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Choice of Generation Volume Models for Electron Beam Induced Current Computation

Oka Kurniawan and Vincent K. S. Ong

Abstract—The spatial distribution of the electron-hole pairs generated by the electron beam is commonly called the generation volume or interaction volume. The generation volume affects the electron beam-induced current (EBIC) profile. This effect of the generation volume on the EBIC profile is particularly true for regions near to the semiconductor junctions. Mathematical models have been proposed for use in the computation of EBIC profiles. Three pear-shaped generation volume distributions were analyzed by comparing the resulting EBIC profiles to the profile obtained from the data using the Monte Carlo simulations. The result shows that the Bonard model gives an EBIC profile that is closest to the one computed using the Monte Carlo simulation. This result is easily observed in the first and the second derivatives of the semilogarithmic EBIC profiles.

Index Terms—Charge carrier processes, charge injection, electron-beam applications, semiconductor materials measurements, simulation.

I. INTRODUCTION

THIS PAPER gives an analysis of some of the generation volume models that can be used in electron beam-induced current (EBIC) computation. The EBIC technique has been widely used for a wide range of semiconductor materials characterizations [1].

The EBIC technique has been used for imaging, failure analysis, minority carrier properties measurement, and identification of inhomogeneities in the materials [1], [2]. In fact, the EBIC profile is quite sensitive around semiconductor junctions [3]. Due to this, it has recently been used to locate the edges of the depletion layer of semiconductor junctions [4].

What makes the EBIC technique sensitive to semiconductor junctions? In this technique, the semiconductor surface is bombarded with electron beam. The energy of the electrons coming from the beam can be up to several kiloelectronvolts.

These primary electrons, which come from the beam, enter the semiconductor crystal and collide with the atoms. Two scattering mechanism occurs: elastic and inelastic. In the elastic scatterings, the primary electrons do not lose energy and experience large angle deflection. In the inelastic scatterings, the primary electrons lose energy and impart their energies to the surroundings. The latter phenomena can ionize electrons

from the atoms and generate what is called the electron-hole pairs (ehps) which can move within the semiconductor materials. The volume in which this generation of ehps occurs is commonly called the interaction volume or the generation volume [5], [6].

Therefore, back to the question on why the EBIC technique is sensitive to the semiconductor junctions. These ehps diffuse away from the generation volume to its surroundings with fewer concentrations. When the ehps encounter a built-in electric field, such as a p-n junction, the minority carrier will be swept across to the other side of the junction. On the other hand, the majority carrier will be repulsed. When the p-n junction is connected to external circuit, this creates a current. This induced current is what people called the EBIC or EBIC profile. Since the separation occurs due to built-in electric field which present in a semiconductor junctions, the EBIC technique is sensitive to the junction regions.

In the EBIC technique, the generation volume where the ehps are generated plays an important role. The size of this volume affects the resolution of the technique [7]. Furthermore, when the EBIC technique is used near semiconductor junctions, the actual shape of the generation volume alters the shape of the EBIC profile. For these reasons, it is important to study and to accurately model the generation volume particularly for regions very near to the semiconductor junctions.

In the early works of the EBIC technique, the theoretical EBIC profile was derived with a point generation source assumption [8]. In order for this assumption to be valid, the generation volume must be much smaller than the vertical and horizontal dimension of the p-n junctions, and the beam has to be located far from the boundaries which comprise the junctions and the contacts. This model is not satisfactory for a realistic EBIC profile near the semiconductor junctions.

Berz and Kuiken [9] used a uniform spherical generation volume. In this model, the generation rate of the ehps within the sphere is a constant, while the rate outside it is zero. In reality, the generation of ehps is distributed continuously and does not change abruptly like the uniform sphere model. Donolato [10], on the other hand, used a Gaussian model. The shape of the volume is a sphere; but here, the generation rate is distributed following the Gaussian distribution. In fact, Donolato used the model proposed by Fitting *et al.* [11]. In this model, the peak is located at $\bar{z} = 0.3R$, where R is the electron penetration range. This model has a constant standard deviation in the x - and z -directions with a value $\sigma = R/\sqrt{15}$.

Cohn and Caledonia [12], however, showed that the actual shape of the generation volume is not perfectly a sphere, but rather it is a pear shaped or a tear-drop shaped. The 3-D

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pear-shaped generation volume was modeled by Donolato [13]. In this model, the radial distribution follows the Gaussian distribution. The depth distribution, however, follows the polynomial given by Everhart and Hoff [14]. A year later, Donolato and Venturi decided to use the depth distribution proposed by Fitting *et al.* [11] instead of the polynomial distribution of Everhart and Hoff.

In 1996, Bonard *et al.* [15], [16] used a different model for the generation volume distribution based on their experimental results. The generation volume was characterized using a multi-quantum well structure. Their model, however, only examined the AlGaAs material. Parish and Russel [17] then generalized the model to be used for all materials.

The many choices of the generation volume models make it difficult for one to determine which of these is suitable for one's application. Therefore, three pear-shape models are analyzed in this paper within the context of computing the EBIC profile at regions very near to the semiconductor junctions. The reason for computing in regions near to the junctions is that the EBIC profile in this region is very sensitive to the distribution of the generation volume. The computed profiles are then compared with the profile computed using Monte Carlo simulations as its generation volume data. Monte Carlo simulations have been frequently used in the literature working on the beam-sample interactions [18], [19]. The Monte Carlo technique simulates the electron trajectory using random number with probability distributions for its scatterings mechanism models. These models in fact can be tuned to fit with experimental results. The work in this paper analyzes the available models and compare it to the Monte Carlo data, and proposes the best mathematical model to be used in EBIC studies.

II. MATHEMATICAL MODELS OF GENERATION VOLUME

Three mathematical models of the generation volume distribution are considered in this paper. The first one is proposed by Donolato [13]. The 3-D distribution can be written as

$$g(r, z; R) = \frac{\Lambda(z/R)}{2\pi R \sigma^2(z, R)} \exp\left(-\frac{r^2}{2\sigma^2(z, R)}\right) \quad (1)$$

where $g(r, z; R)$ is the normalized generation volume distribution, R is the electron range, $\Lambda(z/R)$ is the depth distribution, while $\sigma^2(z, R)$ is the standard deviation of the Gaussian distribution and is given by

$$\sigma^2(z, R) = 0.36d^2 + 0.11z^3/R \quad (2)$$

where d is the beam diameter. The depth distribution in [13] follows the polynomial proposed by Everhart and Hoff [14], which can be written as (3), shown at the bottom of the page. A year later, Donolato and Venturi computed EBIC using the same model as in (1). However, the depth distribution used the

model proposed by Fitting *et al.* The depth distribution can be written as

$$\Lambda(z/R) = 1.14 \exp(-7.5(z/R - 0.3)^2). \quad (4)$$

It can be seen that the depth distribution follows an exponential function with a peak at $\bar{z} = 0.3R$.

It is important to note that (1) is a 3-D generation volume. For simplicity, the EBIC computation is done in the projected x - z plane. Therefore, (1) must be projected into this plane by integrating along the y -axis, i.e.,

$$h(x, z) = \int_{-\infty}^{\infty} g(x, y, z) dy. \quad (5)$$

This results in

$$h(x, z) = \frac{\Lambda(z/R)}{\sqrt{2\pi} R \sigma} \exp\left(-\frac{x^2}{2\sigma^2}\right). \quad (6)$$

In the above equation, both σ and R have a dimension of a unit length, while the other terms are unitless. Therefore, we can see that the unit of $h(x, z)$ is ehp/(unit area). Substituting (2) and (3) into (6) gives a pear shape distribution, which shall be called the Donolato model. On the other hand, substituting (2) and (4) into (6) gives another pear shape distribution. This distribution shall be called the Donolato-Venturi model in this paper.

The model proposed by Bonard *et al.* [15], [16] and is used by Parish and Russel [17] is slightly different. The expression in 2-D can be written as

$$h(x, z) = \frac{1}{2\sqrt{\pi\sigma_x\sigma_z^3}} z^2 \exp\left(-\frac{z}{\sigma_z}\right) \exp\left(-\frac{x^2}{\sigma_x^2}\right) \quad (7)$$

where σ_x is the lateral electron range and σ_z is the depth electron range. These parameters are functions of the material and the beam parameters. Parish and Russel proposed to obtain these parameters by fitting the data from Monte Carlo simulations. It was shown that the distribution can be separated into

$$\begin{aligned} h(x, z) &= k(x)j(z) \\ k(x) &= A \exp(-x^2/\sigma_x^2) \\ j(z) &= B z^2 \exp(-z/\sigma_z) \end{aligned} \quad (8)$$

where A and B are constants. These expressions can be fitted separately in the x - and z -axes into the Monte Carlo simulations data. The function $k(x)$ and $j(z)$ can be linearized by taking the natural logarithm of these functions

$$\ln[k(x)] = \ln(A) - \frac{x^2}{\sigma_x^2} \quad (9)$$

$$\ln[j(z)] - 2\ln(z) = \ln(B) - \frac{z}{\sigma_z}. \quad (10)$$

$$\Lambda(z/R) = \begin{cases} 0.6 + 6.21(z/R) - 12.4(z/R)^2 + 5.69(z/R)^3, & 0 \leq z/R \leq 1.1 \\ 0, & z/R > 1.1 \end{cases} \quad (3)$$

Fig. 1. Normal-collector configuration of EBIC measurement.

Equations (9) and (10) can be fitted separately into the Monte Carlo simulations data.

The analysis is to be done on the EBIC profile near the junction. The EBIC configuration is shown in Fig. 1. To compute this, we follow the approach of Czaja [20] who divided the current into three regions: the n-region, the depletion layer region, and the p-region. In each region, the current is computed by calculating the convolution of the generation volume distribution with respect to the charge collection probability. This can be written as

$$\begin{aligned}
 I_N(x') = & \int_0^\infty \int_{-\infty}^{x_n} h(x-x', z) Q(x, z) dx dz \\
 & + \int_0^\infty \int_{x_n}^{x_p} h(x-x', z) dx dz \\
 & + \int_0^\infty \int_{x_p}^\infty h(x-x', z) Q(x, z) dx dz \quad (11)
 \end{aligned}$$

where $I_N(x')$ is the normalized EBIC current when the beam is located at x' . In this equation, x_n and x_p are the locations of the edges of the depletion layer, and $Q(x, z)$ is the charge collection probability. The above equation simply says that the collected current is a convolution of the spatial distribution of the generation volume, i.e., $h(x, z)$, and the EBIC due to a point source, which is the charge collection probability $Q(x, z)$. For the EBIC configuration shown in Fig. 1, the charge collection outside the depletion layer was derived by Donolato [10] and is given by

$$Q(x, z) = \exp(-\lambda x) - \frac{2s}{\pi} \int_0^\infty \frac{k}{\mu^2(\mu+s)} \exp(-\mu z) \sin(kx) dk \quad (12)$$

where $\lambda = 1/L$ and L is the diffusion length of the material. The term $\mu = (\lambda^2 + k^2)^{1/2}$, and $s = v_s/D$ is the semi-normalized surface recombination velocity. In this equation, the x -axis starts from the depletion layer edge. Therefore, if the calculation uses the metallurgical junction as $x = 0$, then

we need to replace x with either the absolute value of $(x - x_n)$ or $(x - x_p)$ in (12). When the surface recombination velocity is zero, the only term left is the exponential term. Taking the natural logarithmic of this exponential term gives us $-\lambda x$ or $-x/L$. In other words, when we plot the current in semilogarithmic plot, the slope is $-1/L$. The effect of the second term is simply to reduce the current due to the surface recombination velocity. This agrees with the experiments that show the diffusion length L can be obtained from the negative reciprocal of the semilogarithmic plot when the surface recombination velocity is zero [1].

Note that the charge collection for the region within the depletion layer is assumed to be unity in (11) [20]. This explains why the second term in (11) does not have $Q(x, z)$. Computing (11), (12), and the corresponding expression for $h(x, z)$ gives the EBIC profile around a semiconductor junction.

III. CALCULATION OF GENERATION VOLUME MODEL

The EBIC profiles were computed numerically from (11) and (12). Four profiles were computed, three of which used the mathematical models for the generation volume distributions, i.e., the Donolato model, the Donolato–Venturi model, and the Bonard model. These three profiles were then compared with the EBIC profile computed using energy distributions obtained directly from a Monte Carlo simulation program.

In the Monte Carlo simulation, the electron trajectories in the semiconductor solids due to the bombardment of the electron beam are calculated. The elastic and the inelastic scatterings are modeled using a scattering cross section and a stopping power. The scattering cross section gives the probability distribution when the electron is scattered. This determines the next trajectory after scatterings. On the other hand, the stopping power determines the loss of energy of the electrons. When the energy of the electron is lower than a certain threshold value, the calculation for that particular electron trajectory is stopped.

The Monte Carlo simulation was done with the program developed by Raynald Gauvin's group [21]–[23]. The computation in this paper used the tabulated Mott elastic scattering cross section of Czyzewski. It has been shown by Ivin *et al.* [19] that the Mott elastic cross section is in better agreement with experiment than the Rutherford elastic cross section. Kuhr and Fitting [18] also used the Mott elastic cross section in their Monte Carlo simulation for low-energy electrons. The inelastic scattering is usually modeled using the stopping power expression. The model used for the stopping power expression was from Joy and Luo [24] who modified the Bethe expression for low-beam-energies computation. The Monte Carlo simulation stops when the energy of the computed electron is no longer able to ionize an electron. The model used in this paper to compute the effective ionization energy is based on the work by Casnati *et al.* [25]. The same model has been used in a previous work to determine the electron range in silicon and GaN materials for energy below 5 keV [26].

In this simulation, the beam energy was set to 3 keV with a 10-nm beam radius. The projected energy distribution in the x – z plane was then obtained and stored in a matrix. This matrix was used in the computation of (11) as the generation volume

Fig. 2. Computed EBIC profiles for the region around the edges of a depletion layer. The depletion layer edge is located at $0.3 \mu\text{m}$.

distribution. The sample material was chosen to be silicon. A density of 2.33 g/cm^3 was used in the calculation.

For the EBIC profile calculation, the minority carrier diffusion length was set to $3 \mu\text{m}$. The structure of the EBIC configuration was the normal-collector configuration such as shown in Fig. 1. The depletion layer's edges were located at $\pm 0.3 \mu\text{m}$. For simplicity, the top surface of the sample was assumed to have zero surface recombination velocity. The profile was computed from $x = 0$ to $x = 0.5 \mu\text{m}$, with a spacing of $\Delta x = 0.01 \mu\text{m}$. The profiles were computed only for one side of the junction due to its symmetry.

To compute the profiles using the Donolato and the Donolato-Venturi models, the electron penetration ranges was to be calculated first. The electron range for silicon was computed from [14]

$$R = 4 \times 10^{-2} \frac{E_b^{1.75}}{\rho} \quad (13)$$

where R is the electron range in micrometers, E_b is the beam energy in kiloelectronvolts, and ρ is the density of the sample in grams per cubic centimeter. Besides the electron range, the beam diameter (or the beam radius) must be specified to compute (2). The same beam radius of 10 nm was used in the calculation.

The data from Monte Carlo simulations were used to obtain the fitted parameters of the Bonard model. Equations (9) and (10) were fitted into the data from the simulation. The data was integrated in the z - and x -axes before fitting into the parameters of the functions $k(x)$ and $j(z)$.

The first and the second derivatives of the semilogarithmic EBIC profiles were computed using the centered difference formula [27]. Before computing the first or the second derivative, the natural logarithm function ($\ln$) was applied to the EBIC profiles to give the semilogarithmic EBIC plots. The differences in the EBIC profiles due to the differences in the generation volume distributions will be enhanced when their derivatives are plotted.

IV. RESULTS

Fig. 2 shows the computation results of all four profiles. The differences between the profiles cannot be easily observed in

Fig. 3. First derivative plots of semilogarithmic EBIC profiles. The depletion layer edge is located at $0.3 \mu\text{m}$.

Fig. 4. Second derivative plots of semilogarithmic EBIC profiles. The depletion layer edge is located at $0.3 \mu\text{m}$.

Fig. 2. Figs. 3 and 4, on the other hand, enhance the difference between the four profiles. It can be seen that the profile using the Donolato model is close to the one using the Donolato-Venturi model. On the other hand, the Bonard model is closer to the one using the Monte Carlo data compared to the other two.

Another observation is that the profiles using the Donolato and the Donolato-Venturi models change more rapidly than the Bonard model and the one using the Monte Carlo data (Fig. 3). This can also be seen in the second derivative plots of Fig. 4. The second derivative plots seem to give some indication of the lateral dimensions of the generation volumes.

V. DISCUSSION

The results show that the Bonard model gives an EBIC profile that is closer to the one using the Monte Carlo data. This is partly because of the parameter fitting process. This result also shows that the mathematical expression in (7) can be used to accurately describe the distribution obtained from the Monte Carlo simulations.

In the region around the edges of the depletion layer, the Bonard model changes less rapidly than the other two models. The second derivative plots indicate that this could be due to the lateral dimension of these models. The contours of the energy ionization distributions are shown in Fig. 5. It can be seen that the Donolato model and the Donolato-Venturi model closely resemble one another. The latter has a slightly larger lateral

Fig. 5. Contour of the energy ionization distributions. (a) Monte Carlo simulation results. (b) Donolato model. (c) Bonard model. (d) Donolato-Venturi model. The scales of the x - and z -axes are in nanometers, and the intensity is in electronvolts.

dimension. The lateral dimensions of these two, however, are much smaller than the Monte Carlo simulation result. The Bonard model, on the other hand, has about the same lateral dimension as the Monte Carlo simulation.

However, the contour plots show that the shape of the Bonard model differs slightly in shape compared to the Monte Carlo simulation result. The reason for this is that the distribution of the Monte Carlo simulation result drops faster as it moves away from the beam axis. The distribution then decreases rather slowly after that. The Bonard model, on the other hand, drops at approximately a constant rate. This can be seen from the gradation of the contour. The lateral size of the Bonard model, however, is about the same as that of the Monte Carlo simulation result.

The EBIC profiles plots also give the same conclusion. The second derivative plots show that the Monte Carlo data has a higher peak and drops faster near to edge of the depletion region. The shape of the EBIC profile seems to depend more on the lateral distribution of the generation volume. In this regard, the Bonard model gives better EBIC profiles than those computed using the Monte Carlo simulation result directly.

It is interesting to note that in the first derivative plots, all models intersect at the edge of the depletion region. This is confirmed by the plots of the second derivative. The minimum of all four models are located at the edge of the depletion region.

This gives rise to an alternative method to accurately determine the location of the depletion layer's edges. In other words, it is possible to determine the depletion layer's edges from either the minimum of the second derivative plots, or from the

intersection points of the first derivative plots. The intersection points of the first derivative plots can be obtained when the EBIC is measured with different sizes of generation volumes, or in other words, by using different beam energies.

The difficulty in using the second derivative plots is that the EBIC profiles are usually noisy. This noise is amplified when the first derivative is taken. Taking the second derivative amplifies the noise even further to such an extent that the minimum point cannot be clearly distinguished.

Finally, one would ask why it is that we do not simply use the Monte Carlo data in the computation of EBIC profile. Why would one have to resort to mathematical models which introduce more errors? The answer lies in the convenience of manipulating and computing the mathematical expression instead of dealing with a distribution of data given by the Monte Carlo simulations. If one needs an accurate distribution of the generation volume, then the best results will be obtained by using Monte Carlo distribution data. However, if one only needs to compute the EBIC profile, then this is not required at all. Figs. 2, 3, and 4 show that a mathematical expression using the Bonard model is accurate even to the second derivative plots.

VI. CONCLUSION

This paper analyzes the choice of generation volume models that can be used in the computation of EBIC profiles near to the semiconductor junctions. The EBIC profiles computed using three pear-shaped mathematical models were compared to the one using the data from the Monte Carlo simulation. It was found that the Bonard model gives a closer profile compared

to the Donolato and the Donolato–Venturi models. This is due to the flexibility of the fitting parameters in the Bonard model. The second derivatives of the semilogarithmic EBIC plots give a qualitative indication of the lateral dimension of the generation volume. Some possible alternative ways to determine the edges of the depletion layer were also mentioned in the discussion.

We also gave a choice of the generation volume model to be used for EBIC profile computation around the junction. This is useful for many applications that require EBIC profiles at or near these regions. One example is the extraction of the depletion width of a p-n junction.

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