INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS D: APPLIED PHYSICS
J. Phys. D: Appl. Phys. **38** (2005) 3845–3849 doi:10.1088/0022-3727/38/21/002

Monte Carlo simulation of the contrast of SEM charge-collection images of dislocations in semiconductors

M Ledra[1] **and N Tabet**[2]

[1] Physics Department, University of Biskra, Biskra 07000, Algeria
[2] Physics Department, KFUPM, 31261 Dhahran, Saudi Arabia

E-mail: m-ledra@caramail.com and natabet@kfupm.edu.sa

Received 24 August 2005
Published 24 October 2005
Online at stacks.iop.org/JPhysD/38/3845

Abstract

We describe a Monte Carlo algorithm that we have developed to simulate the electron beam induced current (EBIC) contrast of a surface perpendicular dislocation. The contrast was obtained by simulating the random diffusion and collection of the carriers that are generated at point-like sources S_i randomly distributed within the generation volume. The dislocation is described as a cylinder with a radius r_D where the minority carrier lifetime (τ_D) is lower than that in the bulk (τ_B).

The dependence on the electron range R_e of the simulated EBIC contrast profiles, their full width at half maximum (FWHM) and their maximum (C_{max}) is analysed for a germanium sample. It is shown that with increasing R_e, the FWHM of the contrast profile increases steadily in agreement with experiment while the maximum contrast goes through a maximum and converges to zero for $R_e \to 0$. The variation of C_{max} upon the diffusion length L_D within the dislocation cylinder is analysed too. The results of our simulations show that the values of the contrast obtained by the analytical approach using the first order approximation are underestimated for dislocations of strength exceeding 5.

1. Introduction

Extended defects such as dislocations, grain boundaries and precipitates greatly affect the electrical properties of semiconductors. In general, they contribute to the carrier scattering and recombination. They reduce the mobility and the lifetime of the majority and minority carriers, respectively. As a result, the presence of these defects drastically affects the performance of semiconductor devices. The scanning electron microscope (SEM) in the charge-collection mode electron beam induced current (EBIC) has been extensively used to observe the electrically active defects in semiconductors [1,2]. The recombination of the carriers at the defects leads to a current loss and the formation of a dark contrast.

The first comprehensive model of the EBIC contrast of localized defects was published by [3]. Since then, many authors have used the approach suggested by that model to analyse the contrast of various defects. The approach consists in describing the diffusion and the collection of the electron beam generated minority carriers by an integral equation, from which a first approximation solution, analogous to the Born approximation in quantum mechanics, is derived. The representation of a dislocation as a geometrical line (i.e. as the cylinder of vanishing radius) [4, 5] is convenient for describing its EBIC images in the usual conditions where the diameter $2r_D$ of the dislocation cylinder is smaller than the electron beam range R_e. However, this scheme cannot be retained at low beam energies, i.e. when R_e becomes smaller than $2r_D$. In [6] and [7], an analysis of the EBIC contrast of a straight dislocation perpendicular to the surface of a Schottky diode or a p–n junction was performed. The calculations were based on the bulk recombination model describing a dislocation as a cylinder with radius r_D where the lifetime τ_D is lower than outside the cylinder. Simplifications are usually made in order to derive an analytical solution; a spherically symmetrical Gaussian and a uniform generation function of the carriers have been used by [6] and [7], respectively.

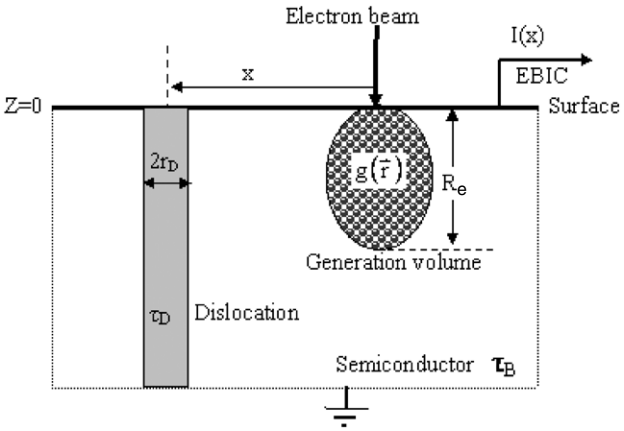

Figure 1. Schematic diagram of the EBIC analysis of a dislocation normal to the surface of a Schottky contact.

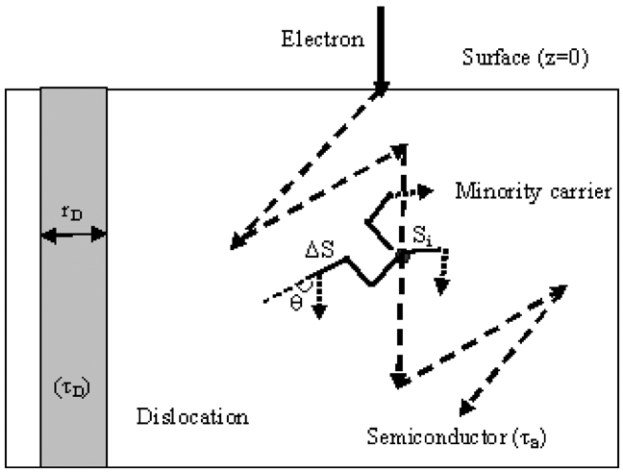

Figure 2. Schematic diagram of the random diffusion of the minority carriers.

In addition, the first-order approximation describes the excess minority-carrier density within the defect using the linear response whose validity is restricted to the dislocation of sufficiently weak recombination efficiency. The Monte Carlo (MC) simulation is an alternative method that can provide a more realistic analysis of the recombination contrast of extended defects [8–13]. In [13], the EBIC contrast of a dislocation normal to the surface was investigated. A good agreement was obtained between the MC simulations and the theoretical models regarding the variation of the contrast versus the electron beam range R_e and the carrier lifetime within the dislocation τ_D. However, the absolute values of the contrast obtained by simulation were about three times higher than the theoretical ones [13] and have no clear argument that could explain the observed discrepancy. In this study, we have developed a new MC algorithm to simulate the EBIC contrast that results from a three-dimensional generation function. The dislocation was considered as a cylinder of radius r_D perpendicular to the surface (figure 1). The depletion region of the Schottky contact was neglected. Notice that this approximation is no longer justified if slightly doped materials are considered. The effect of the thin metallic film of Schottky contact has been neglected too. The minority-carrier lifetime within the dislocation has a value τ_D smaller than the value τ_B in the bulk. The collection of minority carriers by the surface depletion layer of a shallow Schottky diode is described by an infinite surface recombination velocity.

In this paper, we present the results of an MC simulation of the EBIC contrast based on the above description of a surface perpendicular dislocation. We have carried out a computation to establish the variation versus the electron range of the contrast profiles and their full width at half maximum (FWHM) and maximum C_{max}. The variation of C_{max} upon the diffusion length L_D within the dislocation cylinder is analysed too.

2. MC simulation algorithm

The MC algorithm simulates, first, the generation function of the excess carriers as in [11–13]. This was achieved by simulating the 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. The number of carriers generated at the point S_i whose coordinates are x_i, y_i, z_i, is given by

$$\mathrm{Ncg}(x_i, y_i, z_i) = \frac{\Delta E(x_i, y_i, z_i)}{\varepsilon_{\text{e-h}}}, \tag{1}$$

where $\Delta E(x_i, y_i, z_i)$ is the energy loss and $\varepsilon_{\text{e-h}}$ is the formation energy of the electron-hole in the semiconductor.

In the second step, the algorithm simulates the random diffusion and collection of the carriers that originate from the point-like sources S_i (figure 2). The random diffusion of the 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 carrier lifetime τ, ($\Delta t = \tau/N$), depending on the location of the carrier, in the bulk ($\Delta t_B = \tau_B/N$) or in the defect ($\Delta t_D = \tau_D/N$). During the time Δt, the carrier crosses a distance ΔS given as follows:

$$\Delta S = \sqrt{D\Delta t}, \tag{2}$$

where D is the diffusion constant of the carrier.

The constant D was given the same value in the bulk and inside the defect as it is usually done in the analytical models. We have considered values of Δt that give a step length ΔS much smaller than the diameter $2r_D$ of the dislocation. This constraint is necessary otherwise a carrier reaching the vicinity of the dislocation may cross it without 'seeing it' leading to an underestimation of the simulated contrast.

The two scattering angles θ and φ (figure 2) are calculated randomly as follows:

$$\varphi = 2\pi R_1, \tag{3}$$

$$\cos\theta = 1 - 2R_2, \tag{4}$$

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

A carrier was considered as collected if it reaches the surface taken as the edge of the Schottky contact. The collection probability of the carrier generated at a point-like source S_i was calculated as the ratio of the collected carriers to the number of carriers generated at S_i. A carrier was

Table 1. Comparison of semi-simulated I_0^{SS} and simulated I_0^{mcs} current in the absence of defect in a germanium sample, $\tau_B = 10^{-8}$ s, $N = 1600$, $N_t/N = 2.5$.

E (keV)	5	8	10	15	20
I_0^{SS}	0.929	0.866	0.815	0.679	0.549
I_0^{mcs}	0.929	0.865	0.811	0.654	0.497

considered as recombined if it does not reach the surface after N_t steps, where N_t is the total number of steps. Notice that, in [13], the recombination probability is calculated after each step of the simulation. In the new algorithm, the number of steps N_t is adjusted by carrying successive simulations of the collected current I_0^{mcs} when the incident electron beam is impinging on the surface far away from the defect until it coincides with the semi-simulated value I_0^{SS}. This value, I_0^{SS}, corresponding to the simulated distribution of sources S_i, can be obtained by multiplying the number of carriers $Ncg(x_i, y_i, z_i)$ generated at the depth z_i by the collection probability $P_i = \exp(-z_i/L_B)$ and summing over all sources.

We have reported in table 1 the values of I_0^{SS} and I_0^{mcs} for different incident electron beam energies E in the germanium sample. One can notice that the differences between I_0^{SS} and I_0^{mcs} values do not exceed 10%. The number of point sources S_i varied from about 33 000 for $E = 5$ keV to more than 113 000 sources at $E = 20$ keV. The simulations were carried out on a personal computer using a 1.7 GHz Pentium 4 processor. The computing time varied from less than 1 h to many days depending on the number of sources, carriers considered and the values of N and N_t.

The program was run for any given positions x of the incident electron beam. The first position, far away from the dislocation, gives the current I_0 in the absence of defect; the other positions give the current $I(x)$ collected when the incident electron beam is at a distance x of the dislocation (figure 1). The contrast $C(x)$ was obtained as the ratio

$$C(x) = \frac{I_0 - I(x)}{I_0} = 1 - \frac{I(x)}{I_0}. \tag{5}$$

The maximum contrast C_{max} is obtained when the primary beam normal to the surface is on the top of the dislocation (i.e. $C_{max} = C(x = 0)$). It is given by

$$C_{max} = \frac{I_0 - I(x = 0)}{I_0} = 1 - \frac{I(x = 0)}{I_0}. \tag{6}$$

The theoretical model, using the first approximation, gives the maximum EBIC contrast as follows (see equation (7) of [6]):

$$C_{max} = \gamma F(R_e\tau_B, r_D), \tag{7}$$

where γ is the recombination strength of the dislocation given by

$$\gamma = \frac{\pi r_D^2}{D}\left(\frac{1}{\tau_D} - \frac{1}{\tau_B}\right). \tag{8}$$

The function $F(R_e, \tau_B, r_D)$ gives principally the effect of the generation function and the lifetime τ_B of minority carriers in the bulk on the contrast. One can notice that the function F is independent of the lifetime τ_D within the dislocation. Therefore, in the first approximation, the maximum contrast is proportional to $1/\tau_D$.

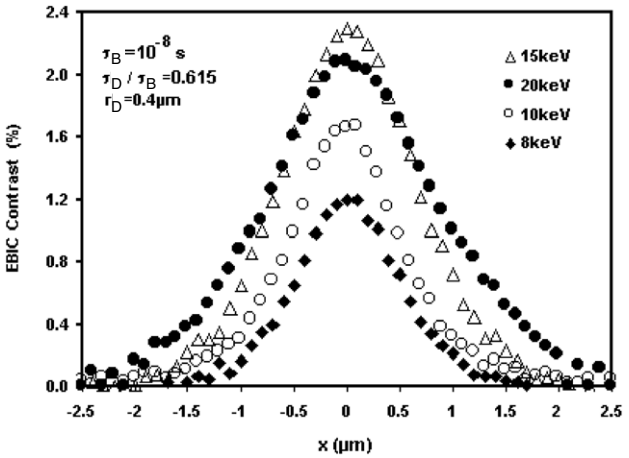

Figure 3. Simulated EBIC contrast profiles of a straight dislocation perpendicular to the surface for different beam energies in germanium.

3. Results

A major practical problem in the EBIC observation of defects in semiconductors is the choice of the beam energy that gives an image with maximum resolution and maximum contrast. We shall investigate this point by applying the MC simulation to a definite case and examining the dependence of the characteristics of the image on the electron range R_e. The electron range R_e has been related to the beam energy E through the empirical expression [14]:

$$R_e(\text{cm}) = \frac{3.98 \times 10^{-6}}{\rho(\text{g cm}^{-3})}(E(\text{keV}))^{1.75}. \tag{9}$$

Taking values of the parameters: $\tau_B = 10^{-8}$ s, $\tau_D/\tau_B = 0.615$, $r_D = 0.4\,\mu$m (according to (8), these values correspond to $\gamma = 0.1\pi$) and considering E values between 8 and 20 keV (for germanium, according to (9), these values correspond to R_e in the range 0.284–1.412 μm), we obtain the contrast profiles $C(x)$ reported in figure 3. This figure shows that the FWHM of the profiles increases rapidly as E increases. However, the peak height of the curves $C(x = 0)$, that is the maximum contrast C_{max}, goes through a maximum.

To study this behaviour in more detail, the contrast parameters, FWHM and C_{max}, have been simulated for a germanium sample with the following parameters: $\tau_B = 10^{-8}$ s, $\tau_D/\tau_B = 0.615$, $r_D = 0.4\,\mu$m and assuming R_e values between 0.025 and 2 μm (for a germanium sample, according to (9), this corresponds to beam energies E in the range 2–25 keV). The results are shown in figures 4 and 5.

Figure 4 shows the variation of FWHM versus the electron range R_e. It can be observed that FWHM increases linearly with R_e and being of the order of R_e. The image resolution will follow an $E^{1.75}$ dependence (see equation (9)). This result is in agreement with experiment [15].

Figure 5 shows the dependence of the maximum contrast upon the electron range R_e. The values of the maximum contrast reported in figure 5 were obtained by simulating two values of the EBIC current only for each beam energy. The first value I_0^{mcs} corresponds to the current collected in the absence of the dislocation and the second to that obtained in the

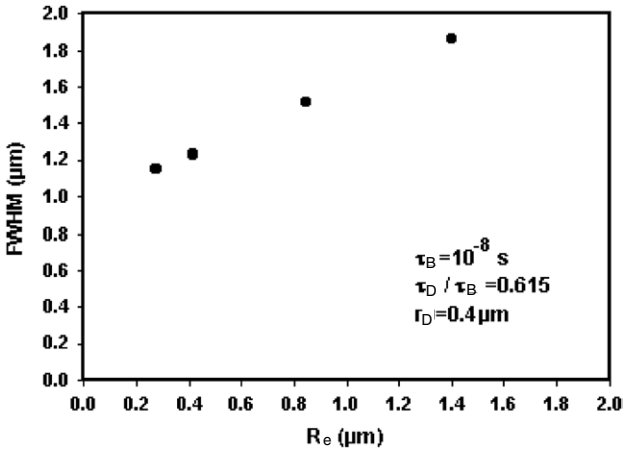

Figure 4. The FWHM of the contrast profile of a straight dislocation perpendicular to the surface versus the electron range in germanium.

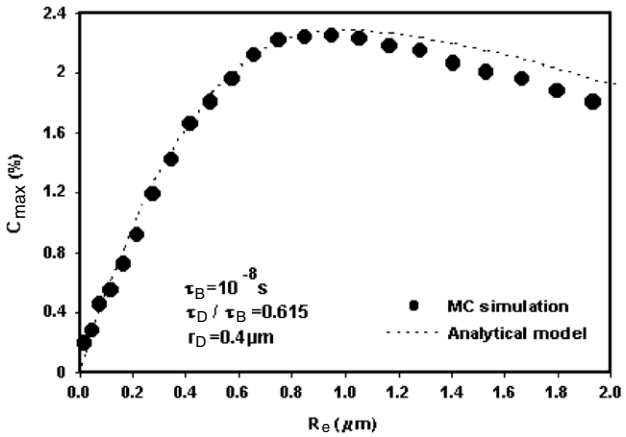

Figure 5. Maximum EBIC contrast of a straight dislocation perpendicular to the surface versus the electron range in germanium.

presence of the dislocation, the electron beam being at position $x = 0$. We have also reported in the same figure the maximum contrast variation that was obtained by using equation (7) of [6]. The results show that C_{max} is characterized by a maximum and converges to zero for $R_e \to 0$. A comparison of figure 5 with figure 6 of [7] and figure 3 of [13] shows that all curves yield the same dependence of the maximum contrast upon R_e. The absolute maximum contrast values of figure 3 of [13] obtained by the MC simulation, however, were about three times higher than the corresponding theoretical ones, but the differences between our simulated values and those calculated using equation (7) of [6] do not exceed 10%. Our simulated values are lower than those derived from the first order approximation model as one could expect. Indeed, the actual excess density of the minority carriers within the dislocation is expected to be less than its value in the perfect semiconductor under excitation used in the model.

We have carried out a computation to establish the variation of the maximum contrast upon the minority carrier diffusion length $L_D = \sqrt{D\tau_D}$ within the dislocation cylinder in a germanium sample. The results are reported in figure 6. We have also reported in the same figure the contrast variation that was obtained by using equation (7) of [6]. As expected, one observes a decrease of the contrast as L_D increases and

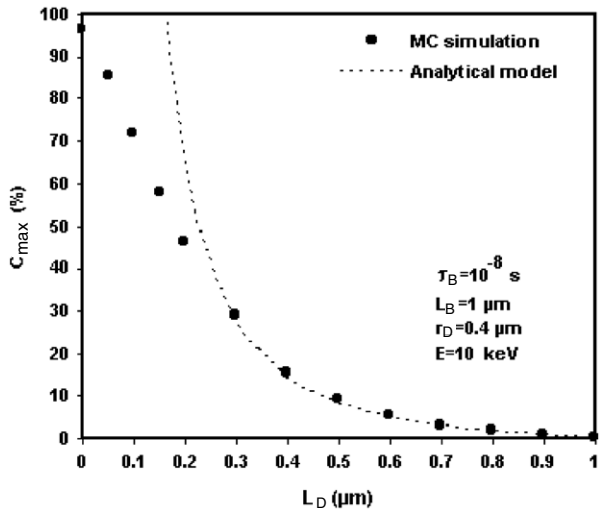

Figure 6. The variation of the maximum contrast upon the minority carrier diffusion length L_D within the dislocation cylinder.

becomes close to the bulk diffusion length $L_B = \sqrt{D\tau_B}$. The figure shows an excellent agreement between our computations and the first order approximation for values of L_D higher than $0.3\,\mu$m which corresponds to a recombination strength less than $\gamma = 5$ (see equation (8)). The differences between our simulated values and those calculated using equation (7) of [6] do not exceed 10% for values of $\gamma \leqslant 5$. The value $\gamma = 5$ can be considered as an upper limit for the validity of the first order approximation in the conditions that are considered in figure 6. Beyond this limit, the first order approximation calculations overestimate the rate of change of the contrast upon L_D.

4. Conclusion

We have developed a MC algorithm that simulates the three-dimensional generation, the random diffusion and the collection of carriers in semiconductors. The algorithm presented is used to compute the EBIC contrast of a straight dislocation, represented as a cylinder of finite diameter perpendicular to the surface of a Schottky contact. Our computations show that, as the electron range R_e increases, the FWHM of the contrast profile increases steadily in agreement with experiment while the maximum contrast goes through a maximum and converges to 0 for $R_e \to 0$. Both absolute values of the maximum contrast and its dependence upon the electron range and the diffusion length L_D within the dislocation cylinder are in good agreement with those obtained by the analytical models for values of the dislocation strength γ less than 5. The differences between our simulated values and those calculated using equation (7) of [6] do not exceed 10% for values of $\gamma \leqslant 5$.

References

[1] Holt D B and Joy D C 1989 *SEM Microcharacterization of Semiconductors* (London: Academic)
[2] Tabet N 1991 *Structure and Property Relationships for Interfaces* ed J L Water *et al* (Materials Park, OH: ASM Publications) p 361
[3] Donolato C 1978/79 *Optik* **52** 19

[4] Donolato C 1979 *Appl. Phys. Lett.* **34** 80
[5] Donolato C and Klann H 1980 *J. Appl. Phys.* **51** 1624
[6] Donolato C 1991 *J. Appl. Phys.* **70** 7657
[7] Pasemann L 1991 *J. Appl. Phys.* **69** 6387
[8] Akamatsu B and Henoc J P 1981 *J. Appl. Phys.* **52** 7245
[9] Joy D C 1986 *J. Microsc.* **143** 233
[10] Stemmer M 1994 *Mater. Sci. Eng.* B **24** 180
[11] Tabet N and Ledra M 1996 *Mater. Sci. Eng.* B **42** 181
[12] Tabet N 1998 *Semicond. Sci. Technol.* **13** 1392
[13] Tabet N 1998 *Solid State Phenom.* **63–64** 89
[14] Everhart T E and Hoff P H 1971 *J. Appl. Phys.* **42** 5837
[15] Leamy H JE 1982 *J. Appl. Phys.* **53** R51