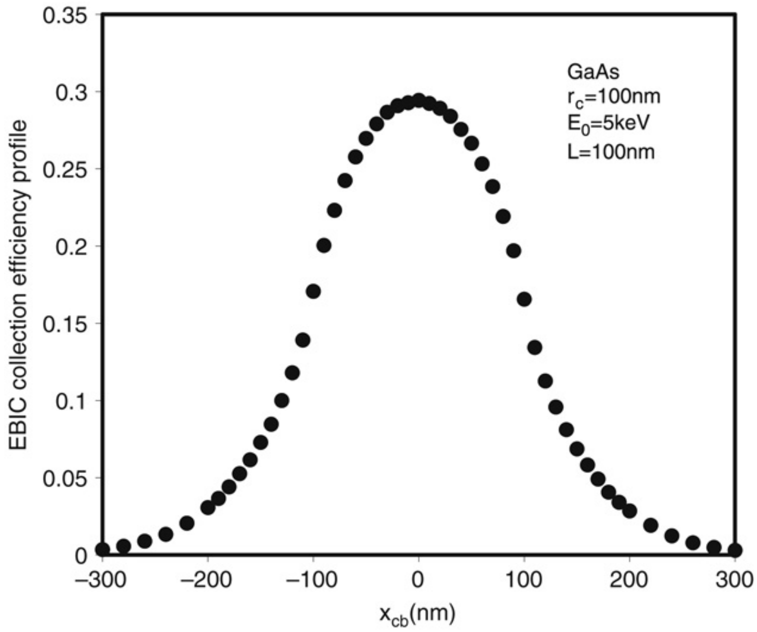

Fig. 3. The simulated EBIC collection efficiency profile $\eta^{mcs}(x_{cb})$ of a nano Schottky contact in GaAs.

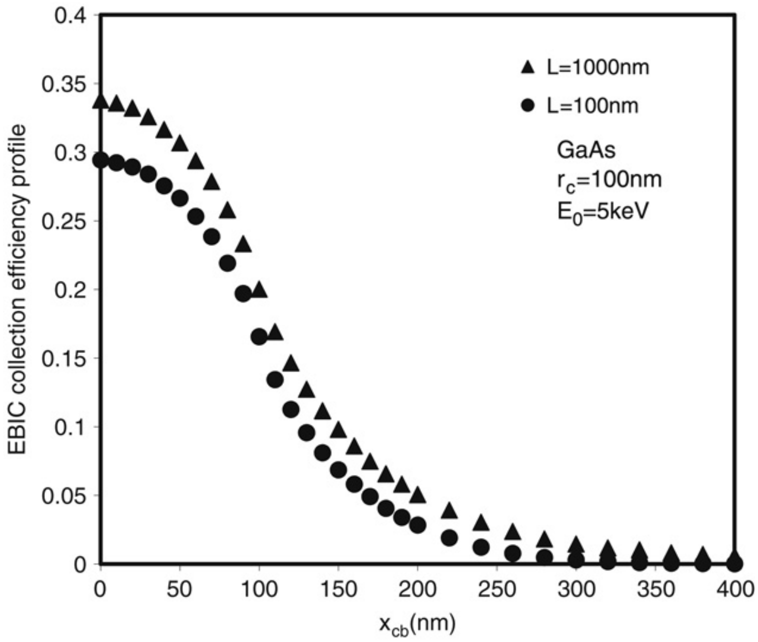

Fig. 4. The simulated EBIC collection efficiency profiles $\eta^{mcs}(x_{cb})$ of a nano Schottky contact for two different values of the diffusion length L (100 and 1000 nm) at 5 keV in GaAs.

increases as the minority carrier diffusion length L increases but FWHM remains approximately equal to 200 nm.

We have carried out also computations to establish the variation of the maximum values of the EBIC collection profiles $\eta^{mcs}_{\max} = \eta^{mcs}\ (x_{cb} = 0)$ upon r_c for two different beam energies E_0 (5 and 10 keV) and two minority carrier diffusion lengths L (100 and 1000 nm) in a GaAs sample. The results are reported in Figs. 5 and 6. These figures show that, as the radius r_c increases, $\eta^{mcs}_{\max}$ increases and converges to a constant value for large values of r_c. It can also be observed that the max-EBIC efficiency $\eta^{mcs}_{\max}$ increases as the minority carriers diffusion length L increases. This behavior is quite similar to that obtained for a large Schottky contact.

We have investigated the variation of $\eta^{mcs}_{\max}$ upon the beam energies E_0 for $r_c = 100$ nm and an infinite value of r_c for two different values of $L = 100$ and 1000 nm in GaAs sample. The results are

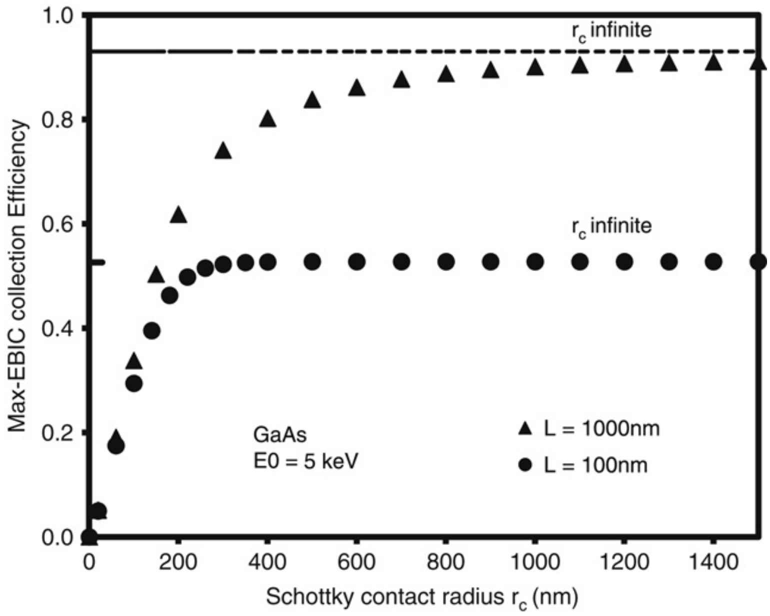

Fig. 5. The variation of the simulated maximum EBIC collection efficiency $\eta_{\max}^{mcs}$ upon the nano Schottky contact radius r_c for two different values of L at 5 keV in GaAs.

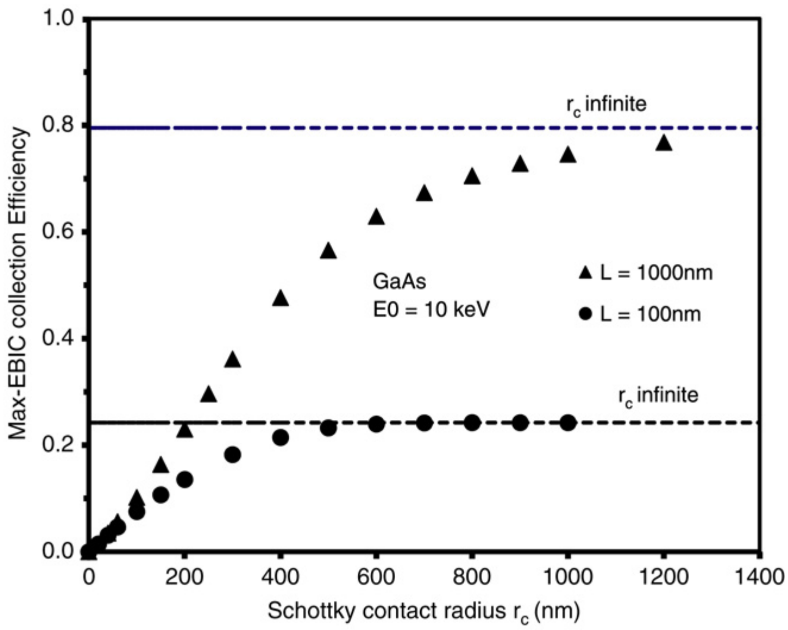

Fig. 6. The variation of the simulated maximum EBIC collection efficiency $\eta_{\max}^{mcs}$ upon r_c for two different values of L at 10 keV in GaAs.

reported on the Figs. 7 and 8 respectively. It can be observed that the collected current decreases significantly as the energy of the incident beam increases regardless of the size of the contact. However, it is important to note that the effect of the diffusion length on the collected current is drastically reduced as the size of the contact decreases (Fig. 7). This result can also be observed on Figs. 5 and 6 as the curves corresponding to two different diffusion lengths come closer to each other as the contact radius decreases. A practical consequence of this result is the difficulty of measuring the diffusion length around small contacts using the energy dependence of the collected current, as traditionally done for large contacts.

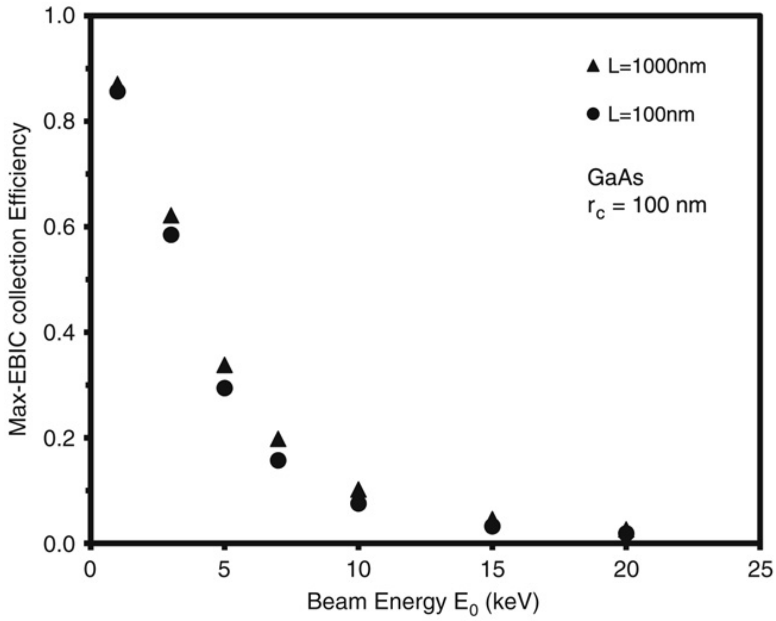

Fig. 7. The variation of the simulated maximum EBIC collection efficiency $\eta_{\max}^{mcs}$ upon the energy E_0 for $r_c = 100$ nm and $L = 100$ and 1000 nm in GaAs.

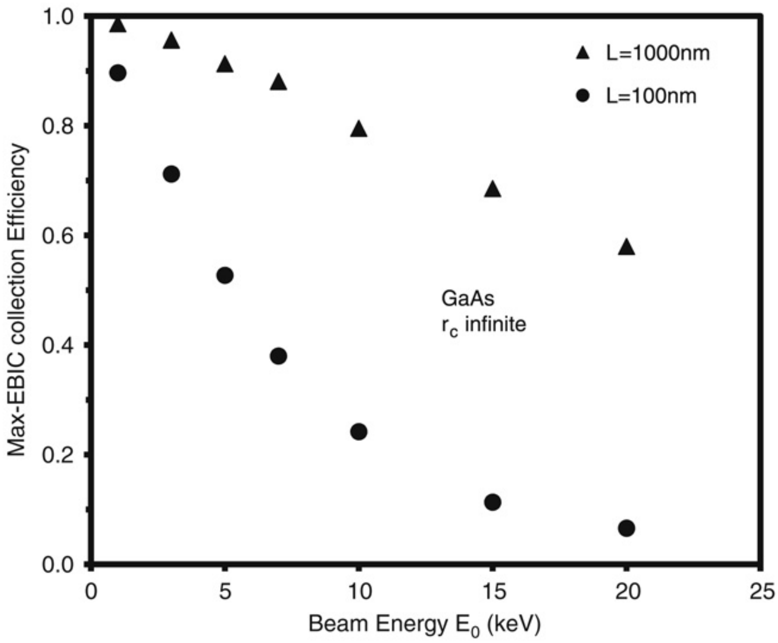

Fig. 8. The variation of the simulated maximum EBIC collection efficiency $\eta_{\max}^{mcs}$ upon E_0 for an infinite value of r_c and $L = 100$ and 1000 nm in GaAs.

4. Conclusion

We have developed a Monte Carlo algorithm that simulates the three dimensional generation, the random diffusion and collection of carriers in semiconductors. The algorithm presented is used to compute the EBIC efficiency of a nano Schottky contact, represented as a circle of finite diameter surrounded by a surface of infinite recombination velocity. Our computations show that, as the radius r_c increases, the maximum EBIC collection efficiency of the contact increases and converges to a constant value, as r_c becomes comparable to the carrier diffusion length. It is also shown that the collected current decreases as the incident beam energy increases, regardless of the size of the contact. In addition, the effect of the carrier diffusion length on the curve collection efficiency, versus incident beam energy, was very small for the small values of the contact radius.

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