Device parameters characterization with the use of EBIC

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2008

Oka Kurniawan. (2008). Device parameters characterization with the use of EBIC. Doctoral thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/41843>

<https://doi.org/10.32657/10356/41843>

DEVICE PARAMETERS CHARACTERIZATION WITH THE USE OF EBIC

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A thesis submitted to the Nanyang Technological University
in partial fulfillment of the requirement for the degree of
Doctor of Philosophy

2008

Acknowledgements

The author is indebted to Associate Professor Vincent Ong Keng Sian for his constant support and guidance throughout his candidature as a research student. The author is also very grateful to Dr. Grigore Moldovan and Prof. Colin J. Humphreys from the Department of Material Science and Metallurgy, Cambridge University (UK), for allowing the author to use their EBIC data measurements on the GaN LED. Dr. Grigore Moldovan was also involved in the discussion in developing the technique to determine the edges of the depletion layer of a p-n junction. Next, the author would like to thank Ms Seow-Guee Geok Lian for her help in giving technical supports in IC Design Laboratory II, where the author worked on his project. The author also would like to express his gratitude to NTU for the research grant to do his further study as a PhD student. Lastly, the author wants to thank Ms Maya Kristandyo for her help in checking the manuscript of the Thesis, as well as the author's family for their continual support and encouragement.

"omne quod spirat, laudet Dominum" (Psalmus 150:5)

Abstract

The performance of bipolar and photodiode devices is determined by the transport properties of the minority carriers, such as the minority carrier diffusion lengths and the surface recombination velocities. The Electron Beam Induced Current (EBIC) technique of the Scanning Electron Microscopy (SEM) has been widely used to characterize these two parameters. One of the most widely used methods involves a fitting process with the use of a fitting parameter called alpha. The accuracy of extracting the minority carrier diffusion lengths using this method is affected by several parameters, such as the surface recombination velocity and the exact locations of the edges of the depletion layer. Moreover, this method is only applicable when the p-n junction depth is assumed to be either very deep or very shallow. The present work aims to analyse the parameters affecting the accuracy, as well as to develop techniques to characterize diffusion lengths from a p-n junction that has a finite junction depth.

The effect of the surface recombination velocities on the extraction of the diffusion lengths comes from the fitting parameter, termed alpha, used in the method. The present work analysed the factors affecting this alpha parameter and provided the required conditions for accurately determining the value of the surface recombination velocity. On the other hand, a technique to locate the edges of the depletion layer was developed. Thus, more accurate locations of the edges of the depletion layer can be obtained from

the same measurement data used in extracting the diffusion lengths of the materials.

In order to extract the diffusion lengths from a finite junction depth, the most commonly used method in the field was generalized to take into account the depth of the p-n junction. This generalized method is capable of extracting the diffusion lengths accurately when the beams scan outside of the junction well. For the case when the beams scan inside of the p-n junction well, no analytical expression was currently available. The present work then derived the analytical equations for two different junction geometries; one is an L-shaped junction well, while the other one is a U-shaped junction well.

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Chapter 1

Introduction

1.1 Background

The performance of electronic devices is dictated by the transport properties of the carriers inside the materials. In particular, the performance of bipolar and photoelectronic devices is influenced by the minority carrier properties. The need to characterize these minority carrier properties derives from the fact that some materials give better transport properties than others for some particular applications. Moreover, the device can be designed in such a way so as to improve the transport properties of the materials and, therefore, to improve the performance of the device.

In bipolar and photoelectronic devices, minority carrier diffusion lengths (or diffusion lengths in short) have significant roles. For example in an NPN Bipolar Junction Transistor (BJT), the current gain (β) is proportional to the ratio of the square of the diffusion length (L) of the base region to the width of the base region. Furthermore, the base transport factor (α_T) is

approximately proportional to one minus the square of the ratio of the width of the base region to the diffusion length of the base region. Therefore, to increase either the current gain or the base transport factor, materials with large minority carrier diffusion lengths should be chosen. The other way around to increase the performance is to reduce the base width to be much smaller than the diffusion length.

Another example using photoelectronic devices can help to illustrate the importance of this parameter. For a p-n junction photodiode, the quantum efficiency and the leakage current can be improved by using materials with large diffusion lengths. The diffusion lengths of the materials, however, are reduced when defects are present. Therefore, characterization of diffusion lengths is able to provide information about the defects.

One of the most widely used techniques to characterize the minority carrier diffusion lengths is the Electron Beam Induced Current (EBIC) technique of the Scanning Electron Microscopy (SEM) [1]. The reason for its acceptance is its application for wider range of materials, both direct and indirect band gap materials. Optical techniques, such as photoluminescence, can be used effectively only for direct band gap materials. Furthermore, the EBIC technique can be implemented using an SEM machine, which is widely used for materials characterizations. This also means that the same instrument can be used for several characterizations. Therefore, it gives an advantage to correlate the data obtained from the EBIC technique with the data obtained from the other signals of SEM, such as the secondary electron, the cathodoluminescence, the backscattering, the x-rays, etc.

Another advantage in using electron beams technique is that it does not

require knowledge of the absorption coefficient of the materials [2]. The optical methods, on the other hand, usually require the knowledge of the absorption coefficient for the exciting radiation, and this may vary greatly with the semiconductor or its impurity concentration. These advantages have been attested by the abounding number of papers using the EBIC measurements found in the literature. EBIC has found widely acceptance for minority carrier properties measurements, defect and inhomogeneities observations, IC failure analysis, and many others.

1.2 Electron Beam Induced Current

In this section, a literature review of the EBIC technique is presented, particularly in the area of minority carrier parameters extraction. The term EBIC used in this thesis refers to the current induced in a semiconductor due to an electron beam bombardment when a built-in electric field is present in the material. Researchers in the field of scanning electron microscopy (SEM), however, do not recommend the use of the term EBIC since it obscures the distinction of different contrast mechanisms in conductive mode microscopy [3]. Nevertheless, since many of the works in device parameter measurements use the term EBIC, we will follow the practice here to refer to the contrast signal which we have defined.

A brief historical account of EBIC is first presented, followed by the physical explanation of EBIC. The literature review then focuses on the applications of EBIC in the area of device parameters measurements, particularly in the extraction of the minority carrier properties such as the

minority carrier diffusion lengths and the surface recombination velocities. The section is then closed with a review of the challenges in measuring these two parameters accurately in today's devices.

1.2.1 Early Works

The first observation of EBIC can be traced back to an experiment by Ehrenberg *et al.* in 1951 [4]. It was observed that photovoltaic cells, an example of which is a solar cell, are sensitive to electron beam bombardment. In these series of experiments, a selenium cell was bombarded with electron beams up to 80 keV energy. The plot of the gain, that is the ratio of the short circuit current to the beam current, was plotted against the beam energy. It was shown that the gain increases with the beam energy. This increase seems to be proportional to the number of ion pairs generated. The term *electron voltaic effect* was first introduced in this paper.

A few years later, Rappaport [5] studied the electron voltaic effect phenomena in p-n junctions bombarded by beta-particles. It was shown that the diode current-voltage characteristic under electron bombardment is similar to photovoltaic cells under light illumination. The term electron voltaic effect was used to emphasize the close analogy with the better known photovoltaic effect in solar cells.

In a seminal paper of charge collection contrast, Lander *et al.* [6] showed that electron beams can be used to observe crystal imperfections near the space-charge region of p-n junctions. In this paper, the observation of dislocations, inversion layers, and the depletion region of p-n junctions were

reported. The beam scans the material and the signal of the charge collection was displayed for the first time in a cathode-ray tube to give the image of the p-n junctions.

In 1964, Everhart *et al.* [7] used EBIC for semiconductor device measurements. The article discussed the effects of electron penetration into the material and the scattering with the atom lattice. The theories of this electron penetration and the scattering effect were being developed during this period of time. In fact, few years later, Everhart [8] proposed a universal curve for calculating the electron penetration range in solids, deriving from the Bethe expression.

1.2.2 Basic Physical Principles

As mentioned before, the first to observe the EBIC phenomena were Ehrenberg *et al.* [4]. In that paper, the term *electron voltaic effect* was used since the observed phenomena is similar to those found in photovoltaic devices. A detailed literature review, including on the photovoltaic phenomena, can be found in [9].

The term photovoltaic comes from two words, *photo* which is the Greek root for light, and *volt* which is a common measurement of electricity named after Alessandro Volta. This term expresses the phenomena of semiconductor devices which generate current or voltage when it is illuminated with light [10]. The photon absorbed generates electron-hole pairs within the device.

Similarly, in EBIC, the electron-hole pairs (ehps) are generated inside

the semiconductor materials. However, unlike the photovoltaic phenomena, the ehps in this case are generated by the electron beam.

The electrons coming from the beam, which is usually termed as the primary electrons, can have energy up to several kilo-volts. As the primary electrons enter the semiconductor materials, they interact with the atom lattices through scattering mechanisms. There are two primary mechanisms for electron scatterings in solids. The first one is elastic scatterings while the second one is inelastic scatterings [11].

Figure 1.1: Schematics of the primary electron scatterings in solid [3].

In the elastic scattering, the primary electrons undergo large angular deflections due to scatterings by the strong coulomb field of the nucleus. There is essentially no energy transfer and the collision is elastic. This mechanism causes the spread of the primary electrons within the sample. On the other hand, in the inelastic scattering, the primary electrons lose their energy through electron-electron interaction in which the atomic electrons

are excited into vacant higher energy states leaving the holes in the valence band. In this mechanism, the energy is being transferred from the primary electrons to the atomic electrons. Thus an electron-hole pair is generated. A schematic representation of electron scatterings in a target material is shown in Fig. 1.1.

Figure 1.2: Schematics of the ehps generation and collection [12].

When the primary electron interacts with an atomic electron, it transfers its energy and excites the atomic electron. This is illustrated in Fig. 1.2 where the electron is excited from the valence band into the conduction band.

The volume in which this ehps generation occurs is often called the generation volume or the interaction volume. The ehps diffuse away from the generation volume, and when there is a built-in electric field in the range of the material's minority carrier diffusion length, the minority carrier charge is separated from the majority carrier charge. This segregation is often termed as *collection* in nuclear instrumentation field [3, 13], and thus the term charge collection is commonly used to describe the phenomena. Some

Figure 1.3: The configurations of collectors for EBIC measurement. The built-in potential is shown by the shaded area. Figs (a) and (c) are commonly called the normal-collector configurations, while (b) and (d) are commonly called the planar-collector configurations. Fig (e) is common for transit time measurement in time-of-flight technique. Taken from [13].

common collector configurations for EBIC measurements are shown in Fig. 1.3

The process of diffusion and collection is also shown in Fig. 1.2. In this figure, the built-in electric field is caused by the barrier of a p-n junction. Another approach to create a built-in electric field is to use a Schottky barrier. In any case, the built-in electric field collects the minority carrier charge and repels the majority carrier charge. And when an external circuit is connected to the two ends of the p-n junction, a short circuit electric current flows. This short circuit current, or the induced current, can be measured

from the current-voltage profile such as the one given in [5]. The changes in the conductivity can also be measured from this current by changing the generation rate. In fact, this change in conductivity is the one observed by Ehrenberg *et al.* in [4]. This induced current is what most people call the *electron beam induced current*.

1.2.3 EBIC for Diffusion Length Measurements

The basic idea of minority carrier transport measurements is to inject minority charge carriers into the sample and measure the signals from a certain collector configuration so as to reveal the properties of interest. The minority carriers can be injected either by biasing, illumination (by photon or light), or bombardment of particles (such as electrons as in the case of EBIC). The injected carriers are then transported inside of the materials either through diffusion or drift. These carriers can then be collected in a certain way so as to reveal their transport properties.

Techniques to measure minority carrier diffusion lengths are similar. The ehps are generated by the bombardment of an electron beam. These ehps then diffuse away from the generation volume to the surroundings. If there is a nearby built-in electric field, the minority carriers can be separated or collected. Since the minority carriers diffuse before they are collected, these carriers tend to recombine with the majority carriers. How far the minority carriers can travel before they recombine is determined by the diffusion length of the material.

If the semiconductor crystal is perfect, the minority carriers in the con-

duction band will recombine with the majority carriers in the valence band. However, when impurities or defects are present, some allowed energy levels are introduced in the band gap. These energy levels can also act as recombination centres. In other words, defects or impurities increase the probability of the minority carriers to recombine. Since the probability of recombination increases, the diffusion length, in turn, decreases.

Another parameter that usually affects the value of the diffusion length is the surface recombination velocity. It is a Shockley-Read-Hall (SRH) recombination process through surface states in the band gap. The recombination rate of this process depends on the density and the distribution of the surface states, their associated cross sections, the band bending near the surface, and the injection level. This recombination process introduces another boundary condition at the surface. In many EBIC profile calculation, the surface recombination velocity is usually assumed to be constant. Correig *et al.* [14] analysed the region where this assumption is valid.

These recombination processes are important in understanding the EBIC technique to measure the diffusion lengths of the materials. This is simply because the diffusion length parameter is a measure of the recombination process happening inside of the material.

1.2.3.1 Transient Methods

One of the first papers to extract the minority carrier diffusion length was written by Loferski and Rappaport [15]. In the experiment, an electron voltaic cell was bombarded with high-energy electrons. It was shown that the transient short circuit current is proportional to the square root of the

lifetime, i.e. $I_{sc} \propto \sqrt{\tau}$. The minority carrier diffusion length was then determined from the following equations,

$$L = \sqrt{D\tau} \quad (1.1)$$

and

$$D = \mu \frac{kT}{q} \quad (1.2)$$

where D is the diffusion coefficient or the diffusivity in cm^2/s , μ is the mobility of the carrier in $\text{cm}^2/(\text{V.s})$, k is the Boltzman constant, T is the temperature, and q is the unit charge.

One of the problems with this method is its inaccuracy. Zimmermann [16] showed that the current is not proportional to the square root of the lifetime, but rather, decays following an exponential behaviour. The decay is given by

$$I/I(t=0) = \exp(-t/\tau) \quad (1.3)$$

where t is the time of measurement. However, Kuiken [17] claimed that the simple exponential function is not enough. The reason is that there is a delay after the injection is stopped. Kuiken derived a more complicated function involving the error function to describe the EBIC decay in a normal-collector configuration (Fig. 1.3 (a)). This function, however, is only applicable for zero and infinite surface recombination velocities. It was shown that the surface recombination velocity affects the profile of the decay and, in turns, the extraction of the lifetime.

Jakubowicz [18] derived an EBIC equation for the planar-collector configuration (Fig. 1.3 (b)) for various values of surface recombination velocities.

The thickness of the junction was comparable to or less than the diffusion lengths. It was shown that the increase of the surface recombination velocity results in a more rapid decay of the current. Moreover, the decay in a thin layer sample is different than that of a thick layer. This shows that the layer thickness must be taken into account when using this configuration. The solutions for various surface recombination velocities were obtained numerically. The analytical solutions are only available for zero, one, and infinite surface recombination velocities.

Ioannou [19] bombarded the sample just beneath a Schottky barrier to eliminate the problem caused by the surface recombination velocity. It was found that the EBIC can be expressed as

$$I(t) \propto \exp(-t/\tau)/t^{1/2} \quad (1.4)$$

where t is the time after the beam is turned off. Plotting $\ln(I t^{1/2})$ versus t results in a straight line and the lifetime can be obtained simply from the slope. The derivation of Eq. (1.4) was based on several assumptions. First, the sample is considered to be semi-infinite, which means that the sample thickness must be greater than about five diffusion lengths. Second, the Schottky diode is considered to be infinite. The size of the diode, however, cannot be too large, since it may impose capacitance limitations on the measurement. Another assumption is that the electron penetration depth is much smaller than the diffusion length. The last condition, however, was rather restrictive, that is the plot only results in a straight line when $t^{1/2} \gg \tau^{1/2}$.

The difficulty with these transient methods is that they are less robust than the steady state methods in obtaining the diffusion lengths. In order to obtain the diffusion lengths from the lifetime measurements, it is required to know the diffusivity accurately. This, in turn, requires the determination of the mobility. Even though the mobility can be determined by methods like time-of-flight which also uses electron beam bombardment [20], it is preferred to obtain the diffusion lengths directly in some particular devices. As discussed previously, in devices like bipolar and photodiode, the parameter of interest is the diffusion lengths, and therefore, it is desirable to obtain the diffusion lengths directly for these cases.

1.2.3.2 Steady State Methods

One of the first experiments to determine the diffusion length directly by scanning the electron beam across the junction was done by Higuchi and Tamura [21]. A p-n junction of a normal-collector configuration (Fig. 1.3 (a)) was scanned by an electron beam. The electron beam scanning direction was perpendicular to the collecting p-n junction, and so the normal-collector term was used for this configuration. Previously in [22], a light spot was scanned across a p-n junction and the diffusion length was obtained from the logarithmic plot of the induced current. The slopes of the resulting straight lines give the diffusion lengths of the material. In [21], Higuchi and Tamura did something similar but with electron beams. Since Goucher *et al.* [22] has shown that the EBIC profile is exponential, Higuchi and Tamura then estimated the diffusion length by measuring the distance from the junction where the profile drops to about $1/e$ of the value at the junction.

The reasoning is as follows. If the EBIC profile follows an exponential form such as

$$I(x) = I_m \exp(-x/L) \quad (1.5)$$

where I_m is the maximum current at the junction, x is the distance from the junction, and L is the diffusion length. The natural logarithmic of the profile is simply a straight line, which was the one found in [22]. It can be written as

$$\ln I(x) = \ln I_m - x/L \quad (1.6)$$

In this way, the diffusion length is simply the negative reciprocal of the slope. This is what was done by Goucher *et al.* by using a light spot. Higuchi and Tamura used a slightly different approach. The diffusion length was obtained by measuring the x distance from the junction that gives the value $I_m \exp(-1)$. Substituting this into Eq. (1.5) gives

$$\begin{aligned} I_m \exp(-1) &= I_m \exp(-x/L) \\ -1 &= -x/L \\ x &= L \end{aligned} \quad (1.7)$$

Holt [3], however, argued that this method cannot be recommended. The reason is that it does not take into account the size of the generation volume. The size of the generation volume depends on the beam voltage, and increases as the beam voltage increases. Thus, the distance of decay to $1/e$ is dependent on the beam voltage. This can be seen in an experiment done by Fuyuki *et al.* [23, 24]. Fig. 1.4 shows some experimental results

Figure 1.4: Experimental results for a sample with $\rho = 1 \Omega\text{cm}$, where $L = 8 \mu\text{m}$ and $S = 20$. Δ $E_b = 50 \text{ keV}$, $\circ$ $E_b = 30 \text{ keV}$, $\bullet$ $E_b = 10 \text{ keV}$. Each full curve is the theoretical one of that value [23].

on a normal-collector configuration similar to Fig. 1.3(c). Holt [3] preferred to use the slope of the semi-logarithmic plot in order to obtain the diffusion lengths.

In the same year of the paper by Higuchi and Tamura, another paper was published by Wittry and Kyser [25] which explained the exponential behaviour of the EBIC profile. The exponential dependency on the distance from the junction was derived from a steady-state diffusion equation of the minority carrier concentration by assuming a point source with a spherical symmetry. Assuming that the minority carrier is of n-type, the diffusion equation outside the generation source can be written as

$$D\nabla^2 n - (1/\tau)n = 0 \quad (1.8)$$

By using Eq. 1.1, it can be simplified to

$$\nabla^2 n - (1/L^2)n = 0 \quad (1.9)$$

Assuming a point source with spherical symmetry, this differential equation can be solved to obtain the distribution of the minority carrier. There are two boundary conditions in this problem. The first is zero concentration of minority carriers at the junction. This condition means that all minority carriers approaching the junction are collected and transported to the other side of the junction and become a majority. The second is that a zero surface recombination velocity is assumed. The induced current was then calculated from the concentration gradient at the junction. Assuming that the junction is located at $x = 0$, this can be written as

$$J = \int_0^\infty -D \partial n / \partial x|_{x=0} dz \quad (1.10)$$

The final solution for the EBIC current is given by Eq. (1.5). A more detailed calculation is given in Appendix A.

The solution, as given in Eq. (1.5) or Eq. (1.6) (in natural logarithmic), assumed that the generation volume was a point source. Moreover, the surface recombination velocity was assumed to be negligible. Therefore, in order to obtain the diffusion length from the negative reciprocal slope of Eq. (1.6), these assumptions must be taken into account.

The point source estimation can be used when the beam is far away from the junction. The straight line curve under a semi-logarithmic plot for the case when the beam position is far away from the junction was shown by Munakata [26]. Extrapolating the linear region to the junction gives an

estimated maximum current that can be generated inside of the material, i.e. I_m . However, the observed maximum current is usually less than that due to a finite generation volume. The profile deviates from a straight line for beam positions around the junction.

In 1966, Czaja [27] measured the diffusion lengths of Si and GaP from a planar-collector configuration such as shown in Fig. 1.3(b). The approach, however, was slightly different. The diffusion lengths were fitted into the following equation.

$$I = I_n + I_{scr} + I_p \quad (1.11)$$

$$I = \frac{1}{\epsilon} \int_0^{x_n} h(\xi) \exp((\xi - x_n)/L_n) d\xi + \frac{1}{\epsilon} \int_{x_n}^{x_p} h(\xi) d\xi + \frac{1}{\epsilon} \int_{x_p}^R h(\xi) \exp((x_p - \xi)/L_p) d\xi \quad (1.12)$$

where the first term accounts the collection in the n region, which was from 0 to x_n , the second term accounts the collection in the space charge region, and the third term accounts the collection in the p region. The collection is an integration of the generation volume distribution multiplied with the collection probability of a point source.

The advantage of this approach is that it takes into account the three regions, even the depletion layer, as well as the distribution of the generation volume. The diffusion lengths at both the p and the n regions can be obtained simultaneously. The diffusion length in the top surface was divided

into the surface diffusion lengths and the bulk diffusion lengths. This is to take the effect of the surface recombination velocity into consideration. The approach of Czaja gives insight that it is important to take into account the surface recombination velocity as well as the distribution of the generation volume. Nevertheless, the diffusion lengths were obtained by fitting a rather complicated function into the data.

One way to use a simpler expression for a planar-collector configuration (Fig. 1.3(b)) is to scan the electron beam on an angle-lap surface [28–30]. In this way, as the beam scans horizontally, the distance of the generation volume to the junction varies. Therefore, an exponential behaviour can still be observed, i.e. $I(z) = C \exp(-z/L)$. If the surface is angle-lapped by θ degrees, the current expression with respect to the horizontal axis can be written as

$$I(x) = I_m \exp(-x \sin \theta / L) \quad (1.13)$$

where $z = x \sin \theta$. Hackett derived a more thorough expression starting from the result of van Roosbroeck [31] for the solution of a differential equation due to a light source. The above result is a simplification for the case when $\bar{z} \gg L$, where $\bar{z}$ is the depth, or the centre of mass, of the generation volume. When this condition is satisfied, the effect of the surface recombination velocity is negligible. This angle-lap method, therefore, is suitable for measuring small diffusion lengths. The disadvantage of this method lies in a more complicated specimen preparation that is required to create the angle-lap surface. Some correction to the original expression was made by von Roos [32]. The expression by Hackett was shown to be accurate for

small angle $\theta < 10^\circ$.

It has been shown in [2, 30] that the surface recombination velocity does affect the EBIC current. The measured diffusion length is then the *effective* diffusion length rather than the true value of the diffusion length of the material. As the beam energy decreases, the effective diffusion length also tends to decrease. This is mainly due to more recombinations at the surface. This was shown in [33]. Jastrzebski *et al.* [34] analysed quantitatively the effect of the surface recombination velocity on the effective diffusion length. The analysis, however, was found to be inaccurate by Donolato [35], Ong *et al.* [36], and Luke [37]. The surface recombination velocity extracted using the method in [34] tends to underestimate the true value of the surface recombination velocity.

In 1976, Berz and Kuiken [38] derived a point source EBIC expression for any values of surface recombination velocities. The analytical expressions for special cases zero and infinite surface recombination velocities using a normal-collector configuration were also given. In the calculations, the method of images was used to satisfy the boundary conditions. The expression for the zero surface recombination velocity simplifies to Eq. (1.5). The expression for the infinite surface recombination velocity, however, involves a modified Bessel function. Nevertheless, when the beam positions satisfy $x/L \gg 1$, the current approaches

$$I(x) = kx^{-1/2} \exp(-x/L) \quad (1.14)$$

where k is a constant with respect to the beam position.

It was shown also that larger surface recombination velocities cause the

curve to concave upward in the semi-logarithmic profile. For the case of zero surface recombination velocity, the curve is a straight line; while for the case of infinity surface recombination velocity, the curve is concave upward.

This enables one to extract the diffusion lengths for two extreme conditions, that are the zero and the infinite surface recombination velocities. These conditions can be satisfied after some surface treatments. Without a surface treatment, however, the surface recombination velocities usually fall between these two extremes. In this case the accuracy would be affected. A derivation of the EBIC profile expression for a finite width device was given by Burk and Sundaresan [39] using the same method of images.

Berz and Kuiken also gave an expression to calculate the surface recombination velocities by varying the beam energies. The current as a function of beam energies can be written as

$$\frac{I}{I_b E_b} = A \left(1 + \frac{v_s}{D} \bar{z} \right) \quad (1.15)$$

where I_b is the beam current, which can be measured by using a Faraday cup, E_b is the beam energy, v_s is the surface recombination velocity in cm/s, A is a constant independent of I_b and E_b , and $\bar{z}$ is the centre of mass of the generation volume, which was found to be approximately $0.41R$ [35], where R is the electron penetration range and is a function of the beam energy. Plotting the left hand side with respect to $\bar{z}$ gives a straight line, from which the surface recombination velocity can be extracted. The surface recombination velocity is obtained from the ratio of the slope to the intercept.

Watanabe *et al.* [40] also gave an expression to extract the surface re-

combination velocity based on the calculation of Hacket in [30]. The EBIC current as a function of the depth is given as

$$\frac{\partial}{\partial \bar{z}} \ln I|_{\bar{z}=0} = \frac{v_s}{D} \quad (1.16)$$

The surface recombination velocity is obtained from the first derivative with respect to the $\bar{z}$ axis and extrapolating them to $\bar{z} = 0$. It was claimed that the method is valid for any collector geometry. Luke in [41] gave the conditions to use this technique accurately. It was shown that the condition of $\bar{z} \rightarrow 0$ must be observed and the beam width must be kept constant as the beam energy is varied.

The two approaches by Berz and Kuiken and Watanabe *et al.* are commonly called the voltage-varying methods. Instead of scanning the beam across the sample, the beam is bombarded at one point with varying energies. Luke [42] generalized the two methods and showed that the two approaches actually derived from a common origin. The generalized method by Luke requires two extrapolations and uses a correction factor to obtain the surface recombination velocity.

Wu and Wittry [43] eliminated the effect of the surface recombination velocity by utilizing a Schottky barrier at the surface. The barrier creates a depletion region at the sample's surface and thus all excess carriers going to the surface are collected as an induced current. The beam bombarded the sample at one location with varying beam energies. The diffusion length was then calculated by comparing the experimental data with the theoretical equation. This enables several other parameters to be obtained. The disadvantage is that the fitting involves a complicated function. Moreover,

it is only applicable to planar-collector configuration.

In the following few years, the planar-collector configuration had gained interests. The reason was that the configuration can be used for both diffusion length measurements as well as defect observations. Ioannou and Davidson [44] showed that the diffusion lengths can be extracted by slowly scanning the beam away from the Schottky diode in the horizontal direction. It was found that the EBIC decay for an infinite surface recombination velocity can be described by the following equation

$$I(x) = k_1 x^{-3/2} \exp(-x/L) \quad (1.17)$$

where k_1 is a constant whose value depends on the beam energy, the beam current, the atomic number, and the diffusion length of the sample. The diffusion length can then be obtained by plotting $\ln(Ix^{3/2})$ versus x . The negative reciprocal of the slope gives the value of the diffusion length of interest. The equation holds under several conditions. It is required that the dimensions of the Schottky diode as well as the sample thickness to be much larger than the diffusion lengths. This expression was later confirmed theoretically. Ioannou and Dimitriadis [45] derived Eq. (1.17) from the steady state diffusion equation.

One of the conditions in using the previous method is that the sample thickness must be much larger than the diffusion lengths. Therefore, the method is not valid for thin semiconductor layer. In 1981, Dimitriadis [46] showed that for a thin semiconductor layer, the slope approaches

$$1/L_{\text{eff}}^2 = 1/L^2 + 1/L_g^2 \quad (1.18)$$

where L_{eff} is the measured slope, $L_g^2 = w^2/\pi^2$ is a *geometrical diffusion length*, with w as the thickness of the thin layer, and L is the true diffusion length of the bulk material. Plotting $1/L_{\text{eff}}^2$ versus $1/w^2$ results in a straight line. The diffusion length can then be obtained from the intercept. The problem with this approach is that it requires several samples with different values of w . And the diffusion length can only be obtained by extrapolating the data to the case where w is very large.

Some advancements of the determination of diffusion lengths using the normal-collector configuration also happened around this year. Oelgart *et al.* [47] measured the diffusion lengths and the surface recombination velocities by comparing the theoretical and the experimental data. The theoretical expression used a Gaussian approximation for the depth distribution. Donolato, on the other hand, derived an EBIC profile for this collector configuration in a form of Fourier transform with an expression containing elementary functions only [48]. The same paper also gave a derivation for the case when the width of the p-n junction is not infinitely large. The result was the same as those obtained by von Roos some years back [49].

Based on his derivation, Donolato [35] proposed a method to determine the diffusion length based on the evaluation of the first moment of two EBIC profiles at different beam energies. Since it involves two equations, the method is able to solve two unknowns simultaneously. In this paper, the diffusion length and the surface recombination velocity were obtained by solving this system of equations.

It was also shown that the error is sensitive on two factors. They are the assumed value of the electron range and the exact locations of the depletion

layer's edges. The system of equation involves a parameter termed *the mean generation depth* which can be approximated to be about $0.41R$. On the other hand, the evaluation of the first moment requires knowledge of the location of the edges of the depletion layer. Donolato followed Oelgart *et al.* [47] by taking the location of the inflection point of the profile as the edges of the depletion layer. This, however, was supported only by qualitative arguments.

Luke and van Roos also derived equations for the normal-collector configuration [50, 51]. The expression for the case of finite width collector was given in integral rather than summation as the case of Donolato. This resulted in a faster convergence. Luke and Cheng [52] then tried to extract the diffusion length by fitting this expression to experimental data. This, however, involves a complicated function for the fitting process.

Besides for the normal-collector configuration, Donolato also derived an expression for the planar-collector configuration, but only for the case of zero surface recombination velocity [53]. The derivation for the finite surface recombination velocity is complicated since it involves mixed boundary conditions. The case for the finite surface recombination velocity can be solved by using a more complicated technique such as Weiner-Hopf as done by Boersma *et al.* [54].

For the case of the zero surface recombination velocity, however, the EBIC profile approaches asymptotically to

$$I(x) = k_2 x^{-1/2} \exp(-x/L) \quad (1.19)$$

where k_2 is a constant, and x is the beam distance from the edge of the

barrier as the beam scans further away. The equation is valid for large values of x , and only for the case of zero surface recombination velocity. An alternative method by using the moment of the derivative of the profile was also proposed in this paper. This technique was demonstrated for the planar-collector [55] and the normal-collector configuration [56] to extract the diffusion lengths.

The extraction of the diffusion lengths has so far been restricted to special cases of zero or infinite surface recombination velocities. The extraction of any finite surface recombination velocities usually requires fitting of a complicated function to experimental data. Some works were done to use simpler expressions. One of them is the work by Kuiken and van Opdorp [57]. Kuiken and van Opdorp provides several methods to extract the diffusion lengths and the surface recombination velocities for planar-collector configuration based on the expression provided by Boersma *et al.* [54]. They claimed that obtaining diffusion lengths from the tangent of the logarithmic plot of Eq. (1.17) overestimated the true value of the diffusion length by about 25%. This could be due to the validity of the equation for infinitely large surface recombination velocities. Kuiken and van Opdorp proposed to extract diffusion lengths for $S = v_s L/D \gg 1$ by taking the tangent twice, and using the previous result as a correction factor for the next calculation, and then evaluating the mean value of the two measurements.

They also provided several techniques to measure surface recombination velocities for various regions of the S range. The disadvantage is that the technique is only valid for certain region of S , and thus, one does not have a general technique for all values of surface recombination velocities.

It was only in 1994 that a generalized expression in the form of an exponential was proposed by Ong *et al.* [36] to take into account the surface recombination velocities of any values. The original paper was written for the normal-collector configuration, however, it was found that the method is also applicable for the planar-collector configuration [58]. In general, the EBIC profile can be expressed as

$$I(x) = k_3 x^\alpha \exp(-x/L) \quad (1.20)$$

where k_3 is a constant, x is the beam distance from the junction for the case of the normal-collector, or the beam distance from the edge of the Schottky barrier for the case of the planar-configuration. The parameter α (alpha) is the linearization coefficient which is obtained by fitting the equation into the data. The name of the linearization coefficient comes from the fact that when the EBIC is plotted as

$$\ln(Ix^{-\alpha}) = \ln k_3 - x/L \quad (1.21)$$

, it yields a straight line. The alpha parameter determines the concavity of the curve. The curve is concave due to the surface recombination velocity. The values of alpha, therefore, depend on the surface recombination velocities. For the case of the normal-collector configuration, the alpha value varies from 0 to -1/2, with zero for the zero surface recombination velocity, and -1/2 for the infinite surface recombination velocity. On the other hand, the alpha value varies from -1/2 to -3/2 for the case of the planar-collector configuration, with -1/2 for the zero surface recombination velocity, and -3/2 for the infinite surface recombination velocity. These values agree with previous results as shown in Eqs. (1.5), (1.14), (1.19), and (1.17).

The technique was found to be very accurate when the following conditions are satisfied [38].

$$(w - x) > 2L \quad (1.22)$$

$$R \ll L \quad (1.23)$$

$$\bar{z} \ll L \quad (1.24)$$

$$x > 2L \quad (1.25)$$

where w is the location of the back contact. The first condition means that the device width must be larger than two diffusion lengths. The second and the third conditions mean that the electron penetration depth or the centre of mass of the generation volume must be much smaller than the diffusion length. The last condition states that the beam must scan further away from the junction by about two diffusion lengths. The limitation of this technique lies in the requirement that the beam scanning range must be $2L$ away from the junction as well as from the back contact. The accuracy is also affected by the locations of the depletion layer's edges. This is particularly true for small diffusion lengths materials since the error perturbs the x values in the fitting process.

Nevertheless, this technique also enables one to obtain the surface recombination velocities simultaneously. It is shown in [59] that the alpha parameter seems to depend only on the surface recombination velocities and can be used to extract them by using

$$S = \eta + \sigma_1 \sqrt{2 \ln \left(\frac{A}{\alpha + B} \right)} \quad (1.26)$$

where $S = v_s L/D$ is the normalized surface recombination velocity, α is the parameter from Eq. (1.21), and the rest are fitted parameters to Gaussian distribution, which values are given as follows: $\eta = -20$, $\sigma_1 = 4.7$, $A = 5047$, and $B = 0.6$. It was shown that the finite surface recombination velocities in the range of $0.05 < S < 5$ can be extracted with errors less than 20%. The advantage of this method is that the surface recombination velocities can be obtained directly from the alpha parameter obtained from the same EBIC line scan used to extract the diffusion lengths.

In 2003, Zhu *et al.* [60] proposed that the diffusion lengths can be obtained without fitting the equation. Starting from Eq. (1.21), the first derivative of the natural logarithmic EBIC profile can be written as follows.

$$\frac{d \ln I}{dx} = \alpha/|x| + 1/L \quad (1.27)$$

The diffusion lengths for finite surface recombination velocities (i.e. finite α) can be obtained from the asymptote plot as $x \rightarrow \infty$. The difficulty with this method is that it requires a large device since the measurement must be taken at a very large x . The accuracy, therefore, is limited by the x range that can be taken in the measurement.

In that same paper, however, it was stated that the alpha parameter was found not only a function of surface recombination velocities, as it was thought, but also a function of the beam energy. If this is the case, then the accuracy of Eq. (1.26) would be affected.

In the recent years, several techniques for region close to the collectors and contacts have been proposed. The asymptotic techniques require the data to be taken from a certain distance from the junction as well as from

the back contacts. For example, Eq. (1.21) requires the beam distance to be larger than two diffusion lengths from the junction as well as from the back contacts. As dimensions of devices get smaller, the accuracy of these techniques would be affected.

It was first pointed out by von Roos [49, 61] that the presence of the back contacts affects the accuracy of the extraction of the diffusion lengths. An analytical equation was derived. This equation contains non-elementary functions such as the Error Function. It was shown that the diffusion lengths extraction produces error when the distance between the collector and the back contact is comparable to the diffusion lengths.

Donolato [48] in 1982 also gave a derivation when the back contact is present. This equation composed only of elementary functions. The extraction of diffusion lengths can be done through fitting these functions into the data. Luke [62], on the other hand, proposed a simpler, yet a non-asymptotic, technique to measure the diffusion lengths from a planar-collector configuration. The diffusion lengths can be extracted from a region $0.5 < x/L < 2$ by evaluating the following equation

$$L = -\frac{1}{\text{slope}} \frac{1}{(L_\alpha/L)_{\text{ave}}} \quad (1.28)$$

where the slope is taken from the plot of $\ln(Ix^\alpha)$ versus x , and the second ratio is a correction factor. The correction factor $(L_\alpha/L)_{\text{ave}}$ is taken from the tabulated value given in the paper for a given alpha value. The alpha value was obtained by fitting Eq. (1.21) in the region of $0.5 < x/L < 2$. Once the alpha value is known, the correction factor $(L_\alpha/L)_{\text{ave}}$ is obtained by evaluating the numerical equations derived by Boersma *et al.* [54].

The difficulty with this technique is that it is based on tabulated correction factors. For values not given in the table, one is required to interpolate the data. Moreover, since the tabulated data is based on the fitting in the region of $0.5 < x/L < 2$, it requires an estimate of the diffusion length (cf. the term x/L). In practice, this estimate will create error in the x range and thus in the correction factor used to calculate the diffusion lengths.

Ong and Wu [63] proposed a non-asymptotic technique for the case of zero surface recombination velocity. It is shown that the diffusion lengths can be obtained from

$$L = \sqrt{\frac{I(x)}{I''(x)}} \quad (1.29)$$

where $I''(x)$ denotes the second derivative of EBIC with respect to x . This can be calculated by the finite difference method as follows.

$$I''(x) = \left. \frac{I(x + \Delta x) - 2I(x) + I(x - \Delta x)}{\Delta x^2} \right|_{\Delta x \rightarrow 0} \quad (1.30)$$

The accuracy of the technique depends on how small Δx can be taken experimentally. Luke [64] analysed this question. In order to extract the diffusion lengths accurately, the value of Δx must be very small and close to zero. On the other hand, the error-to-signal ratio increases as Δx decreases. To reduce this ratio, the value of Δx must be as large as possible. These are some considerations that have to be taken when using this technique.

The above technique, however, is only valid for zero surface recombination velocity. The same authors [65] improved the technique to make it applicable for any values of surface recombination velocities. Since the EBIC profile has been known to be sensitive when it is scanned vertically,

the authors showed that the diffusion lengths can be obtained by scanning the sample horizontally and vertically. The relationship was given as

$$I_{xx}(x, z) + I_{zz}(x, z) = \lambda^2 I(x, z) \quad (1.31)$$

where $I_{xx}(x, z)$ and $I_{zz}(x, z)$ are the second derivative of the EBIC profile with respect to x and z axis respectively, and $\lambda = 1/L$. The product of the beam energy and the beam current must be kept constant when the beam scans vertically by varying the beam energy. These techniques, however, requires quite a high accuracy since it involves a second derivative of the EBIC profile in the x and z direction. The method has given a high potential for measuring the diffusion lengths, and more works still need to be done for its implementation.

A recent development is on the work of single contact EBIC (SC-EBIC). It has been shown that the wirings can be reduced significantly by using this configuration [66–70]. The configuration only requires one connection at the substrate. The technique has been used for failure analysis [71] and IC imaging [72]. The theory of the EBIC signal has been presented in as short paper in [73]. In year 2000, Ong and Wu showed that the same EBIC signal can be obtained from the transient SC-EBIC signal in the region just after the beam is turned on [74]. It was shown as well that the same EBIC technique proposed by Ong *et al.* using the alpha parameter can be used to measure the diffusion length.

To sum up the survey, the overall picture basically shows that there are two practical techniques to measure diffusion lengths. The first involves comparing the analytical function to the data. This requires certain assump-

tions on the distribution of the generation volume. The second one uses an asymptotic approach. The later, which usually developed from the former, is preferred by many experimentalists due to its simplicity. The development of the techniques for certain configurations shows that analytical expressions must be available. This is then followed by certain simplifications which results in an asymptotic technique.

Currently, the most commonly used technique is the one proposed by Ong *et al.* [36]. The asymptotic approach was generalized by introducing a fitting parameter called the alpha parameter, i.e. α . This enables us to extract both the diffusion lengths and the surface recombination velocities simultaneously.

1.3 Problems Formulation and Motivation

1.3.1 Factors Affecting the Alpha Parameter

The last section shows that, currently, most measurements of diffusion lengths use Eq. (1.21) with a linearization coefficient alpha. This alpha parameter has been used to extract the surface recombination velocities [59] through the use of Eq. (1.26). The advantage of using this method for the extraction of surface recombination velocities is that it can be obtained simultaneously from the same line scan measurements of diffusion lengths.

Zhu *et al.* [60], however, stated that the alpha parameter seems to be affected by the beam energy. If this is the case, the accuracy of Eq. (1.26) would be affected. However, no further analysis was given to support the

statement. Up to the present time, there is no thorough analysis on the factors affecting the alpha parameter.

1.3.2 Depletion Edges Determination

In many diffusion length measurements, the accuracy of the technique is also affected by the location of the depletion layer's edges which determine the x range values of the fitting equation. This is particularly true when the diffusion length is comparable to the depletion layer width and when the surface recombination velocity is not zero. Since most diffusion length measurements are for non-zero surface recombination velocities, it is important to determine the edges of the depletion layer. This becomes more important in measuring small diffusion length materials.

The depletion width and its edges can be determined experimentally by many techniques such as capacitance-voltage (C-V) [75], scanning capacitance microscopy (SCM), scanning tunneling microscopy (STM) [76], as well as optical beam induced current (OBIC) [77], and EBIC [78, 79]. Nevertheless, when the diffusion lengths are obtained from EBIC, it is advantageous to obtain the depletion width directly from the same profile.

The capability of EBIC for depletion width measurements was first demonstrated by MacDonald and Everhart [80] in 1965. The depletion width was obtained from the width of the maximum EBIC profile in the micrograph. The depletion widths for several reverse biased p-n junctions were plotted. The accuracy was claimed to be about $1\text{ }\mu\text{m}$, which is not accurate for high doping materials.

Oelgart *et al.* [47] used the inflection point of the EBIC profile as the position of the depletion edges. Though this is supported only by some qualitative arguments, the method was used by Donolato in [35].

A more accurate extraction of depletion width was provided in a review paper by Yakimov [78]. He used an equation that involves both diffusion lengths and depletion width to fit into the EBIC profile. The fitting gives the value of both the diffusion lengths as well as the depletion width. The technique, however, suffers the same disadvantage from other fitting techniques that involve complicated functions. The analytical function for the choice of configuration must be known beforehand. Moreover, the technique only gives the width of the depletion layer and not the exact position of the edges.

In 2002, Chiu and Shih [79] improved the accuracy of the depletion width extraction by using a small energy of electron beam bombardment. The depletion width can be obtained from the following equation

$$W = W_0 + 2 \times 0.1R \quad (1.32)$$

where W_0 is the width of the maximum flat region in the EBIC profile, and the second term was added to take into account the lateral dimension of the depletion region. The maximum flat region can be observed when $W \gg R$, where R is the electron penetration range. The difficulty with this technique, however, comes from the determination of the value W_0 . The reason is that it is rather difficult to determine the exact edges of the maximum flat region in an EBIC profile.

Another thing that would affect the accuracy is the assumed expression

of the lateral dimension of the generation volume ($0.1R$) and the calculation of the R value. Currently there is no consensus on which semi-empirical expressions of the range-energy relationships to use [81], particularly for low beam energy range. This is further discussed in the following section.

1.3.3 Range-Energy Relationship for Low Beam Energy Range

The previous discussion showed that one of the parameters affecting the accuracy is the calculation of the electron penetration range value, i.e. R . This parameter characterizes the size of the interaction volume between the beam and the sample, or the generation volume of the electron-hole pairs. There are two principle ways to calculate the electron penetration range: semi-empirically or statistically using the Monte Carlo simulation.

The three most commonly used semi-empirical expressions are due to Gruen [82], Everhart and Hoff (E-H) [8] and Kanaya and Okayama (K-O) [83]. Gruen measured the variation of energy dissipations with penetration distance for air. He found that the shape of the distribution was almost independent of the beam energy when plotted as a function of an *extrapolated* range. This extrapolated range is commonly termed the Gruen range and is a function of beam energy. Everhart and Hoff, then, derived a universal curve from the Bethe stopping power expression. The calculation of the electron range is a function of the beam energy as well as the material properties such as the atomic number and the atomic weight. They also corrected the Gruen range based on their calculation from the universal curve. A

year later, Kanaya and Okayama derived an expression for the electron range based on a hemi-sphere model of its generation volume.

Currently, there is no consensus on which semi-empirical range-energy expressions to use [81]. Luke in [81] analysed both Everhart and Hoff as well as Kanaya and Okayama expressions with Si and GaAs as the sample materials. However, in the computation of the E-H electron range for GaAs, the universal curve from the original paper was not used. Rather, it used the corrected Gruen range expression that was given by Everhart and Hoff. Moreover, the analysis is applicable only for beam energies above 5 keV, and no discussion is found for lower beam energy range. Low beam energy range has become significant in order to achieve higher resolution in EBIC applications. This is due to the fact that smaller beam energy results in a smaller generation volume. Therefore, it is necessary to investigate and propose an expression to describe the relationship between the electron range and the beam energy, particularly for low beam energy range.

1.3.4 Measurements from a Diffused Junction

Most collector configurations are restricted to either the normal-collector or the planar-collector configurations. The technique involving the alpha parameter has been found to be valid for both configurations. In the case of the normal-collector configuration, for example, the junction depth is assumed to be infinitely deep. In today's planar technology devices, however, most p-n junctions are fabricated as diffused junctions with finite junction depths.

Some works have been done to study the EBIC profile for this finite junction depth. Dimitriadis [46] used a Schottky barrier in a thin semi-conducting layer where the bottom part of the device behaves just like a collecting junction. Holloway [84] studied the induced current profile when a spot light impinges a semiconductor's surface outside the diffused junction. It was shown that the thickness of the specimen affects the decay of the current profile. Thin samples have slower decay while thick samples have faster decay. This is caused by more collection in the thin samples, particularly when the bottom part is assumed to have zero surface recombination velocity. The depth of the junction seems to affect the decay of the induced current profile as well. The profiles of the shallow junction depths decay faster compared to larger ones.

A thorough analysis for the induced current by an electron beam was done by Soukup and Eskstrand [85]. The junction well has a sharp L-shaped geometry. The effect of the junction depth was found to be the same as those by Holloway. In the analysis, theoretical expressions were derived using the method of images for the case when the beam is located at the outside of the diffused junction. The diffusion lengths were obtained by comparing theoretical functions to the experimental data. The theoretical functions, however, involve non-elementary functions, such as the Bessel Function. This complicates the computations and the extraction of diffusion lengths. Moreover, the expression is only valid for the case of high surface recombination velocities.

Artz [86] tried to simplify the matters by using a second order polynomial as a fitting expression for the EBIC profile outside the diffused junction.

Most experimentalists, however, would still prefer a simpler asymptotic approach such as done by Boudjadi [87] in 1995. The diffusion length of the base region of the BJT was obtained from the negative reciprocal slope of Eq. (1.6). The configuration of a finite junction depth was simplified to a normal-collector configuration by making some assumptions. It was assumed that the junction is large enough and the penetration depth of the electron beam is very close to the surface. Nevertheless, the trend of device scaling prevents these assumptions in the future.

The same technique used by Boudjani also assumed a negligible surface recombination velocity. However, no approach using the asymptotic technique seems currently available for the extraction of diffusion lengths from a finite junction depth for any values of surface recombination velocities.

1.3.5 EBIC Expressions for Collection from within a Diffused Junction Well

The success of an EBIC technique have arisen from the availability of the analytical equations of the EBIC profile. For the case of the normal-collector and the planar-collector configuration, the analytical expressions have been available in the literature. This makes the configurations become the two most widely used configurations in EBIC measurements.

In planar technology, however, many devices are constructed from p-n junctions with finite junction depths. This means that one must make certain assumptions in order to use the available expressions from either the normal-collector or the planar-collector configuration. Some studies for this

finite junction depth have been presented in the last section. The previous discussion considered only the EBIC profile when the beam is bombarded outside the diffused junction. For the collection from within the diffused junction, the expression provided by Soukup and Ekstrand is the only analytical expression currently available. As mentioned before, this expression contains non-elementary functions which complicate the computations.

Moreover, the expression by Soukup and Ekstrand assumes that the width of the junction is infinitely large. In today's devices, most junctions have finite widths. Therefore, the shape of the junction is no longer an L-shaped junction well but rather U-shaped junction well. Currently, there has been no available EBIC expressions for the case of the finite width and the finite junction depth collectors. The availability of an analytical expression would help to enhance the study of the charge collection in today's devices, where the dimension of the junction can no longer be assumed to be infinite.

1.4 Objectives of the Present Work

The objective of the present thesis is to fill in the gaps presented in the previous section. The first objective is to give a thorough analysis on the factors affecting the alpha parameter, which in turns, affecting the accuracy of extracting the surface recombination velocities. The second is to investigate and propose a more accurate technique to measure the edges of the depletion layer from the EBIC profile. Besides that, the thesis aims to analyse and propose methods to measure diffusion lengths from non-conventional collectors, such as the L-shaped diffused junctions found in many of today's

devices. And lastly, in order to enhance the study of charge collection in today's devices, the thesis also aims to provide analytical expressions of the EBIC profiles for two junction geometries. They are the L-shaped and the U-shaped junction wells. In this way, charge collection from smaller dimension devices can be analysed.

1.5 Major Contributions of the Thesis

The contributions of the thesis can be summarized as follows:

1. The thesis gives a thorough analysis on the factors affecting the alpha parameter, which in turn affects the accuracy of extracting the surface recombination velocities. This is the first time such approach has been made.
2. It develops a technique to obtain the edges of the depletion layer from the first derivative of a semi-logarithmic plot of the EBIC profile. This technique improves the one proposed by Chiu and Shih [79].
3. It generalizes the technique proposed by Ong *et al.* [36] by taking into account the depth of the junction. This enables one to extract the diffusion lengths from any values of surface recombination velocities and junction depths. This is for the case when the beam scans outside of the junction well.
4. The thesis also derives two analytical EBIC expressions for the L-shaped and the U-shaped junction well geometries. The expression for the L-shaped junction comprises of only elementary functions, which is

simpler than the one given by Soukup and Ekstrand [85]. On the other hand, the expression for the U-shaped junction is the first analytical expression provided for this geometry, as far as the author knows.

1.6 Organization of the Thesis

This chapter gives a literature review of the EBIC technique particularly for the extraction of the minority carrier diffusion lengths. Some gaps for further research have also been identified. The present work aims to address these gaps.

The following chapter gives a brief review of the diffusion lengths and surface recombination velocities measurements using the most commonly used technique proposed by Ong *et al.* [36]. Some discussion on the accuracy of the technique is also given in this chapter. One of the most important parameter of this technique is the alpha parameter, which can also be used to extract the surface recombination velocities. The third chapter discusses the factors affecting this alpha parameter. Conditions for accurate measurements are also given in that chapter.

The fourth chapter addresses the challenge of obtaining the depletion layer's edges or the depletion width directly from the EBIC profile. A thorough analysis was done on the proposed technique using a design of experiment approach. Experimental results are then presented to verify the application of the proposed technique. Two issues that affect the analysis and the accuracy of this technique are addressed in the following two chapters. The first one discusses the range-energy relationships to use in Silicon

and Gallium Nitride, particularly for low beam energy region. The second one discusses the generation volume model to be used in the mathematical analysis of the EBIC profile across the junction.

The next two chapters deal with non-conventional collector configurations. The first of these proposes a generalized method to extract the diffusion lengths from when the beam scans the outside of the L-shaped collector junction. The second one, which is the last chapter, derives an analytical EBIC profile expressions for two collector geometries: the L-shaped and the U-shaped p-n junction geometries. The thesis is then closed with a conclusion, which also discusses some recommendations for future works.

Chapter 2

Extraction of Diffusion Lengths and Surface Recombination Velocities

2.1 Introduction

This chapter gives a short introduction to the diffusion lengths and surface recombination velocities extraction by using the technique proposed by Ong [36]. In the first section, some theories on linear regression are presented. This section is then followed by some examples to obtain the diffusion lengths and the surface recombination velocities from the normal-collector configuration. The data used in the example is generated from the most commonly used theoretical EBIC profile equation found in the literature.

Figure 2.1: Normal-collector configuration.

2.2 Theory

One of the most commonly used configurations in EBIC measurements is the normal-collector (Fig. 2.1). In the normal-collector configuration, the electron beam scans the surface of the sample in a direction normal to the collecting junction.

It was shown by Ong *et al.* [36], and then by Chan *et al.*, [58] that the EBIC profile can be written as

$$I = kx^\alpha \exp(-x/L) \quad (2.1)$$

The diffusion length can then be extracted from the negative reciprocal of the slope from the plot

$$\ln(I/x^\alpha) = \ln(k) - x/L \quad (2.2)$$

In the original papers, the linearization coefficient α was varied until the

coefficient of determination r^2 reached a maximum value. This work can be much simplified by applying the theory of linear regression.

Instead of Eq. (2.2), we can express Eq. (2.1) as

$$\ln(I) = \ln(k) + \alpha \ln(x) - x/L \quad (2.3)$$

It can be easily seen that this equation is linear with respect to its fitting parameters. In fact, the above equation can be written as

$$y = \beta_0 x_0 + \beta_1 x_1 + \beta_2 x_2 \quad (2.4)$$

where

$y = \ln(I)$	$x_0 = 1$	(2.5)
$\beta_0 = \ln(k)$	$x_1 = \ln(x)$	
$\beta_1 = \alpha$	$x_2 = x$	
$\beta_2 = -1/L$		

The problem can then be written in a more compact form by using a matrix notation [88],

$$\mathbf{X}\beta \cong \mathbf{y} \quad (2.6)$$

where $\mathbf{y}$ is a column vector with length m , and m is the number of data points used in the fitting process. The term β is also a column vector but with length n , where n is the number of the fitting parameters. In our case, $n = 3$. The matrix $\mathbf{X}$ is an $m \times n$ matrix with $m > n$.

The problem is then simplified to finding the matrix β . The least square linear regression technique requires that the sum of square of the residual

to be a minimum. If we define $\mathbf{r} = \mathbf{y} - \mathbf{X}\beta$, then the problem is to find the minimum of the following function.

$$\begin{aligned}
 \phi(\beta) &= \|\mathbf{r}\|_2^2 = \mathbf{r}^T \mathbf{r} \\
 &= (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) \\
 &= \mathbf{y}^T \mathbf{y} - 2\beta^T \mathbf{X}^T \mathbf{y} + \beta^T \mathbf{X}^T \mathbf{X} \beta
 \end{aligned} \tag{2.7}$$

The necessary condition for a minimum is that $\nabla \phi(\beta) = 0$. Thus, we must have

$$\begin{aligned}
 \mathbf{0} &= 2\mathbf{X}^T \mathbf{X} \beta - 2\mathbf{x}^T \mathbf{y} \\
 \mathbf{X}^T \mathbf{X} \beta &= \mathbf{X}^T \mathbf{y}
 \end{aligned} \tag{2.8}$$

This is the $n \times n$ symmetric linear system and is commonly called the normal equation. This equation can be solved by the usual techniques such as the Gaussian-Jordan elimination.

In numerical computation, however, the linear system is not commonly solved from the normal equation [88]. It is more common to factorize the matrix $\mathbf{X}$ as

$$\mathbf{X} = \mathbf{Q} \begin{bmatrix} \mathbf{R} \\ \mathbf{O} \end{bmatrix} \tag{2.9}$$

where $\mathbf{Q}$ is an $m \times m$ orthogonal matrix, $\mathbf{R}$ is an $n \times n$ upper triangular matrix, and $\mathbf{O}$ is a matrix which elements are all zero. This transformation

is called the *QR factorization*. The squared residual norm now becomes

$$\begin{aligned}
 \|\mathbf{r}\|_2^2 &= \|\mathbf{y} - \mathbf{X}\beta\|_2^2 \\
 &= \|\mathbf{y} - \mathbf{Q} \begin{bmatrix} \mathbf{R} \\ \mathbf{O} \end{bmatrix} \beta\|_2^2 \\
 &= \|\mathbf{Q}^T \mathbf{y} - \begin{bmatrix} \mathbf{R} \\ \mathbf{O} \end{bmatrix} \beta\|_2^2 \\
 &= \|\mathbf{c}_1 - \mathbf{R}\beta\|_2^2 + \|\mathbf{c}_2\|_2^2
 \end{aligned} \tag{2.10}$$

where

$$\mathbf{Q}^T \mathbf{y} = \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \end{bmatrix} \tag{2.11}$$

The problem now is to find the minimum just as before. The fitting parameter matrix β can be found by solving the $n \times n$ triangular system

$$\mathbf{R}\beta = \mathbf{c}_1 \tag{2.12}$$

and the minimum residual norm is given by

$$\|\mathbf{r}\|_2 = \|\mathbf{c}_2\|_2 \tag{2.13}$$

In this way, all the fitting parameters (k , α , and L) are found simultaneously from the linear system. The QR factorization algorithms are common in many numerical computation software (e.g. in Matlab, $[\mathbf{Q}, \mathbf{R}] = \text{qr}(\mathbf{X})$ gives the $\mathbf{Q}$ and $\mathbf{R}$ matrix factorization of $\mathbf{X}$).

A question might arise about the goodness of the fit. In order to give a quantitative measure, the coefficient of determination, r^2 , is calculated. An

r^2 whose value approaches unity suggests that the linear regression model fits the data closely. The value of this coefficient can be calculated from the ratio of the variance of the fitted line over the variance of the actual data [89].

$$r^2 = \frac{\text{var}(\hat{y})}{\text{var}(y)} \quad (2.14)$$

where y is the actual data, in our case $y = \ln I$, and

$$\hat{y} = \hat{\beta}_0 x_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 \quad (2.15)$$

The corresponding $\hat{\beta}$ are the estimated fitting parameters.

2.3 EBIC Data Generation

To illustrate the extraction of the diffusion lengths and the surface recombination velocities, EBIC data from a normal-collector configuration were generated from a theoretical EBIC equation. For this purpose, the expression proposed by Donolato was used [48].

$$Q(x, z) = \exp(-\lambda x) - \frac{2s}{\pi} \int_0^\infty \frac{k}{\mu^2(\mu + s)} \exp(-\mu z) \sin(kx) dk \quad (2.16)$$

where $\lambda = 1/L$, $\mu = (\lambda^2 + k^2)^{1/2}$, $s = v_s/D$, and $Q(x, z)$ is the EBIC current for a point source located at (x, z) . The term x is the beam position measured from the junction as shown in Fig. 2.1. Since this is the equation for point source generation volume, the centre of mass ($\bar{z}$) is just the value of z .

For example purpose, the material was set to have $L = 3 \mu\text{m}$, with v_s varying from 0 to $1 \times 10^7 \text{ cm/s}$, and $z = 0.3 \mu\text{m}$. To compute the reduced

($s = v_s/D$) and the normalized surface recombination velocity ($S = v_s L/D$), it was assumed that the mobility of the minority carrier electron is 252 cm²/(v.s), which corresponds to a diffusivity value of 6.527 cm²/s. The EBIC data was computed at beam positions $x = 0$ to $x = 40$ with interval 1 μm . The Matlab function to compute the charge collection probability was given in Appendix C.3.2.

The expression for the charge collection probability involves an improper integral with one of the limit at infinity. To overcome this problem, we followed the technique proposed in [88] by transforming the variable as follows.

$$k = \frac{t}{1+t} \quad (2.17)$$

and

$$dk = -\frac{1}{(t+1)^2} dt \quad (2.18)$$

Therefore, the limit of the integration with respect to t becomes from 0 to -1.

2.4 Extraction of Diffusion Lengths

In order to obtain the diffusion lengths for the case of the normal-collector configuration, Eq. (2.3) was fitted into the generated EBIC data. The surface recombination values were chosen to follow that of [36, 59]. The data used for the fitting purpose were from the region $x = 6 \mu\text{m}$ to $x = 33 \mu\text{m}$. The matrix and vectors of Eq. (2.6) were constructed using the relationships given in Eq. (2.5).

Table 2.1: Extraction of Diffusion Lengths for Various Values of Surface Recombination Velocities for the Case of the Normal-Collector Configuration.

v_s (cm/s)	k	α	L (μm)	Error (%)	r^2
0	1.0000	0.0000	3.0000	0.00	1.0000
1.00×10^2	1.0002	-0.0021	2.9988	-0.04	1.0000
1.00×10^3	1.0018	-0.0213	2.9894	-0.35	1.0000
3.16×10^3	1.0056	-0.0666	2.9729	-0.90	1.0000
1.00×10^4	1.0064	-0.1941	2.9548	-1.51	1.0000
3.16×10^4	0.8955	-0.4248	2.9783	-0.72	1.0000
1.00×10^5	0.5592	-0.5798	3.0178	0.59	1.0000
1.00×10^6	0.2335	-0.6106	3.0248	0.83	1.0000
1.00×10^7	0.2047	-0.6387	3.0432	1.44	1.0000

A QR factorization was performed using Matlab to obtain the matrix $\mathbf{R}$ of Eq. (2.12) and the matrix $\mathbf{Q}$ of Eq. (2.11). Once $\mathbf{Q}$ is known, the vector $\mathbf{c}_1$ can be obtained by solving Eq. (2.11). Thus, the vector β was solved from Eq. (2.12). The values of the physical parameters can be obtained from the vector β by using the relationship in Eq. (2.5).

In this procedure, the alpha value is not varied manually, but is obtained simultaneously together with the other fitting parameters as a result of solving Eq. (2.12). The Matlab code is given in Appendix C

Table 2.1 shows the results of the fitting process. It can be seen from the r^2 value that the linear regression model fits the data closely. The errors in extracting the diffusion lengths for any values of surface recombination velocities are about 1%. This agrees with the statements given in [36].

Table 2.2: Extraction of Surface Recombination Velocities for the Case of the Normal-Collector Configuration.

v_s (cm/s)	S	Extracted		
		α	v_s (cm/s)	Error (%)
0	0.0000	0.0000	-	-
1.00×10^2	4.5963×10^{-3}	-0.0021	-	-
1.00×10^3	4.5963×10^{-2}	-0.0213	4.7193×10^2	-52.81
3.16×10^3	1.4524×10^{-1}	-0.0666	2.4242×10^3	-23.28
1.00×10^4	4.5963×10^{-1}	-0.1941	8.9041×10^3	-10.96
3.16×10^4	1.4524×10^0	-0.4248	2.8267×10^4	-10.55
1.00×10^5	4.5963×10^0	-0.5798	7.4684×10^4	-25.31
1.00×10^6	4.5963×10^1	-0.6106	-	-
1.00×10^7	4.5963×10^2	-0.6387	-	-

2.5 Extraction of Surface Recombination Velocities

It was shown in [59] that the surface recombination velocity in a normal-collector configuration can be extracted from

$$S = \eta + \sigma_1 \sqrt{2 \ln \left(\frac{A}{\alpha + B} \right)} \quad (2.19)$$

where

$$S = v_s L / D \quad (2.20)$$

and $A = 5047$, $B = 0.6$, $\eta = -20$, and $\sigma_1 = 4.7$. Substituting the alpha values from Table 2.1 into Eq. (2.19) gives the *normalized* surface recombination velocities. The actual values can then be obtained from Eq. (2.20).

Table 2.2 gives the results of extracting the surface recombination velocities from the normal-collector configuration. It can be seen that the technique is valid only for $0.05 \leq S \leq 5$. Fortunately, the case of $S < 0.05$

can be considered as the zero surface recombination velocity, while for $S > 5$ can be considered as the infinite surface recombination velocity [36].

2.6 Discussion

The two previous sections show the simultaneous extraction of the diffusion lengths and the surface recombination velocities from the same EBIC line scan. It has been shown that the technique gives errors of about 1% for the case of diffusion lengths and about 25% for the case of the surface recombination velocities.

The small error in extracting the diffusion length is possible only when the conditions specified are satisfied ((1.22) to (1.25)). The first and the last conditions mean that the data used in the fitting process must be away from either the junction or the back contact by about two diffusion lengths. In this chapter, the EBIC data was generated from the Donolato equation which assumes that the back contact is at infinity. Thus, the first condition is satisfied. Moreover, the last condition is also satisfied in our case, since the diffusion length was set to have the value of $3 \mu\text{m}$, while the equation is fitted starting from $x = 6 \mu\text{m}$.

The second and the third conditions related to one another since $\bar{z} \approx 0.41R$. In the data set which we used, the depth of the generation volume is $z = 0.3 \mu\text{m}$, and so these two conditions were satisfied as well. These conditions basically resulted from the size of the generation volume, which in turn would affect the resolution of the technique.

In this technique, it is assumed that we know precisely the value of x ,

which is the beam distance from the junction. The distance is measured from the edge of the depletion layer rather than from the metallurgical junction. For materials with large diffusion length, this difference does not make a significant impact on the results. However, for materials where the diffusion length is comparable to the depletion width, this difference becomes significant.

Another important consideration is that the collecting junction dimension in the z axis is infinitely large. This applies when the junction depth is large enough compared to the depth of the generation volume. Moreover, the thickness of the device must be large enough compared to the diffusion length. When it is comparable, the surface recombination velocity at the bottom must be ensured to be negligible.

In this example, the surface recombination velocities were extracted from the alpha parameter. The values were obtained from Eqs. (2.19) and (2.20). It can be seen that all the parameters are constant. In other words, the extraction of the surface recombination velocities depend only on the values of the alpha parameter. This issue is analysed further in the following chapter.

2.7 Summary

This chapter gives an example of a simultaneous extraction of diffusion lengths and surface recombination velocities. The technique involves the use of a fitting parameter termed alpha, which make it possible to extract the diffusion length from any values of surface recombination velocities. This same parameter is also used to obtain the surface recombination velocity.

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A theory on linear regression was presented which simplify the fitting process of the EBIC profile. Afterwards, an EBIC profile was generated from the theoretical equation provided by Donolato for the case of normal-collector configuration. The diffusion lengths and the values of the alpha parameter were then extracted using the technique previously presented. The surface recombination velocities were then obtained from the values of the alpha parameter using the normal distribution equation proposed by Ong.

The accuracy of the extraction of the diffusion lengths and the surface recombination velocities agrees with the one claims by the original papers. Discussions on the techniques have also been given.

Chapter 3

Factors Affecting the Alpha Parameter

3.1 Introduction

This chapter gives an in-depth analysis of the factors affecting the alpha parameter which is used for extracting the surface recombination velocities in EBIC line scan measurements. It has been shown by Ong [36] that a simultaneous extraction of diffusion lengths and surface recombination velocities can be done from the following EBIC expression.

$$I = kx^\alpha \exp(-x/L) \quad (3.1)$$

where L is the minority carrier diffusion length, k is a constant, α (alpha) is a fitting parameter, and x is the beam distance from the junction as shown in Fig. 3.1.

Figure 3.1: Normal-collector configuration of EBIC measurements.

In this method, the fitting parameter α is used to straighten the $\ln(I)$ versus x curve, thereby enabling the minority carrier diffusion length to be extracted accurately for any values of surface recombination velocities. The α parameter obtained from the fitting process can then be used to extract the surface recombination velocity.

In 1998, it was shown [59] that the α parameter was related directly to the normalized surface recombination velocity. The relationship between the α parameter and the normalized surface recombination velocity can be modeled using a Normal distribution function. The results of the experiments seemed to suggest that the variation of the α parameter with respect to the normalized surface recombination velocity was independent of both the minority carrier diffusion length and the depth of the generation volume. Thus, the surface recombination velocity can be extracted from

alpha value alone from

$$S = \eta + \sigma_1 \sqrt{2 \ln \left(\frac{A}{\alpha + B} \right)} \quad (3.2)$$

where

$$S = v_s L / D \quad (3.3)$$

and $A = 5047$, $B = 0.6$, $\eta = -20$, and $\sigma_1 = 4.7$.

In Eq. (3.3), v_s is the surface recombination velocity with unit cm/s, while S is its dimensionless normalized value. In this equation, D is the diffusion coefficient. The errors reported were less than 20% for the surface recombination velocity range of 1×10^3 cm/s to 3.16×10^4 cm/s.

Recently, Zhu *et al.* [60] gave an alternative method for extracting the surface recombination velocities. Their experiments, however, indicated that the alpha parameter also depended on the depth of the generation volume. Since the depth of the generation volume is a function of the beam energy, this means that the alpha parameter seemed to depend on the beam energy as well. If this is true, then the accuracy in extracting the surface recombination velocities using the Normal distribution function would be in question. This is because the model assumes that the relationship between the alpha parameter and the surface recombination velocity is independent of the beam energy or the depth of the generation volume.

In order to extract the surface recombination velocities accurately by using the alpha parameter, it is important to analyse the dependence of the alpha parameter on the physical parameters, such as the depth of the generation volume, the minority carrier diffusion lengths, and the beam

distance from the junction. This chapter provides a thorough analysis of the parameters that alpha depends on, based on an analytical model of the alpha equation. The analysis of the various parameters is then verified using a computer simulation. The impact on the accuracy as well as the conditions for obtaining accurate surface recombination velocities are also given.

3.2 Analytical Equation for Alpha

The analytical equation for the alpha parameter can be derived from Eq. (3.1). Taking the natural logarithm of both sides and differentiating with respect to the distance would give an equation that consists of alpha, beam distance, and the minority carrier diffusion length. This is elaborated in a more detail in the following paragraphs.

Rearranging the term and taking the natural logarithm of Eq. (3.1) gives

$$\ln(I/x^\alpha) = \ln(k) - x/L \quad (3.4)$$

It can be seen that the right hand side of the equation is a straight line. Fitting this equation into the EBIC current values gives the minority carrier diffusion length and the fitting parameter alpha. It will be shown later that the actual plot does not exactly yield a straight line. The error in this fitting process can be seen from the coefficient of determination, r^2 . Therefore, the above equation needs to be rewritten as

$$\ln(I'/x^\alpha) = \ln(k) - x/L \quad (3.5)$$

where we have changed I with I' to indicate that the current that satisfy

Eq. (3.5) is different with the actual EBIC current. Let

$$I' = \frac{I}{\delta} \quad (3.6)$$

where I is the actual EBIC current and δ gives the error in the fitting process from the straight line.

Substituting Eq. (3.6) into (3.5) gives

$$\ln(I/x^\alpha) - \ln(\delta) = \ln(k) - x/L \quad (3.7)$$

If the fitting process gives $r^2 \approx 1$, then the second term of the left hand side of Eq. (3.7) can be neglected. This is because the actual EBIC current yields almost a straight line when fitted into Eq. (3.4). It was reported in [36] that the coefficient of determination is very close to unity and thus the second term in the left hand side of Eq. (3.7) can be ignored. Table 2.1 in Chapter 2 also gives the values of the alpha parameter that are close to unity.

Fig. 3.2 shows the magnitude of this term for the case where the surface recombination velocity is 1×10^4 cm/s. The figure is obtained by calculating numerically the second term of Eq. (3.7) with a substitution of an analytical equation for the current I . The analytical equation for the current will be presented immediately. It can be seen that within the fitting range ($x = 9$ to 33), the magnitude of the second term is close to zero. Fig. 3.2 also shows that a constant alpha value makes the first term to be close to a straight line only within the fitting range.

Ignoring the second term and differentiating with respect to x gives

$$\frac{d \ln(I)}{dx} - \frac{\alpha}{x} = -\frac{1}{L} \quad (3.8)$$

Figure 3.2: The amount of the second term of the left hand side of Eq. (3.7). The alpha values were obtained by fitting process with $L = 3 \mu\text{m}$, $z = 0.3 \mu\text{m}$, and scanning range from $x = 9$ to $33 \mu\text{m}$. The surface recombination velocity is $1 \times 10^4 \text{ cm/s}$.

Rearranging the term and using the relationship $d \ln I / dx = 1/I(dI/dx)$ gives

$$\alpha = \left(\frac{1}{I} \frac{dI}{dx} + \frac{1}{L} \right) x \quad (3.9)$$

Substituting the EBIC current I and its derivative with EBIC theoretical expressions that contain the surface recombination velocity term gives the analytical expression for the alpha parameter. The actual expressions for I and its derivative depend on the configuration of the collector. One of the more popular methods for the determination of the minority carrier diffusion lengths is the one where the collector is normal to the scanning direction of the electron beam. This is known as the normal-collector configuration and is shown in Fig. 3.1.

Theoretical EBIC profile expressions for the normal-collector configuration are given by several authors. The most commonly used is the expression derived by Donolato in [48]. In this analysis, however, we used the expression given by Luke *et al.* in [90]. A closer look will show that the two expressions are the same. The difference is that the expression given by Luke is written in a normalized form (i.e. $S = v_s L/D$, x/L , and z/L), whereas the one by Donolato is not (i.e. $s = v_s/D$, x , and z). In this analysis, therefore, it is preferable to use the one given by Luke, they are

$$Q(x, z) = \exp(-x/L) - \frac{2S}{\pi} \int_0^\infty \frac{k \exp(-\sqrt{k^2 + 1}z/L) \sin(kx/L)}{(k^2 + 1)(S^2 + \sqrt{k^2 + 1})} dk \quad (3.10)$$

$$\frac{dQ(x, z)}{dx} = -\frac{1}{L} \exp(-x/L) - \frac{2S}{\pi L} \int_0^\infty \frac{k^2 \exp(-\sqrt{k^2 + 1}z/L) \cos(kx/L)}{(k^2 + 1)(S^2 + \sqrt{k^2 + 1})} dk \quad (3.11)$$

where $Q(x, z)$ is the charge collection probability, which is the induced current of a point generation source, z is the depth of the generation volume, and the other symbols have their usual meanings.

For an extended generation source, we use Gaussian model given by Donolato in [48]. After rewriting in terms of normalized variables, the expressions are

$$I_N(x, z) = \frac{2}{\pi} \int_0^\infty \frac{k}{k^2 + 1} \left\{ \exp\left(-\frac{k^2 \sigma^2}{2L^2}\right) \right.$$

$$\begin{aligned}
& -0.57 \exp \left(\frac{\sigma^2}{2L^2} - \sqrt{k^2 + 1} \frac{z}{L} \right) \frac{S}{S + \sqrt{k^2 + 1}} \\
& \times \operatorname{erfc} \left[\frac{\sigma}{\sqrt{2}L} \left(\sqrt{k^2 + 1} - \frac{z}{L} \frac{L^2}{\sigma^2} \right) \right] \Bigg\} \sin(kx/L) dk \quad (3.12)
\end{aligned}$$

$$\begin{aligned}
\frac{dI_N(x, z)}{dx} = & \frac{2}{\pi L} \int_0^\infty \frac{k^2}{k^2 + 1} \left\{ \exp \left(-\frac{k^2 \sigma^2}{2L^2} \right) \right. \\
& -0.57 \exp \left(\frac{\sigma^2}{2L^2} - \sqrt{k^2 + 1} \frac{z}{L} \right) \frac{S}{S + \sqrt{k^2 + 1}} \\
& \times \operatorname{erfc} \left[\frac{\sigma}{\sqrt{2}L} \left(\sqrt{k^2 + 1} - \frac{z}{L} \frac{L^2}{\sigma^2} \right) \right] \Bigg\} \cos(kx/L) dk \quad (3.13)
\end{aligned}$$

where $\sigma = z/(0.3\sqrt{15}) = z/1.162$, and $I_N = I/GI_b$. The term I_b is the beam current while the term G is the generation factor given by [12]

$$G = E_b(1 - f)/E_i \quad (3.14)$$

where f is the backscattering fraction and E_i is the ionization energy, that is the effective average energy required to generate an ehp.

Evaluating Eqs. (3.9) to (3.11) numerically for several values of surface recombination velocities results in an alpha curve. This curve can be computed numerically using any numerical computational software. The computed results is shown in Fig. 3.3. The curve in Fig. 3.3 has the same shape and the same range of values as those given in [36, 59].

Eqs. (3.9) to (3.11) show that the alpha curve for a point generation source depends only on two parameters. They are the normalized scanning range, and the normalized depth of the generation volume, z/L . It is important to note that the term x/L in Eq. (3.9) refers to the location where the alpha parameter is constant.

In the derivation, the alpha parameter was assumed to be a constant fitting parameter. However, Eqs. (3.9) to (3.13) show that the alpha equation

Figure 3.3: The alpha curve from numerically computing Eqs. (3.9) to (3.11) with $x/L = 3$ and $z/L = 0.1$.

has the term x/L . This is because the second term in Eq. (3.7) was ignored in the derivation. Therefore, Eq. (3.9) actually gives an alpha value where $d\alpha/dx = 0$. In other words, Eq. (3.9) gives the alpha value at a particular location x where the derivative of the alpha parameter is zero. In real measurements, the exact location where alpha is almost a constant has to be within the scanning range where the equation is fitted into. This means that varying x/L in Eq. (3.9) would show the actual effect of varying the location of the scanning range with respect to the junction.

For the case of the Gaussian generation source, the alpha parameter also depends on the term σ/L which is the normalized lateral extension of the generation volume. However, since σ is strictly a function of the depth of the generation volume, the alpha equation, then, is also only a function of the normalized beam distance from the junction and the normalized depth

of the generation volume.

The analytical equation for the alpha parameter shows that the alpha curve does not depend on the beam current I_b . This is because the term GI_b cancels out in Eq. (3.9). This means that the only parameters that affect the alpha versus normalized surface recombination velocity curve are the normalized beam depth and the normalized beam distance from the junction. This is true for both the point generation source as well as the Gaussian generation source.

The analysis of the alpha dependencies will, therefore, be done by investigating the effects of these two parameters. Eqs. (3.9) to (3.11) for the point source assumption will be used throughout this analysis. The point source assumption can be justified when the distance between the beam and the junction is greater than the electron penetration range (R) in the material [90]. The accuracy in using the point source assumption will also be justified later in this chapter.

3.3 Analysis

3.3.1 Analysis Using the Analytical Equation

Eqs. (3.9) to (3.11) show that the alpha versus normalized surface recombination velocity curve is affected by two parameters: the normalized scanning location from the junction (x/L) and the normalized depth of the generation volume (z/L). The effect of changing the normalized depth on the alpha curve, computed from Eqs. (3.9) to (3.11), is shown in Fig. 3.4.

Figure 3.4: Effect of the generation volume depth on the alpha curve computed from Eqs. (3.9) to (3.11). The computation used $x/L = 3 \mu\text{m}$ and $L = 3 \mu\text{m}$. The normalized surface recombination velocity (S) changes from 0 to 459.64.

The alpha curve is affected by the normalized depth only at higher values of surface recombination velocities. Larger z/L ratio will cause this portion of the curve to move upward. However, the alpha curve changes imperceptibly for

$$z/L \leq 0.1 \quad (3.15)$$

The curves for different values of normalized depths show that changing z/L affects the alpha parameter only at higher values of surface recombination velocities. This effect can be explained by considering the recombination of minority carriers at the surface for different beam depths. The deeper the generation volume, the less the effect of the surface recombination would be. Another consideration is that for lower values of surface recombination

velocity, the change in the z/L ratio must be sufficiently large for it to affect the collected current. Only when the current is affected would the alpha value change.

When the surface recombination velocity is large, the effect on the current can be readily seen even for small changes in the z/L ratio. As the z/L ratio increases, more minority carriers will be collected instead of recombining at the surface. Therefore, the natural logarithm of the EBIC current will be less concave and the alpha value will be less negative [59]. This is the reason that the curve shifts upward at higher values of surface recombination velocities.

Changing the normalized depth could affect the accuracy in extracting higher values of surface recombination velocities. However, since the change in the alpha curve is negligible for $z/L \leq 0.1$, the accuracy is unaffected when this condition is satisfied.

Increasing the scanning range location will shift the middle portion of the curve upward as shown in Fig. 3.5. The rate of change in the alpha curve decreases as the scanning range location increases. Therefore, the change in the alpha curve due to the change in the scanning range location is only significant at small values.

The results for different values of scanning locations can be used to see the effect of varying the starting location of the scanning range in the EBIC line scan measurement. However, the scanning range of practical measurements has finite scanning width, and thus, this new parameter must come into consideration. The effect of the width of the scanning range, however, cannot be analyzed by using Eqs. (3.9) to (3.11) alone. The following section gives

Figure 3.5: Effect of the scanning range location on the alpha curve computed from Eqs. (3.9) to (3.11). The computation used $z/L = 0.1 \mu\text{m}$ and $L = 3 \mu\text{m}$. The normalized surface recombination velocity (S) changes from 0 to 459.64.

the analysis for the effect of the width of the scanning range.

3.3.2 Effects of the Scanning Range on the Extracted Alpha Parameter

The analytical expression for the alpha parameter (Eqs. (3.9) to (3.11)) is able to show the changes in the alpha curve when either the normalized scanning location from the junction or the normalized beam depth changes. This equation, however, does not give any information on the effect of the width of the scanning range.

Since the alpha values used for extracting surface recombination velocities come from a fitting process within finite width of scanning ranges, it

Figure 3.6: Effect of the scanning range width on the alpha curve. The computation used $z/L = 0.07 \mu\text{m}$ and $L = 3 \mu\text{m}$. The normalized surface recombination velocity (S) changes from 0 to 459.64.

is important to see how this new parameter would affect the alpha curve. In order to do this, the theoretical EBIC values are obtained by using Eq. (3.10). Eq. (3.1) can then be fitted to these theoretical EBIC values which would give the extracted minority carrier diffusion length as well as the alpha parameter. Thus, the effect of varying the width of the scanning range on the alpha curve can also be investigated.

The effect of reducing the scanning range width is similar to reducing the scanning location term x/L , when the alpha value is obtained from the analytical equation (Fig. 3.6). On the other hand, increasing the starting location of the scanning range alone will have a similar effect as increasing the scanning location term x/L , when the alpha value is obtained from the analytical equation (Fig. 3.7). This agrees with the previous analysis.

Figure 3.7: Effect of the starting location of the scanning range on the alpha curve. The computation used $z/L = 0.07\mu\text{m}$ and $L = 3\mu\text{m}$. The normalized surface recombination velocity (S) changes from 0 to 459.64.

Figure 3.8: Effect of the steepness of the alpha curve on the accuracy of the surface recombination velocity extraction.

Figure 3.9: Error in extracting L when the starting location decreases. The value of L is extracted by curve fitting Eq. (3.1) into the theoretical EBIC values computed from Eq. (3.10). The parameters set as $L = 3 \mu\text{m}$, with the scanning width $W/L = 9$, and the depth as $z/L = 0.1$.

It is important to extract the surface recombination velocities accurately in the range of $0.05 < S < 5$ [59]. This is because in practice the case of $S < 0.05$ can be approximated to be zero, while the case of $S > 5$ can be considered as infinity. In order to extract the surface recombination velocities in the range of $0.05 < S < 5$, it is desirable to have a steep alpha curve. This is because a steep alpha curve will give more accurate results in the extraction. This is illustrated graphically in Fig. 3.8. The solid lines in Fig. 3.8 indicate the alpha values for a certain given surface recombination velocity. If a certain amount of error is introduced into the measurement, as shown by the dotted lines, then it can be seen from the figure that this error will result in a smaller variation in S on the steeper curve than the other curve which is less steep.

Fig. 3.6 and 3.7 suggest that in order to have a steep alpha curve, the

starting location and the width of the scanning range must be small. A small starting location, however, should not violate the condition $x > 2L$ [36, 38]. This is because a small starting location will adversely affect the accuracy of the extracted minority carrier diffusion length. (Fig. 3.9)

The inaccuracy of extracting the diffusion length with a small starting location is due to the fact that in this region the EBIC current cannot be fitted exactly into Eq. (3.1) with a constant alpha. This is because the EBIC variation at location very near to the junction no longer follows Eq. (3.1). Equation (3.1) is an asymptotic approach, and therefore, is valid only for large x/L . This can also be seen from Fig. 3.2.

Fig. 3.9 suggests that in order for the extractions of the diffusion lengths to have errors less than 1.5%, the starting location must obey the following relationship:

$$\left(\frac{x}{L}\right)_{\text{start}} \geq 2 \quad (3.16)$$

The minimum width of the scanning range is also determined by the accuracy in extracting the diffusion length. Fig. 3.10 shows the errors in extracting the diffusion lengths for different scanning range values. The results show that the errors in extracting the diffusion lengths increase slightly as the width is reduced. To keep the errors below 1.5%, the normalized width must be greater than or equal to 9, i.e.

$$\frac{W}{L} \geq 9 \quad (3.17)$$

The value of condition (3.17), however, depends on the starting location of the scanning range. The nearer the starting location is from the junction, the larger the width of the scanning range is required to keep the error small.

Figure 3.10: Error in extracting L when the width of the scanning range decreases. The value of L is extracted by curve fitting Eq. (3.1) into the theoretical EBIC values computed from Eq. (3.10). The parameters set as $L = 3 \mu\text{m}$, with the scanning starts from $x/L = 2$, and the depth is $z/L = 0.1$.

3.4 Verification

3.4.1 MEDICI Simulation

The above results, which were obtained from the theoretical equations, were verified by using a computer simulator. MEDICI, 2-D device simulation software, was used for this purpose. A generation radius of $0.1 \mu\text{m}$ was used to simulate the generation source. This point generation source was represented in MEDICI by using a square generation area with sides of $0.2 \mu\text{m}$ [91]. The simulation software requires one to provide the information of the generation rate as well as the location of the generation source.

The depth of the generation volume and the total generation rate can be calculated from the beam energy and the beam current information. The

computation is as follows.

To relate the depth of the generation volume and the beam energy, we used the expression proposed by Everhart and Hoff [8] for the Silicon material.

$$R = 4.00 \times 10^{-2} \frac{E_b^{1.75}}{\rho} \quad (3.18)$$

where R is the electron penetration range in μm , E_b is the beam energy in keV, and ρ is the density, and its value for Silicon is 2.33 g/cm^3 . Moreover, Donolato shows that the centre of mass of this generation volume is located at $\bar{z} \approx 0.41R$ for the range of $0 < R/L \leq 0.5$. Therefore, the centre of mass or the depth of the generation volume is related to the beam energy as

$$z = 7.00 \times 10^{-3} E_b^{1.75} \quad (3.19)$$

The value computed from this expression is about the same as the one obtained in [38].

In order to compute the generation rate, the information on the beam current must be known. It is important to keep the condition of *low injection* satisfied when designing the generation rate. For one Ampere beam current, the ehps produced are

$$G = \frac{E_b(1-f)}{E_i} \quad (3.20)$$

where f is the fraction due to backscattering, and E_i is the ionization energy, that is the energy required to produce one ehp. In Silicon, the value for f is 0.08 and E_i is 3.62 eV [13].

The expression of Eq. (3.20) is called the generation factor in [12]. It gives the number of ehps produced per unit beam current. Thus, the total current generated is

$$I_{\max} = G I_b \quad (3.21)$$

The total number of ehps generated, therefore,

$$g = \frac{I_{\max}}{q} \text{ ehp/s} \quad (3.22)$$

where q is the elementary charge 1.6×10^{-19} C.

In MEDICI, the generation rate is to be given as the rate over a unit volume. Since MEDICI is a two dimensional simulator, the volume of a square with $0.2 \mu\text{m}$ side is $= 0.2 \times 10^{-4} \times 0.2 \times 10^{-4} \times 1.0 \times 10^{-4} = 4 \times 10^{-14} \text{ cm}^{-3}$. Therefore, the generation rate per unit volume can then be easily calculated. In this simulation, 1.5 nA beam energy was used [63, 92]. This gives a generation rate of about 5.22×10^{23} carriers/ cm^3 . Examples of MEDICI input files can be found in Appendix D.

Eq. (3.1) was fitted into the EBIC values obtained from the simulation in order to obtain the diffusion lengths and the values of the alpha parameter, following the technique presented in Chapter 2. The technique for the diffusion length extraction follows the one proposed by Ong *et al.* [36], and the one for the surface recombination velocities follows that of Ong [59] (Chapter 2).

3.4.2 Effects on the Alpha Curves

The alpha curves with various values of the normalized beam depths and the normalized scanning ranges are plotted in Figs. 3.11 and 3.12 respectively.

Figure 3.11: Alpha curves from MEDICI simulations for various values of z/L . The scanning range was from $x/L = 3$ to $x/L = 14$ with $L = 3 \mu\text{m}$. The dotted line shows the shape of the normal distribution function of Eq. 3.2.

Figure 3.12: Alpha curves from MEDICI simulations for two different scanning ranges. The simulation used $z/L = 0.067$ with $L = 3 \mu\text{m}$. The dotted line shows the shape of the normal distribution function of Eq. 3.2.

Comparison of Figs. 3.11 and 3.12 with Figs 3.4 to 3.6 shows that the change in the alpha curves obtained from MEDICI simulations have the same behaviour as those obtained using the analytical equation. Thus, the analytical equation for the alpha parameter can be used to predict the parameters that affect the alpha values, as well as to predict how the alpha values change with these parameters.

This shows that the previous analysis which uses the analytical equations is valid for practical EBIC measurements. Therefore, all conditions stated previously to extract an accurate minority carrier diffusion lengths and the surface recombination velocities have been verified.

Another observation that can be seen in Fig. 3.12 is that the effect of the starting location of the scanning range on the alpha curves is more dominant than the effect of the width of the scanning range. This is because increasing the starting location by one diffusion length while reducing the width by the same amount is similar in effect with increasing the scanning range location term x/L in the analytical equation. In other words, the width must be reduced by more than one diffusion length to compensate the effect of increasing the starting location by the same amount.

3.4.3 Impacts on the Accuracy

It has been shown that the shape of the alpha versus normalized surface recombination velocity curve depends mainly on the normalized depth of the generation volume as well as the normalized scanning range. This means that the accuracy of extracting the surface recombination velocity with the

use of Eq. (3.2) is affected by these two parameters. This is because Eq. (3.2) assumes that the alpha curve is invariant to both the depth and the scanning range. It is, therefore, important to see how changes in the depth and the scanning range would affect the accuracy obtained by using Eq. (3.2).

In order to do this, the alpha values from the MEDICI simulations data were used to extract the surface recombination velocities. To see the impact of depth on the accuracy, the alpha values from Fig. 3.11 were substituted into Eq. (3.2) to obtain the normalized surface recombination velocities. The true values of the surface recombination velocities can then be extracted by using Eq. (3.3). On the other hand, the alpha values from Fig. 3.12 were used to see the impact of changing the scanning range on the accuracy. The errors in extracting the surface recombination velocities are shown in Tables 3.1 and 3.2.

The results from Table 3.1 indicate that the accuracy is not affected much as the z/L ratio change from 0.067 to 0.3. The only obvious impact can be seen for $v_s = 1 \times 10^5$ cm/s. In this case, the error increases as z/L increases. For the impact in changing the scanning range, Table 3.2 shows that the errors for both ranges are below 15% for 3.16×10^3 cm/s $\leq v_s \leq 1 \times 10^5$ cm/s. Therefore, the impact on the accuracy of using Eq. (3.2) is not very significant.

The effect of increasing the z/L ratio is clearly shown at $v_s = 1 \times 10^5$ cm/s. This agrees with the analysis since the effect is most obvious at higher values of surface recombination velocities. However, at $v_s = 1 \times 10^4$ cm/s ($S = 0.460$) and 3.16×10^4 cm/s ($S = 1.452$), the error decreases as z/L

Table 3.1: Impact of the Normalized Depth on the Accuracy of Extracting the Surface Recombination Velocity.

v_s (cm/s)	Error (%)			
	z/L			
	0.3	0.2	0.1	0.067
0	∞	∞	∞	∞
1.00×10^2	-295.34	-291.30	-291.30	-295.34
1.00×10^3	-27.38	-25.70	-25.28	-24.45
3.16×10^3	-4.50	-2.61	-1.88	-1.59
1.00×10^4	5.65	7.71	9.02	9.15
3.16×10^4	-0.07	3.24	5.48	5.93
1.00×10^5	-29.95	-22.50	-15.08	-13.18
1.00×10^6	-	-	-	-
1.00×10^7	-	-	-	-

The scanning range is from $x/L = 3$ to $x/L = 14$ with $L = 3 \mu\text{m}$.

Table 3.2: Impact of the Scanning Range on the Accuracy of Extracting the Surface Recombination Velocity.

v_s (cm/s)	Error (%)	
	$x/L = 2 \text{ to } 14$	$x/L = 3 \text{ to } 14$
0	∞	∞
1.00×10^2	-283.22	-295.34
1.00×10^3	-32.82	-24.45
3.16×10^3	-11.00	-1.59
1.00×10^4	-0.90	9.15
3.16×10^4	-1.55	5.93
1.00×10^5	3.76	-13.18
1.00×10^6	-	-
1.00×10^7	-	-

The depth of the generation volume is $z/L = 0.067$ with $L = 3 \mu\text{m}$.

increases. The reason behind it is due to the shape of Eq. (3.2) as shown in Fig. 3.11. At $v_s = 1 \times 10^5$ cm/s ($S = 4.596$), the alpha curve moves further away from the normal distribution function as z/L increases; while this is not so for the other points. As z/L increases beyond 0.3, the accuracy in using the normal distribution function will deteriorate even further as the alpha values are higher than the corresponding points in the normal distribution function.

The impact of the scanning range, on the other hand, is not very significant when the starting point increases by one diffusion length. Fig. 3.12, however, shows that the normal distribution function is closer to the alpha curve with a scanning range from $x/L = 2$ to $x/L = 14$. As the initial location of the scanning range increases beyond $x/L = 3$, the middle portion of the alpha curve will move further to the left, and the error will become significant at the surface recombination velocity range of $3.16 \times 10^3 \leq v_s \leq 1 \times 10^5$ ($0.145 \leq S \leq 4.596$).

3.5 Accuracy in Using Point Source Assumption

All the previous discussions used a point source assumption in the analysis. This assumption is justified only when the beam distance to the junction is greater than the electron penetration range [90]. If a Gaussian generation source, instead of a point source, is to be used, Eqs. (3.12) and (3.13) can be substituted into Eq. (3.9) to investigate the effect of the finite dimension

Figure 3.13: Deviation in the alpha values when using the point source assumption from the one when using the Gaussian source. The deviation is calculated as follows: $\text{Error} = (\alpha_{\text{point}} - \alpha_{\text{gauss}}) / \alpha_{\text{gauss}} \times 100\%$.

of the generation volume. This gives the analytical expression for the alpha parameter for the case of the Gaussian distribution generation volume.

Fig. 3.13 shows the deviation of the alpha values when using the point source assumption from the alpha values when using the Gaussian source as the distance (normalized to the electron penetration range) is varied. The results suggest that the deviation increases as the ratio of x/R decreases. This is mainly due to the lateral extension effect of the generation volume. In order for the point source assumption to be valid, the beam distance from the junction must be greater than 1.5 times the electron penetration range, i.e.,

$$\frac{x}{R} > 1.5 \quad (3.23)$$

Under this condition the errors can be kept to below 1%.

The electron penetration range is related to the center of mass of the generation volume by the following relationship [35]: $\bar{z} = 0.41R$. Substituting this into Eq. (3.23) gives

$$\frac{x}{z} > 3.66 \quad (3.24)$$

Therefore, in order for the measurement to ignore the lateral extension of the generation volume, either condition (3.23) or (3.24) must be satisfied.

3.6 Conditions for Accurate Extraction

The conditions for an accurate extraction of the surface recombination velocities with the use of the Normal distribution function have been discussed in the previous sections. The two main conditions are to keep the shape of the alpha curve and to have the alpha curve to be as steep as possible. The first condition allows the extraction of the surface recombination velocities directly by using the alpha parameter alone. The second one allows the surface recombination velocities to be extracted more accurately, particularly for the region in the middle portion of the alpha curve.

From the analysis, it can be seen that the shape of the alpha curve can be kept from variation by: (1) satisfying the condition given in Eq. (3.15) for the normalized depth of the generation volume, and (2) using the same normalized scanning range which includes the same normalized starting location with the same normalized scanning width. The steepness of the alpha curve can be increased by two ways: (1) reducing the normalized

starting location of the scanning range, and (2) reducing the scanning width. However, the impact of reducing the starting location of the scanning range is more significant. Therefore, to satisfy the two main conditions for direct and accurate extraction, the conditions for the EBIC measurements can be summarized as follows: for the depth of the generation volume

$$\frac{z}{L} \leq 0.1 \quad (3.25)$$

, while for the scanning range

$$\begin{aligned} &\text{from } \left(\frac{x}{L}\right)_{\text{start}} = 2 \\ &\text{to } \left(\frac{x}{L}\right)_{\text{end}} = 11 \end{aligned} \quad (3.26)$$

Since the fitting parameters for the normal distribution given in [59] were not based on the conditions given above, a new set of parameters would result in a more accurate extraction. It was found by curve fitting that a more accurate set of parameters satisfying the above conditions is given by

$$\begin{aligned} A &= 499.74 & B &= 0.63 \\ \eta &= -17.074 & \sigma_1 &= 4.67 \end{aligned} \quad (3.27)$$

Table 3.3 shows the errors in extracting the surface recombination velocity by using Eq. (3.9) with the parameters given in (3.27). The data was taken from MEDICI simulations which satisfy conditions (3.25) and (3.26).

3.7 Comments on the Alpha Values for Large Surface Recombination Velocities

Berz and Kuiken [38] showed that the alpha value for the infinite surface recombination velocity is -0.5. This alpha value derives from a theoretical

Table 3.3: Error in Extracting the Surface Recombination Velocities Using the Proposed Parameters.

v_s (cm/s)	Extracted v_s (cm/s)	Error (%)
0	-1.2885×10^0	∞
1.00×10^2	9.4568×10^1	-5.43
1.00×10^3	9.8567×10^2	-1.43
3.16×10^3	3.1892×10^3	0.92
1.00×10^4	1.0462×10^4	4.62
3.16×10^4	3.1669×10^4	0.22
1.00×10^5	7.5770×10^5	-24.23
1.00×10^6	-	-
1.00×10^7	-	-

equation. However, computer simulations and the analytical equation for the alpha parameter give value that is lower than -0.5, that is about -0.6.

The reason for this discrepancy comes from the approximation used by Berz and Kuiken to derive the theoretical equation. In [38], it was shown that the current density for the case of infinite surface recombination velocity when the beam scans the n-type region can be expressed as

$$J = \left(\frac{2 D_h}{\pi D} \right) qg \frac{z}{L} K_1 \left(\frac{x}{L} \right) \quad (3.28)$$

where D_h is the diffusion constant for holes and D is the effective diffusion constant. For low injection, $D = D_h$, which is the case we are considering here. The constant g is the total generation rate and $K_1(n)$ is the modified Bessel function of the second kind. The other symbols have their usual meanings.

The above equation can also be written as

$$J = C_1 \times K_1 \left(\frac{x}{L} \right) \quad (3.29)$$

where C_1 is a constant with respect to x . Berz and Kuiken, then, made an approximation for $x/L \gg 1$ by expanding the Bessel function using asymptotic series. For $n \gg 1$, the function $K_1(n)$ can be expanded as [93]

$$K_1(n) \approx \frac{\exp(-n)}{\sqrt{\frac{2x}{\pi L}}} \quad (3.30)$$

Thus, for $x/L \gg 1$, Eq. (3.29) can be expanded and written as

$$J = C_1 \times \frac{\exp(-x/L)}{\sqrt{\frac{2x}{\pi L}}} \quad (3.31)$$

which leads to

$$J = C_2(x/L)^{-1/2} \exp(-x/L) \quad (3.32)$$

where C_2 is another constant. Comparing with Eq. (3.1), the alpha value for this EBIC equation is -0.5.

It can be seen that the asymptotic approximation approaches the actual Bessel function for large values of x/L . However, EBIC measurement usually scan from $x/L \approx 2$. In this region, the two functions differ. Fig. 3.14 shows the logarithmic current of the actual Bessel function which is more concave than its asymptotic approximation. A more concave curve results in a more negative alpha value. This is the reason that the simulation and the analytical equation for the alpha parameter give values of about -0.6 for large values of surface recombination velocities.

3.8 Summary

It has been shown that the analytical expression for the alpha parameter can be used to analyse the alpha curve for the purpose of extracting the

Figure 3.14: Difference between the actual Bessel function and the asymptotic series approximation.

surface recombination velocities. The shape of the alpha versus normalized surface recombination velocity curve depends on two parameters. They are the normalized depth of the generation volume and the normalized scanning range.

The accuracy in extracting the surface recombination velocity using the method given in [59] is not affected very much as the normalized depth changes. The accuracy is affected only when extracting large values of surface recombination velocities. Similarly, changing the starting location of the scanning range affects the accuracy of extraction only slightly. The most affected region is in the middle range of the alpha values.

In order to extract the surface recombination velocities accurately with the use of the Normal distribution function, several conditions must be met.

First, the normalized depth should be less than or equal to 0.1, and second, the scanning range should start close to the junction but with $x/L \geq 2$, and with the smallest possible scanning width. The fitting parameters given in [59] were modified to take into account these two conditions. The errors in extracting the diffusion lengths can be kept to below 1% for any values of the surface recombination velocities, and the error for the surface recombination velocity extraction can be kept to below 25% for the range of 1×10^2 cm/s to 1×10^5 cm/s.

Chapter 4

Depletion Width Extraction

4.1 Introduction

It has been discussed in Chapters 1 and 2 that the accuracy of EBIC techniques for diffusion length measurements depends on the accuracy of determining the exact locations of the depletion layer's edges. The literature review of depletion width extraction using the EBIC technique has also been given in section 1.3.2. This chapter discusses an alternative, yet easier, method of determining the edges of the depletion layer from an EBIC profile across a semiconductor junction.

As mentioned in the literature review, the first experiments that show EBIC's capability to determine the depletion width were done by MacDonald and Everhart [80]. The widths of the depletion layers were obtained from the widths of the maximum EBIC profiles. An EBIC profile, however, does not have sharp edges that enable the determination of this width to be accurate. This is particularly due to the effect of the finite dimension of

the generation volume. This method does not take into account the finite size of the generation volume as well as the finite beam diameter. These two parameters are not significant when the depletion width is large. This is confirmed with the experimental data used by MacDonald and Everhart, which applied reverse bias on the p-n junction. The depletion widths in their data were rather large.

In 2002, Chiu and Shih [79] obtained the depletion widths from

$$W = W_{\text{peak}} + 2 \times 0.1R \quad (4.1)$$

where W_{peak} is the width of the maximum flat region observed in a log scale plot of EBIC profile, which is the depletion width obtained by MacDonald and Everhart. The method proposed by Chiu and Shih is more accurate than the one by MacDonald and Everhart because it takes into account the lateral dimension of the generation volume. Nevertheless, the same problem of identifying the value of W_{peak} is still present.

This chapter proposes a modified technique which enables one to obtain the depletion widths from the EBIC profiles in a more accurate manner. It eliminates the problem of identifying the maximum flat region that occurs in the method proposed by MacDonald and Everhart, as well as by Chiu and Shih.

GaN material was chosen as a sample material used to verify the technique. GaN light emitting diodes (LEDs) emit efficiently at short wavelengths, which are important for full color displays, laser printers, high density information storage, and underwater communication [94]. Its efficiency depends strongly on its diffusion length [95]. The diffusion length mea-

measurements of GaN materials using the EBIC technique can be found in the literature [96–103]. The accuracy of extracting the diffusion lengths depends on the accuracy of obtaining the positions of the edges of the depletion width [100].

The chapter starts with a theoretical consideration of extracting the depletion width or the depletion layer's edges using the EBIC technique. The technique is then applied to an experimental data obtained from a collaborative work with the Cambridge University. The chapter closes with a discussion on the results obtained.

4.2 Theory

4.2.1 Depletion Width and Doping Concentration

If the concentrations of the p and n layers forming the p-n junction are known, then the depletion width can be obtained analytically using [104]

$$W = \sqrt{\frac{2\varepsilon(N_A + N_D)\psi_m}{qN_A N_D}} \quad (4.2)$$

where W is the depletion width, $\varepsilon (= \varepsilon_r \varepsilon_0)$ is the permittivity of the material, ε_0 is the permittivity in vacuum, and ε_r is the relative permittivity. The term q is the elemental charge, N_A and N_D are the doping concentrations of the acceptor (p layer) and the donor (n layer), and ψ_m is the total drop in potential given by

$$\psi_m = \psi_{bi} \pm \psi_{app} \quad (4.3)$$

where ψ_{bi} is the built-in potential and ψ_{app} is the externally applied bias. The positive sign applies under reverse bias while the negative sign under forward bias. The penetration of the depletion layer on the p and n layers can then be obtained by solving these two equations,

$$W = x_n + x_p \quad (4.4)$$

$$N_D x_n = N_A x_p \quad (4.5)$$

where x_n and x_p are the location of the depletion layer's edges in the n and p regions, respectively.

In order to obtain the depletion width and its edges using the above equations, the information on the doping concentrations is required. EBIC has been used to investigate the variation in the doping concentrations [105, 106]. Nevertheless, other techniques are usually used for the determination of an accurate doping concentrations.

Obtaining the depletion width by obtaining the doping first, however, introduces another error in the process of obtaining the depletion width. It is, therefore, desirable to obtain the depletion width directly. The following section shows that the EBIC profile is quite sensitive to the position of the depletion layer's edges and, thus, can be used to obtain the depletion width and its edges directly.

Figure 4.1: Schematic EBIC profile for the case when the depletion width is much larger than the generation volume.

4.2.2 Synthesis of an EBIC Profile Around the Junction

In EBIC, the sample under investigation is bombarded in vacuum with a focused electron beam, generating a large number of ehps in the generation volume. This generation volume affects the EBIC profile around the depletion layer.

Consider the case where a generation volume is completely enclosed within the depletion region. The ehps generated are immediately separated by the electric field of the junction. This, in turn, results in an induced current, termed $I_{\text{depletion}}$. The values of $I_{\text{depletion}}$ remain constant in the depletion region since the amount of carriers collected is constant, which is the amount of ehps generated [12]. This is region C in Fig. 4.1. As the generation volume moves away from the junction, the induced current drops

Figure 4.2: Schematic first derivative of the EBIC profile for the case when the depletion width is much larger than the generation volume and the surface recombination velocity is not negligible.

exponentially. The drop can be expressed in the form of [36, 58]

$$I = kx^\alpha \exp(-x/L) \quad (4.6)$$

where x is the distance from the edge of the depletion region of the p-n junction, L is the diffusion length of the minority carriers, α is a linearization coefficient as described in [36], and k is a constant.

Now, consider the case where the generation volume is approaching, but not yet touching the depletion region. The first derivative of the semilogarithmic EBIC profile with respect to the beam distance from the junction is expected to have either a constant value or increasing in value, depending on the surface recombination velocity (cf. taking $\ln(I)$ in Eq. (4.6)). As mentioned in the previous chapter, zero surface recombination results in a straight line if the current is drawn in semilogarithmic plot. On the other hand, a surface recombination velocity will make the curve to be concaved

upward, or in other words increasing in value when the first derivative of the semilogarithmic plot is drawn. This is labeled as region A in Figs. 4.1 and 4.2. Whether the first derivative profile in region A is constant or increasing in value depends on the coefficient α in Eq. (4.6), which depends on the surface recombination velocity of the material. The surface recombination velocity reduces the amount of minority carriers collected by the p-n junction [38, 48, 59].

When the surface recombination velocity is negligible, the EBIC profile follows an exponential relationship, which is a straight line in a semi-logarithmic plot. This shows up as a constant value in the plot of its first derivative. When the surface recombination velocity is significant, the semi-logarithmic plot is concave upward and the first derivative is a plot with increasing in its absolute value.

As the generation volume begins to enter the depletion region at x_l , the charge carriers generated inside the depletion region are collected more efficiently, causing a departure from Eq. (4.6) and resulting in a local EBIC profile that is concave downwards in the semi-logarithmic plot. The departure from Eq. (4.6) happens because of the effect of the finite size of the generation volume. This change causes an inflection point as mentioned in [35, 47]. The corresponding first derivative, then, produces a range of decreasing positive values, labeled B in Figs. 4.1 and 4.2.

If the depletion width is much larger than the generation volume, then once the generation volume is completely inside the depletion region, a constant maximum value $I_{\text{depletion}}$ is produced in the induced current. This will remain constant until the generation volume begins to leave the deple-

tion region [107]. The corresponding first derivative of this region of constant induced current is zero. This is labeled C in Figs. 4.1 and 4.2. Therefore, it can be seen that the location where the first derivative profile begins to decrease from a maximum value to zero identifies the position where the generation volume begins to enter the depletion region.

If the depletion width is much smaller than the generation volume, then the collection probability in the depletion region is convoluted with the generation volume and the region of a constant induced current is not observed. The peak of this profile is also smaller than the previously considered $I_{\text{depletion}}$, as only a fraction of charge carriers are generated in the depletion region.

The above description applies as the beam moves entering the depletion layer from the left. The same approach can be done to synthesize the other half of the profile. This is true because the same behaviour arises as the generation volume leaves the depletion region. However, in this case, negative values in its first derivative is produced.

4.3 Numerical Computation

4.3.1 Survey of Models

The previous section gave a synthesis of the EBIC profile qualitatively. In this section, we will try to compute the EBIC profiles numerically based on the available analytical equations for the normal-collector configuration. Many works have been done to develop EBIC models for certain collector

geometries. In this survey, we will limit ourselves to the normal-collector geometry.

Berz and Kuiken derived an analytical expression for the EBIC profile with a constant sphere generation volume [38]. The model is valid only when the beam energy is small and so the generation volume distribution approaches a sphere or a point source.

Donolato used a sphere with a Gaussian distribution to derive the analytical expression [48]. This expression however, is only valid for the case when $x > R/2$. In other words, the expression is valid when the generation volume is totally outside of the depletion layer. In reality, the generation volume's shape looks more like a tear drop or a pear shape [13].

The usual EBIC expression is usually only valid for the case when the beam is bombarded in the neutral region, such as the two works mentioned above. This, however, makes one unable to analyse the profile for the region close to the junction. Moreover, they usually use a simplified generation volume model, such as a uniform sphere or a Gaussian sphere, so that the final expression can be simplified.

With the advancement of numerical computation, more complicated models have been derived. Closas and Rubio developed an EBIC model for computer calculations [108]. They analysed two generation volume distributions, the first one is completely Gaussian, while the second one is Gaussian in one coordinate direction and following Everhart and Hoff polynomial [8] in the other coordinate direction. Donolato and Venturi also mentioned about these two models in [109]. In the computation, however, Donolato and Venturi used completely Gaussian model in the x and z directions for simplicity

in calculation. In these works, only the region outside of the depletion layer was considered.

Hungerford gave computation results of EBIC profiles across p-n junctions [107]. His computation included the profile in the depletion layer similar to the work of Czaja [27]. In this work, the generation volume distribution was obtained from a Monte Carlo simulation coded by Napchan [110]. For the region outside of the depletion layer, the generation volume data is convoluted with a point source charge collection probability given in [48]. On the other hand, the collection probability for the region within the depletion layer is assumed to be unity.

We will follow the approach of Hungerford to use the charge collection probability of a point source and to convolute it with the distribution of the generation volume. In the following sections, we will first compare the profiles when using the data from Monte Carlo simulations with the profiles when using the analytical expressions for their generation volume distributions.

4.3.2 Mathematical Model

Two main assumptions are made for the computation. First, it is assumed that the expression for the generation volume distribution is valid for the neutral region, as well as the space charge region or the depletion layer. Second, it is assumed that the charge collection probability within the depletion layer is unity. The first assumption is justified since the distribution of the generation volume depends mainly on the atomic number of the material.

It will be shown later in Chapter 5 that the distribution of the generation volume depends mainly on the atomic number of the material and the beam energy. Since the atomic number does not change in both the neutral region as well as the depletion layer, the first assumption is valid. The second assumption is valid when there is negligible recombination of electron-hole pairs inside the depletion layer. This is the ideal condition used to simplify the derivation. Semiconductor device simulator commonly employs this assumption as well as their default model [143, page 7-15].

Let's consider the case of a two dimensional semi-infinite geometry. In this case, the x and z axes are from zero to infinity. The EBIC profile can then be written as

$$I_N(x') = \int_0^\infty \int_0^\infty Q(x, z) h(x - x', z) dx dz \quad (4.7)$$

where $Q(x, z)$ is the charge collection probability due to a point source, and $h(x - x', z)$ is the generation volume distribution when the beam scans at $x = x'$. The current collected at the junction due to a beam bombarding at $x = x'$ is a convolution of a charge collection probability with a generation volume distribution shifted to $x = x'$.

If the charge collection probability within the depletion layer is assumed to be unity, and the n-region now extends in the x direction to minus infinity, while the p-region extends to the positive infinity, then

$$\begin{aligned} I_N(x') &= \int_0^\infty \int_{-\infty}^{-x_n} Q(x, z) h(x - x', z) dx dz \\ &\quad + \int_0^\infty \int_{-x_n}^{x_p} h(x, z) dx dz \end{aligned} \quad (4.8)$$

$$+ \int_0^\infty \int_{x_p}^\infty Q(x, z) h(x - x', z) dx dz$$

where now the integration includes the locations of the depletion layer's edges, i.e. x_n and x_p for the n and p regions respectively.

The task now is to find the appropriate expressions for both the charge collection probability and the generation volume distribution. The most commonly used expression of the charge collection probability for the normal-collector configuration is the one derived by Donolato [48] and was used in Chapter 2 to generate the EBIC data.

$$Q(x, z) = \exp(-\lambda x) - \frac{2s}{\pi} \int_0^\infty \frac{k}{\mu^2(\mu + s)} \exp(-\mu z) \sin(kx) dk \quad (4.9)$$

Some discussions on the generation volume models can be found on Chapter 6. For the analysis in this chapter, we follow the formula used by Parish and Russell [111] which used the model developed by Bonard and Ganiere [112, 113]. The generation volume in two dimensions can be written as

$$h(x - x', z) = \frac{1}{2\sqrt{\pi}\sigma_x\sigma_z^3} \exp\left(-\frac{(x - x')^2}{\sigma_x^2}\right) z^2 \exp\left(-\frac{z}{\sigma_z}\right) \quad (4.10)$$

where σ_x is the lateral electron range, and σ_z is the depth electron range. These are functions of the material and the beam parameters. The values of these parameters were obtained through fitting Eq. (4.10) into the data generated by Monte Carlo simulations. An example of this procedure is given in Chapter 6.

For 4 keV beam energy with a 20 nm beam diameter, the fitting process in GaN material gives

$$\sigma_x = 4.1618 \times 10^{-2} \mu\text{m} \quad (4.11)$$

Figure 4.3: Computed EBIC profiles across a GaN p-n junction. The diffusion length was set to $3 \mu\text{m}$ and the depletion layer's edges were located at $\pm 0.3 \mu\text{m}$.

$$\sigma_z = 1.0850 \times 10^{-2} \mu\text{m} \quad (4.12)$$

Thus, the EBIC profile across the junction can be computed. The Matlab codes for the numerical computations are given in Appendix C. Fig. 4.3 shows the plot of the computed EBIC profiles across a GaN material p-n junction with $L = 3 \mu\text{m}$ and has its depletion layer's edges at $\pm 0.3 \mu\text{m}$.

4.4 Analysis of the Computed Profile

As shown in section 4.2.2, the locations where the generation volume starts to enter the depletion layer can be best analysed in its first derivative. The first derivative can be computed using the Finite Difference Method [88]. The centred difference formula, which is second-order accurate, can be written

Figure 4.4: First derivatives of the computed EBIC profiles across a GaN p-n junction. The diffusion length was set to $3 \mu\text{m}$ and the depletion edges were located at $\pm 0.3 \mu\text{m}$.

as follows.

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} \quad (4.13)$$

where h is the distance between the points. Applying this formula to the data computed in the previous section gives the first derivative of the EBIC profile across a p-n junction. Fig. 4.4 shows this plot.

Some brief observation is worth to be noted before we go for further analysis. It can be seen from Fig. 4.4 that the first derivative outside of the depletion layer for the case of zero surface recombination velocity is a constant with a value of about ± 0.333 , which is the value of $-1/L$. This agrees with the observation found in the literature that states that the diffusion length can be obtained from the negative reciprocal of the slope [36, 38]. This is a well know result in electron beam induced current theory.

On the other hand, the first derivative for the case $s = 0.15$ is higher, which also means that it has a steeper slope. This again agrees with experimental results. However, the most important observation is that the first derivatives around the depletion layer's edges ($\pm 0.3 \mu\text{m}$) change significantly. This is the region which we shall analyse in this section.

4.4.1 Analysis of Dominant Factors

4.4.1.1 Design of Experiment

The location where the beam starts to enter the depletion layer is uncertain due to a continuous distribution of the generation volume. To overcome this problem, we shall identify the location where the generation volume starts to enter from the intersection of extrapolated lines (Fig. 4.5).

For the analysis, we shall implement the two-level fractional factorial

Table 4.1: Factor Levels of 2^{5-1} Fractional Factorial Design.

Factor	Parameters	(-)	(+)	unit
A	Surface recombination velocities ($s = v_s/D$)	0.15	150	cm^{-1}
B	Diffusion lengths (L)	1	10	μm
C	Beam energy (E_b)	4	8	keV
D	Depletion width (W)	0.3	0.6	μm
E	Beam diameter (d_b)	20	200	nm

design [114]. The theory of shall not be covered in the thesis. We shall only discuss the design and the analysis.

The purpose of the analysis is to identify what are the parameters affecting this point, that is the location of point O in Fig. 4.5. The parameters which we are going to analyse are: the surface recombination velocities, the diffusion lengths, the electron range or the beam energy, the depletion width, and the beam diameter. Therefore, we have five parameters to vary, which are called the main effects. These main effects may interact and affect the location of point O. When the interaction is strong, the indication for main effect cannot be interpreted. It is important in the design to associate highest order interactions with the main effects.

Each main effect is varied in two levels, and so the name two-level factorial design comes from. Table 4.1 gives the levels of each main parameters or effects. It is important to have a sufficient difference between the two levels to reduce the ambiguity caused by the noise. The two levels are decoded as low (-) and high (+) levels.

In the fractional design, the number of runs is reduced. Since in our case $k = 5$, is the number of parameters, then the number of runs is $2^k = 2^5 = 32$.

Table 4.2: Runs, Level Combinations, and Results.

Run	Combination	Basic Design				Generator E=ABCD	Results x_l (μm)
		A	B	C	D		
1	e	-	-	-	-	+	0.182
2	a	+	-	-	-	-	0.158
3	b	-	+	-	-	-	0.171
4	abe	+	+	-	-	+	0.176
5	c	-	-	+	-	-	0.201
6	ace	+	-	+	-	+	0.178
7	bce	-	+	+	-	+	0.210
8	abc	+	+	+	-	-	0.166
9	d	-	-	-	+	-	0.323
10	ade	+	-	-	+	+	0.323
11	bde	-	+	-	+	+	0.327
12	abd	+	+	-	+	-	0.306
13	cde	-	-	+	+	+	0.380
14	acd	+	-	+	+	-	0.313
15	bcd	-	+	+	+	-	0.340
16	abcde	+	+	+	+	+	0.333

The number of runs is reduced by only running a fraction of the total runs. In this case, we choose to have 2^{5-1} or half fractional design, which gives the highest resolution for $k = 5$. Therefore, the total number of runs is 16. The table of runs with the combination of levels for each run is given in Table 4.2. Since the EBIC profile was set to be symmetric, only one side was used in the determination of the location of point O.

The main effect A is computed from

$$A = \frac{1}{16}[-e + a - b + abe - c + ace - bce + abc - d + ade - bde + abd - cde + acd - bcd + abcde] \quad (4.14)$$

where e is the result from the first combination, a is from the second combination, and so on (the value of last column in Table 4.2). The signs follow the level (either - or +) in column A of Table 4.2. The other main effects can be computed in a similar way. For example, the main effect C can be computed from

$$C = \frac{1}{16}[-e - a - b - abe + c + ace + bce + abc - d - ade - bde - abd + cde + acd - bcd + abcde] \quad (4.15)$$

The interaction is computed in the same manner as well. For example the interaction between A and D, which is labeled as AD, can be computed from Eq. (4.14) or (4.15) as well. However, now the signs follow the multiplication of column A and column D.

$$AD = \frac{1}{16}[+e - a + b - abe + c - ace + bce - abc - d + ade - bde + abd - cde + acd - bcd + abcde] \quad (4.16)$$

In this way, the main effects together with their high-order interactions can be calculated.

4.4.1.2 Analysis

One of the easiest ways to visualize the dominant factors is to plot the normal probability plot [114]. A more detailed method to produce this plot can be found in [115], and so will not be reproduced here. Fig. 4.6 shows the

Figure 4.6: Normal probability plot for then location of the intersection of the extrapolated lines, that is point O in Fig. 4.5

normal probability plot of the computed results, which is the location of the intersection of the extrapolated lines. In all the following figures, we only plot the main effects and its second order interaction. This is because higher order interactions are negligible. When no dominant factors are present, all the effects lie in approximately a straight line. On the other hand, a dominant factor will deviate from this straight line in the normal probability plot.

It can be seen that the dominant factor is the depletion width, that is D. This means that the location of point O depends mostly on the location of the edge of the depletion layer. In other words, the location of the depletion layer's edge can be obtained from the location of point O. A question then arises whether the edge of the depletion layer depends only on this point O. To do this, we take the difference,

$$\Delta_1 = x_l - x_{\text{edge}} \quad (4.17)$$

Figure 4.7: Normal probability plot for the difference between point O and the depletion layer's edge, that is Δ_1 .

and recalculate again the normal probability plot. This is shown in Fig. 4.7.

It can be seen that now the main effect D is no longer significant. Some second order interactions become dominant in this case. we know from [79] that the difference is somewhat affected by the lateral dimension of the generation volume. Following [116] which states that 95% of the generation of the ehps is within the range of $0.1R$ in its lateral dimension, where R is the electron range, we can write a new quantity,

$$\Delta_2 = \Delta_1 - 0.1R \quad (4.18)$$

Fig. 4.8 shows the normal probability plot of Δ_2 . Now, the only dominant factor left is A, that is the surface recombination velocity. Unfortunately, we do not know any relationships to take into account the surface recombination velocities.

Figure 4.8: Normal probability plot for the difference between point O and the depletion layer's edge, taking into account the lateral dimension, that is Δ_2 .

So far, the factors D and C have been taken into account. It is interesting to note that factor B, that is the diffusion length, has never come out as an affecting factor for the position of point O. The only left parameter in our investigation is the beam diameter. If we take that into account,

$$\Delta_3 = \Delta_2 - r_b \quad (4.19)$$

where $r_b = d_b/2$ is the radius. Fig. 4.9 shows the normal probability plot. The effect of taking the beam radius seems to worsen the result. Therefore, it seems that the beam radius does not give a large impact on the location of point O. This conclusion can be obtained as well from Fig. 4.10. The data on this figure was taken from Monte Carlo Simulations. The energy distribution was obtained and integrated along the y and the z axis. The figure shows the intensity projected on the x axis, which is the lateral dimension of the

Figure 4.9: Normal probability plot for the difference between point O and the depletion layer's edge, taking into account the lateral dimension and beam diameter, that is Δ_3 .

generation volume. This conclusion, however, is true only when the beam diameter is small. From the analysis done in this chapter, we can at least say that the beam radius of 100 nm and 10 nm does not affect the position of point O. A more detailed study on the effect of the beam radius is beyond the scope of the thesis.

If we ignore the surface recombination velocity, Fig. 4.8 shows that the value of Δ_2 is close to zero. In other words, there are no dominant factors affecting the value of Δ_2 besides the surface recombination velocity. Therefore, when the surface recombination velocity is negligible, the depletion layer's edge can be obtained from

$$x_{\text{edge}} = x_l - 0.1R \quad (4.20)$$

Figure 4.10: Lateral dimensions from Monte Carlo simulations with beam energy of 4 keV on Silicon.

or in terms of the depletion width becomes

$$W = (x_r - x_l) - 2 \times 0.1R \quad (4.21)$$

The data for Fig. 4.8 is given in Table 4.3

4.4.2 Effects of the Surface Recombination Velocity

4.4.2.1 Design of Experiment

The previous section shows quantitatively that the dominant factor affecting Eq. (4.20) or (4.21) is the surface recombination velocity. It is important, then, to study further how this parameter affects the values of the depletion layer's edges obtained.

In order to do this, symmetrical EBIC profiles were generated using the theoretical equations. The surface recombination velocities were varied from

Table 4.3: Effects and Values of the Normal Probability Plot of Fig. 4.8

Effect	Value	j	(j-0.5)/15	z_j	Effect	Sorted Value
A	-1.1313E-02	1	0.03	-1.83	A	-1.1313E-02
B	-1.8125E-03	2	0.10	-1.28	B	-1.8125E-03
C	2.1489E-04	3	0.17	-0.97	AD	-2.4569E-04
D	1.8750E-04	4	0.23	-0.73	AE	-1.3457E-04
E	1.9375E-03	5	0.30	-0.52	DE	-1.1216E-05
AB	3.5843E-04	6	0.37	-0.34	CD	1.0829E-05
AC	6.1481E-04	7	0.43	-0.17	CE	2.0378E-05
AD	-2.4569E-04	8	0.50	0.00	BD	7.1945E-05
AE	-1.3457E-04	9	0.57	0.17	BE	9.5005E-05
BC	1.9392E-04	10	0.63	0.34	D	1.8750E-04
BD	7.1945E-05	11	0.70	0.52	BC	1.9392E-04
BE	9.5005E-05	12	0.77	0.73	C	2.1489E-04
CD	1.0829E-05	13	0.83	0.97	AB	3.5843E-04
CE	2.0378E-05	14	0.90	1.28	AC	6.1481E-04
DE	-1.1216E-05	15	0.97	1.83	E	1.9375E-03

$S = 0$ to 1×10^3 , and the diffusion length was set to $1 \mu\text{m}$. The edges of the depletion layer were set at $\pm 0.3 \mu\text{m}$. Besides using the two beam energies as in the last section, that is 4 and 8 keV, we added another data with 10 keV beam energy.

The values of the depletion layer's edge were then extracted from Eq. (4.20). In order to compute Eq. (4.20), the values of the electron range must be known. These values for GaN for different beam energies were computed using the method of Everhart and Hoff [8], and will be discussed in a more detail in Chapter 5. The computed values of the electron range were 0.16, 0.48, and $0.69 \mu\text{m}$ respectively for the case of 4, 8, and 10 keV beam energies

Table 4.4: Extracted Depletion Layer's Edges for Various Surface Recombination Velocities

S	x_{edge}			Total	Average
	4 keV	8 keV	10 keV	$(y_{i.})$	$(\bar{y}_{i.})$
0	0.301	0.313	0.314	0.928	0.309
1×10^{-3}	0.301	0.313	0.313	0.927	0.309
1×10^{-2}	0.301	0.313	0.312	0.926	0.309
1×10^{-1}	0.299	0.310	0.309	0.918	0.306
1×10^0	0.297	0.298	0.293	0.888	0.296
1×10^1	0.295	0.284	0.270	0.849	0.283
1×10^2	0.293	0.271	0.250	0.814	0.271
1×10^3	0.291	0.263	0.244	0.798	0.266
				$y_{..} = 7.048$	$\bar{y}_{..} = 0.294$

4.4.2.2 Analysis

Table 4.4 shows the extracted values of the depletion edges. In the table, the value of $y_{..}$ was obtained by summing the total column, and $\bar{y}_{..}$ was obtained from $y_{..}/8$. It can be seen that the average value extracted for various surface recombination velocities was $0.294 \mu\text{m}$, which has error of -2.00%. This shows that the Eq. (4.20) is quite accurate for surface recombination velocity range of $0 \leq S \leq 1000$.

This would seem to contradict the previous conclusion when we said that the surface recombination velocity affects the location of the depletion width edges. However, it can be shown that the surface recombination velocity does affect the extracted edge location. Observing the average value column in Table 4.4, it can be seen that the extracted edge position decreases as the surface recombination velocity increases.

Fig. 4.11 shows the plot of the average extracted edge location from three different beam energies. It is obvious that the extracted edge location

Figure 4.11: Predicted values versus the surface recombination velocities.

changes with surface recombination velocity. Observing the y axis scale, however, it can be noted that the change is not significant. This confirms the two previous conclusions which seem to be contradictory. A linear regression was done to model this effect. The curve can be fitted into a Logistic function as follows.

$$x_l - 0.1R = \delta + \frac{\alpha}{1 + \exp(\beta + \gamma \ln S)} \quad (4.22)$$

where $\alpha = 0.0455$, $\beta = -0.7465$, $\gamma = 0.5512$, and $\delta = 0.2648$.

The analysis can be concluded by saying that the surface recombination velocity affects slightly the depletion edges obtained from Eq. (4.20) or the depletion width from Eq. (4.21). The effects can be modelled by the Logistic function. The model shows that higher surface recombination velocities reduce the depletion edges value obtained. The effects, however, are not very significant. The error for surface recombination velocity range

of $0 \leq S \leq 1000$ is about 2.00%. Therefore, in the region of low surface recombination velocities, the depletion edges or the depletion width can be obtained accurately from Eqs. (4.20) and (4.21) respectively.

4.5 Experiment

The experiment was done by Gregory Moldovan in the University of Cambridge, UK. The EBIC profiles were sent to be analysed in the Nanyang Technological University. The work was part of an investigation of a GaN LED structure using the EBIC technique.

4.5.1 Materials

The proposed technique is demonstrated using a GaN LED structure. The GaN LED structure is the same as the work done by Moldovan *et al.* [103]. The undoped GaN has a nominal carrier concentration of $(1-2) \times 10^{17} \text{ cm}^{-3}$, while the Si-doped GaN layer has a carrier concentration of $(2-3) \times 10^{18} \text{ cm}^{-3}$. The Mg-doped GaN was annealed to activate the doping, producing a nominal carrier concentration of $(1-2) \times 10^{17} \text{ cm}^{-3}$.

For the purpose of cross-sectional EBIC, a die was separated from the LED package and then mechanically polished from one side to a mirror finish. To obtain a smoother cross section and reduce the surface damaged introduced by polishing, a final surface treatment was applied with an Ar ion miller.

Figure 4.12: EBIC image of GaN p-n junction with 1keV beam energy.

4.5.2 Method

EBIC profiles across the junction were recorded using a field emission gun FEI XL30 scanning electron microscopy (SEM) operating at acceleration voltage of 1 keV for higher resolution. The beam diameter was about 7 nm.

The EBIC profiles were stored in an image as shown in Fig. 4.12. A calibration was done to adjust the scale of the unit per pixel. Line scans of grey levels were then obtained perpendicular to the junction. The line scans were obtained only for the bottom region of the junction (red circle in Fig. 4.12). ImageJ¹ software was used for this image processing. Since the grey level is proportional to the EBIC level, we can use it to determine the depletion layer's edge.

Since noise is present in the data, the EBIC profile was smoothed before the first derivative was computed. The algorithm that was used is the

¹The software can be freely obtained from <http://rsb.info.nih.gov/ij/index.html>

Figure 4.13: Extrapolated lines to obtain x_l and x_r . The data plotted in this figure is before the smoothing process.

Savitsky-Golay smoothing filter [117]. The three parameters used in the smoothing process were $n_L = 5$, $n_R = 5$, $M = 3$, where n_L and n_R correspond to the number of points at the left and the right of the data to be averaged, and M is the degree of the polynomial to be fitted into the data.

After this, the first derivative of the semi-logarithmic plot was computed from Eq. (4.13). The electron range was computed using the Everhart and Hoff universal curve [8]. The calculations gave the value of 17 nm for beam energies 1 keV. The detail of the method is presented in Chapter 5. Since the surface recombination velocities were found to be quite low [103], the depletion layer's edges and the depletion widths can then be obtained from Eqs. (4.20) and (4.21) respectively. The Matlab code is given in Appendix C.5. The extracted depletion widths were then averaged and analysed. Fig. 4.13 shows the extraction from the extrapolated lines.

Table 4.5: Values of the Extracted Depletion Widths.

No.	x_l (nm)	x_r (nm)	W_0 (nm)	R (nm)	W (nm)
1	234	334	100	17	96.6
2	249	325	76	17	72.6
3	243	332	89	17	85.6
4	241	334	93	17	89.6
5	204	329	125	17	121.6
6	230	308	78	17	74.6
Average					90.1
Std. Dev.					17.9

4.6 Results and Discussion

Significant variations of depletion widths can be observed along the junction. The peak of the EBIC profile also varies with a large minimum at the location of threading dislocations [103]. The data that we are dealing with is only from the region at the bottom of the junction of Fig. 4.12. Table 4.5 shows the extracted data from the EBIC images.

The expected depletion widths can be calculated from Eq. (4.2). In this computation, we used $\varepsilon_r = 9$. For the case of zero bias, the total drop in potential (ψ_m) is the same as the built-in potential and can be obtained from

$$\psi_{bi} = \frac{kT}{q} \ln \left(\frac{N_A N_D}{n_i^2} \right) \quad (4.23)$$

where $n_i = 3.89 \times 10^{-10} \text{ cm}^{-3}$ is the intrinsic carrier concentration of GaN. Table 4.6 shows the expected values of the depletion widths for some doping concentrations. The average value is taken from its geometric average of the minimum and the maximum values.

It can be seen that the extracted depletion widths is smaller compared to

Table 4.6: Expected Values of Depletion Widths.

	unit	min	ave	max
p-type	cm ⁻³	1×10^{17}	1.41×10^{17}	2×10^{17}
n-type	cm ⁻³	1×10^{17}	1.41×10^{17}	2×10^{17}
ψ_{bi}	eV	3.15	3.17	3.19
Wd	nm	250.5	211.3	178.1

the expected values obtained from the doping concentrations calculations.

This could be due to the presence of dislocations in the junction.

The confidence interval can be computed as follows [114]

$$\bar{y} - t_{\alpha/2, n-1} S / \sqrt{n} \leq \mu \leq \bar{y} + t_{\alpha/2, n-1} S / \sqrt{n} \quad (4.24)$$

where $\bar{y}$ is the obtained average value, $t_{\alpha/2, n-1}$ is the inverse of the student-T distribution, S is the standard deviation, and n is the number of data. Substituting the values from Table 4.5 and using a significance level of $\alpha = 0.05$, we can obtain

$$\begin{aligned} 90.1 - 23.1 &\leq \mu \leq 90.1 + 23.1 \\ 67 \text{ nm} &\leq \mu \leq 113 \text{ nm} \end{aligned} \quad (4.25)$$

This means that the depletion width lies within 67 nm to 113 nm with 95% confidence level.

The sources of error comprise the estimated lateral dimension of the generation volume as well as the accuracy of the position x_l and x_r . The study of the lateral dimension of the generation volume can be done by doing Monte Carlo simulations or by doing experiments utilizing a multiquantum

well structure [113, 118, 119]. The accuracy of the x_l and x_r position can also be improved by using the phase sensitive detection methods [13, 120, 121].

Another point that should be studied further is the effect of the surface bend bending. The surface states creates a depletion region in the surface interface between the material and the air. Hence, the value of the material depletion width will reduce near the surface due to this surface bend bending. For low beam energy it is possible that the whole electron range lies completely in the surface depletion region. This would affect the value of the depletion width extracted. The discrepancy will be smaller for larger beam energy since the portion of the generation volume lies in the depletion region reduces. The study of the surface bend bending, however, is beyond the scope of this thesis. This should be considered as a future work.

4.7 Conclusion

This chapter provides an alternative technique of extracting the depletion widths and the locations of the depletion layer's edges. It was proposed that the depletion layer's edges can be obtained from the first derivative of the semi-logarithmic EBIC profile and by taking into account the lateral dimension of the generation volume.

The chapter started with a synthesis of a hypothetical EBIC profile. A theoretical profile was then computed using an analytical EBIC expression for a normal-collector configuration and a generation volume model following Bonard and Ganiere. This theoretical model was then analysed to show the dominant factors that would affect the depletion layer's edges extraction.

It was shown that the edges of the depletion layer can be obtained from Eq. (4.20) while the depletion width from Eq. (4.21). The dominant factor affecting the position of x_l and x_r is the surface recombination velocity. The effect, however, is insignificant when the surface recombination velocity is low (i.e. $S \leq 10$).

The technique was then applied to measure the depletion width of a GaN LED. The measured depletion width was smaller than the expected value obtained from the doping concentration calculation. This could be due to the presence of dislocations in the junction.

The accuracy can be improved by studying the parameters used to estimate the lateral dimension of the generation volume and increasing the accuracy of obtaining the position of x_l and x_r . The study of the lateral dimension can be done using Monte Carlo simulations or through experiments. The determination of the positions of x_l and x_r , on the other hand, can be improved using the phase sensitive detection methods.

Chapter 5

Investigation of Range-Energy Relationships for Low Energy Electron Beams in Si and GaN

5.1 Introduction

The resolution of an EBIC technique is affected by many factors, such as the carrier re-distribution due to drift, sample geometry, contamination, vibration, and the beam interaction with the sample [122], which is the one to be considered in this chapter. The interaction between the electrons from the beam with the sample results in an interaction volume, or commonly termed the generation volume. An example of how the generation volume affects the EBIC technique was shown in the discussion of the previous Chapter.

Within this volume, the electron-hole pairs are created. Higher beam

energies result in larger generation volumes. Therefore, in order to have a higher resolution, a smaller generation volume is commonly required, or in other words, a lower beam energy [123].

The size of this generation volume is characterized by what is called the electron penetration range, or simply the electron range. The contour of the ionization rate of a normalized generation volume is shown in Fig. 3 of [13]. It can be observed that the size of the generation volume has a diameter of approximately the electron range.

There are two principal ways in which the electron range can be calculated: semi-empirically or statistically using the Monte Carlo simulation technique [122]. Semi-empirical methods were claimed to be valid down to about 5 keV in a single layer systems [8]. However, it was recently claimed that the semi-empirical method gives reasonable agreement down to beam energies as low as 1 keV [122]. The three most commonly used expressions are due to Gruen [82], Everhart and Hoff (E-H) [8] and Kanaya and Okayama (K-O) [83].

Everhart and Hoff corrected the Gruen range [12, 82] and proposed the following expression to be used for an Al-SiO₂-Si system. This is given as

$$R_G = 40 \frac{E_b^{1.75}}{\rho} \quad (5.1)$$

where R_G is the corrected Gruen range in nm, E_b is the beam energy in keV, and ρ is the density in g/cm³. This expression was claimed to be valid within the energy range of 5 keV $\leq E_b \leq$ 25 keV.

In the same paper, Everhart and Hoff also provided a universal curve to calculate the electron range down to 5 keV. This universal curve takes into

account the material properties such as the atomic number and the atomic weight of the material. The expression was derived for non-relativistic electrons (beam energies lower than 30 keV) from the Bethe stopping power expression. This Bethe expression can only be used for energies well above 1 keV [124].

Kanaya and Okayama derived an expression for the maximum electron range. This expression also takes into account the atomic number and the atomic weight of the material. In their paper, the expression was claimed to be in good agreement with experiments over the energy range of 10 to 1000 keV.

Currently, there is no consensus on which semi-empirical range-energy expressions to use [81]. Luke in [81] analysed the Everhart and Hoff as well as the Kanaya and Okayama expressions for EBIC applications using Si and GaAs as the sample materials. However, in the computation of the E-H electron range for GaAs, the universal curve from the original paper was not used. Rather, it used the Gruen range expression as given in Eq. (5.1) which depends only on the beam energy and the density of the material. The universal curve, on the other hand takes into account the density, the atomic number, and the atomic weight of the material. Moreover, the analysis is applicable only for beam energies above 5 keV, and no discussion is found for a lower beam energy range.

The current trend is to use Monte Carlo simulation to study the generation volume and the electron range [123, 125]. Electron transport in the solid is modeled via multiple scatterings within the atomic matrix of the solid. This approach assumes that the differential cross section of elastic

and inelastic scatterings with the atoms are known [126]. The accuracy of this technique, therefore, is determined by the accuracy of the differential cross section. Moreover, the accuracy is also determined by the energy loss model used in the simulation.

The current chapter analyses the three semi-empirical range-energy expressions, particularly in comparison with the electron range values obtained from the Monte Carlo simulation. In this analysis, the Gruen range, the universal curve of E-H, and the K-O range are calculated. The materials chosen as samples for the calculations are Si and GaN. The choice of Si is based on its widespread use in semiconductor technology, including CMOS and photodiode applications. As for GaN, interest on this material has grown since it has a wide band gap and has shown promise for applications in ultraviolet photodiodes. The potential of GaN for applications in high frequency optoelectronics and at high temperatures is well documented [95].

A discussion on the validity of the three expressions at low energies is presented. The proposed range-energy expressions for Si and GaN at these low beam energies are then given. These expressions are obtained using data from the Monte Carlo simulations for beam energies below 5 keV.

5.2 Theory

5.2.1 Semi-empirical Expression

There are several definitions of the electron range in the literature. The choice of which electron range definition to use depends on the specific ap-

plications that the parameter is to be used for. This section discusses the three definitions that are most commonly used in the calculations of EBIC applications.

Experimentally, the *maximum* electron range can be obtained by measuring the transmission of electrons through a film. The energy at which the transmission coefficient cuts the zero axis corresponds to this *maximum* energy [127]. Cosslett and Thomas did the same measurement but they obtained the electron range from the *extrapolated* linear curve of the distribution. They called this a *practical* or *extrapolated* range. They found that the *mass* range, that is the density multiplied by the electron range, is approximately the same for all elements for a given incident beam energy. This was the basis of using Eq. (5.1) for materials other than Si.

Gruen [82] measured the variation of energy dissipations with penetration distance for air. He found that the shape of the distribution was almost independent of the beam energy when plotted as a function of an *extrapolated* range. This range is commonly termed the Gruen range and is given as

$$R_G = 45.7 \frac{E_b^{1.75}}{\rho} \quad (5.2)$$

where R_G is in nm, E_b is in keV and the density ρ is in g/cm³. This equation is valid for the energy range $5 \text{ keV} \leq E_b \leq 25 \text{ keV}$. Everhart and Hoff bettered this expression to the one given in Eq. (5.1). The constant was modified from 45.7 to 40. This decreases the value by about 14% [8].

The universal curve of E-H, however, was derived from the Bethe expression for stopping power expression. The electron range obtained from this universal curve is usually called the Bethe range [8, 12]. The Bethe range

Table 5.1: Tabulated Normalized Energy from Everhart and Hoff Universal Curve.

ξ	$\mathfrak{R}_B$
5 to 50	$0.95 \xi^{1.51}$
10 to 100	$0.68 \xi^{1.62}$
50 to 500	$0.34 \xi^{1.78}$

is the total length of the multiply deflected, drunkards-walk-type, electron path.

From the definition of the Bethe range, we would expect this range to be slightly greater than the one calculated from an extrapolated range like the Gruen range. The Bethe range is computed from

$$R_{E-H} = K \frac{\mathfrak{R}_B}{\rho} \quad (5.3)$$

where R_{E-H} is the Bethe range due to Everhart and Hoff in cm, ρ is the density in g/cm³, $\mathfrak{R}_B$ is the normalized range which can be obtained from the curve of a universal Bethe range versus the normalized energy ($\xi = 1.1658E_b/I$, this is used to obtain $\mathfrak{R}_B$ from the universal curve, which is reproduced in Table 5.1, and the term I will be defined below). And finally, K in Eq. (5.3) is given as

$$K = \frac{9.40 \times 10^{-12} I^2 A}{Z} \text{ g/cm}^2 \quad (5.4)$$

In the above expression, Z is the atomic number of the material and A is the atomic weight. The term I is the mean excitation energy given by the following empirical equation.

$$I = (9.76 + 58.8Z^{-1.19})Z \text{ eV} \quad (5.5)$$

It is important to note that the Bethe stopping power expression, and therefore, the Bethe range, is only as good as the I value that is used in this expression. The electron range from the E-H universal curve can then be calculated from Eqs. (5.3) to (5.5) and with reference to Table 5.1.

Kanaya and Okayama, on the other hand, derived an expression for the *maximum* range. One can also expect this range to be slightly larger compared to the extrapolated range. This is because the maximum range is defined as the length of a straight path perpendicular to the surface and is measured from the surface. According to [12], this range is smaller than the Bethe range, which is the total length of the multiply deflected path. The expression for this maximum range by Kanaya and Okayama is given by

$$R_{K-O} = \frac{2.76 \times 10^{-11} A E_b^{5/3} (1 + 0.978 \times 10^{-6})^{5/3}}{\rho Z^{8/9} (1 + 1.957 \times 10^{-6})^{4/3}} \quad (5.6)$$

where R_{K-O} is in cm, and E_b is in eV. As stated previously, this expression was claimed by Kanaya and Okayama to be in good agreement with experiments for beam energies of 10 keV to 1000 keV.

5.2.2 Monte Carlo Simulation

The Monte Carlo technique simulates the complicated trajectories of the electrons in the specimen. Each path consists of free flights of finite length, at the end of which a collision takes place. This collision changes the energy and the direction of the electron. This event can either be elastic or inelastic scatterings events. In the elastic scatterings, the electrons interact with the nuclei of the atom and undergo large angle deflections with little change in energy. On the other hand, in the inelastic scatterings, the electrons

interact with the outer shell electrons of the atoms and lose energy. The accuracy of Monte Carlo simulations depends on the physical models used in the computation.

It has been shown by Ivin *et al.* [126] that the Mott elastic cross section is in better agreement with experiment than the Rutherford elastic cross section. Kuhr and Fitting [123] also used the Mott cross section for their Monte Carlo simulation of low energy electrons. Since the tabulated data gives the Mott cross section at selected values of atomic number, electron energy, and scattering angle, the use of such data requires an interpolation between adjacent data points.

With regards to inelastic scatterings, the Joy and Luo model was found to be the best. The inelastic scatterings are usually modeled from a stopping power expression. The most commonly used stopping power expression is the Bethe expression from which Everhart and Hoff derived their universal curve. This is given by

$$-\frac{dE}{ds} = \frac{2\pi q^4 N Z}{E} \ln \left(\frac{1.1658 E}{I} \right) \quad (5.7)$$

where q is the unit charge, N is the Avogadro's number, E is the electron energy, and I is given by Eq. (5.5). This expression describes the mean energy loss per unit path length.

The Bethe expression is valid for beam energies well above 1 keV. In order to use the Bethe model for lower beam energies, Joy and Luo made a semi-empirical modification to the original Bethe expression for stopping powers in order to make it more accurate at low beam energies. The modified equation was claimed by Joy and Luo to agree well with estimates from other

calculations.

The computation is done by the simulator for both the primary and the secondary electron trajectories. The computation stops when the energy of the computed electron is not sufficient to ionize an electron. The model that is usually used to compute the effective ionization energy is that of Casnati *et al.* [128].

5.3 Methods

For analysis purposes, the electron range values were calculated from both the analytical expressions as well as from the Monte Carlo simulations. The values of the electron range were calculated for beam energies of 0.2 keV up to 50 keV. The three semi-empirical expressions were used and then compared. The E-H Bethe range values were calculated from Eqs. (5.3) to (5.5) with a reference to Table 5.1 for the values of $\mathfrak{R}_B$, while the K-O maximum electron range values were calculated from Eq. (5.6). The Gruen range values were obtained from Eq. (5.1).

The materials for which the electron range was calculated were Si and GaN. The following atomic numbers and atomic weights were used for Si and GaN respectively, $Z_{Si} = 14$ and $A_{Si} = 28.086$, $Z_{GaN} = 19$ and $A_{GaN} = 41.865$. The atomic number for GaN was calculated from the weighted average values. Substituting the above values into Eqs. (5.4) and (5.5) results in the values of K equals to 5.60×10^{-7} and 9.94×10^{-7} g/cm², and the values of I equals to 172.25 eV and 219.05 eV, for Si and GaN respectively. The values of the density used in the calculation are 2.33 g/cm³

for Si, and 6.15 g/cm^3 for GaN. Substituting all these values, one can obtain the electron range values for the E-H and the K-O expressions.

The electron range from the Monte Carlo simulations were obtained as follows. In this work, the Monte Carlo computation used the CASINO software developed by Raynald Gauvin *et al.* [129–131]. This program is a Monte Carlo simulation of electron trajectories in solids, specially designed to simulate the interaction of low energy electron beams with bulk samples and thin foils. The computation for the current work used tabulated Mott elastic scattering cross sections of Czyzewski [129], stopping powers model of Joy and Luo [132], and effective section ionization model of Casnati *et al.* [128].

Si and GaN substrate materials were used in the simulation. The beam energy was then set from 0.2 keV to 50 keV. In the simulations, 5000 electrons were used. The beam radius was set to 10 nm. The physical model was then chosen. The Mott model with interpolation was selected for the total cross section, and the stopping power used was that of Joy and Luo. The model for the effective section ionization used follows that of Casnati. A distribution of the energy ionization depths was then generated from the simulation.

The electron range values were then obtained by extrapolating the linear region of the negative slope of the distribution down to the zero of the y axis. The value where the extrapolated line intersects the zero of the y axis was taken as the value of the electron range. This approach was used by Cosslett and Thomas as well as by Gruen. An example of this technique is shown in Fig. 5.1.

Figure 5.1: Electron range extraction from Monte Carlo simulations for the case of 1 keV beam energy in Silicon.

5.4 Results

The values of the electron range from the Gruen, the E-H, and the K-O calculations, as well as from the Monte Carlo simulations are plotted in Figs. 5.2 and 5.3. It can be seen that all curves are approximately parallel to one another, especially for beam energies larger than 5 keV.

It is rather difficult to observe the difference between the semi-empirical values and the Monte Carlo simulation values. In order to analyse further, we define a ratio as follows, $Ratio = R_{semi-empirical}/R_{Monte-Carlo}$. This is shown in Fig. 5.4. The plot shows the same trend. At around 5 keV, the ratio changes drastically to below unity. Above 5 keV, the ratios of both E-H and K-O electron range values are above unity, while the ratios of the Gruen range are always below unity. The E-H range values are larger than

Figure 5.2: Electron range in Si. R_{M-C} is from the Monte Carlo simulation, R_{K-O} is from the K-O method, R_{E-H} is from the E-H universal curve calculation, and R_G is from Eq. (5.1).

Figure 5.3: Electron range in GaN. R_{M-C} is from the Monte Carlo simulation, R_{K-O} is from the K-O method, R_{E-H} is from the E-H universal curve calculation, and R_G is from Eq. (5.1).

Figure 5.4: Ratio of the semi-empirical range values to the Monte Carlo simulation values.

the K-O range, and both are larger than the Gruen range. This agrees with the electron definitions stated in the previous section.

Observing the lower beam energies region, we can see that the ratios for the E-H range are quite constant down to about 2 keV. From the definition of the electron range, the ratio below unity cannot be explained. This region indicates that the semi-empirical expressions are no longer valid. It is logical to suspect that the expressions become invalid before reaching this point. This result agrees with the definitions.

5.5 Discussion

There are some differences between the values obtained from the E-H universal curve and the one from Eq. (5.1) which was proposed by E-H as a

correction to the earlier Gruen range expression. This difference is due to the definition of the electron range. The E-H universal curve gives the Bethe range while Eq. (5.1) is the corrected Gruen range which is an extrapolated range. It can be seen that the Gruen range is quite close to the results of the Monte Carlo simulations for beam energies larger than 10 keV. In fact, using the original constant of 45.7 as proposed by Gruen would give a ratio which is even closer to unity. Averaging the ratio for Si and GaN for beam energies 10 to 50 keV, we obtained the values of 0.90 and 1.03, when using constants of 40.0 and 45.7 respectively.

The difference between the E-H range, K-O range, and the Monte Carlo simulation is also due to the electron range definition. It is worth noting that the electron range from the Monte Carlo simulation was extracted by extrapolation. The results agree with the definition since we would expect an extrapolated range to be the smallest while the Bethe range to be the largest. In summary, we can expect the following relationship.

$$R_{\text{ext}} \leq R_{K-O} \leq R_{E-H} \quad (5.8)$$

where R_{ext} is the extrapolated range, which in this case includes the results from the Monte Carlo as well as the Gruen calculation.

For beam energies larger than 5 keV up to about 50 keV, a fitted expression can be obtained for the electron range from the Monte Carlo simulation, and is given as $R_{M-C} = 23.17E_b^{1.73}$ nm for Si and $R_{M-C} = 10.46E_b^{1.68}$ nm for GaN. We can see that the exponents are very close to the 1.75 value of Eq. (5.1), especially for the case of Si.

For the case of beam energies lower than 5 keV, the ratios of the K-O

Figure 5.5: Fitted expressions for Si with beam energies lower than 5 keV.

range drop to below unity faster than the ratios of the E-H range. This shows that the E-H universal curve is slightly better in this region. This agrees with the theory since the lower limit of the E-H universal curve is lower than the limit that K-O stated in their original paper.

Since both the Gruen range and the results obtained from the Monte Carlo simulations are extrapolated ranges, they are comparable. Therefore, we would expect the ratio between the two to be a constant. The point where this ratio drops from unity is the point where the expression is no longer valid. From Fig. 5.4, this point is around 5 keV, which is the minimum beam energy stated in [8].

The three semi-empirical equations are questionable when used for calculating the electron ranges for beam energies lower than 5 keV. Since currently there are no semi-empirical expressions for this energy range, we need to turn to Monte Carlo simulation for a solution.

Figure 5.6: Fitted expressions for GaN with beam energies lower than 5 keV.

For low beam energies, fitted expressions can be obtained from the Monte Carlo electron ranges. This is given in Figs. 5.5 and 5.6. These expressions can be used to obtain the electron range for Si and GaN for the case where the beam energies are lower than 5 keV. It is interesting to observe that as the energy decreases, the constant in front of the beam energy variable increases, while the exponent decreases. This holds true for the entire energy range from 50 keV down to 0.2 keV. The same trend can be observed in Table 5.1 for the universal curve of E-H. The approach used here can also be applied to obtain the fitted expressions for other materials besides Si and GaN.

5.6 Conclusion

This chapter analysed the three semi-empirical expressions to calculate the electron range with reference to the values obtained from Monte Carlo sim-

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ulations. It was found that the original constant of the Gruen range agrees better with the Monte Carlo simulation than the one corrected by Everhart and Hoff. In the case of low beam energies, it was found that the E-H expression performs better compared to the K-O expression. However, the validity of all the three expressions is questionable for energies lower than 5 keV. In this region, it is suggested to use the Monte Carlo simulation instead.

Fitted expressions for beam energies lower than 5 keV were provided for both Si and GaN materials. The physical models used in the Monte Carlo simulations affect the accuracy of these expressions. A brief explanation of the models used for the simulation has been provided.

Chapter 6

Generation Volume Models

6.1 Introduction

This chapter discusses the generation volume model to be used in computing the EBIC profile across a normal-collector junction. A choice of models is based on the accuracy to predict the EBIC profile at the region around the collectors. The purpose is to have a model that can be computed numerically and convoluted with the charge collection probability to obtain the EBIC profile. The models are compared with data obtained from the Monte Carlo simulation.

A review on the generation volume models is presented first with some analysis. A choice of the models is then made. An example of the use of the generation volume model for EBIC profile computation has been presented in Chapter 4, and so will not be repeated here.

6.2 Mathematical Models

In the early years, EBIC profiles were derived with an assumption of point source generation volume [25]. In order for this assumption to be valid, the generation volume must be small and located far away from the boundaries. This assumption is not satisfactory for a realistic EBIC profile near the collectors.

Several models of finite generation volumes have been used in the calculation of EBIC profiles. Berz and Kuiken [38] used a uniform sphere generation volume. In this model the generation rate within the sphere is constant, while the rate outside of the sphere is zero. In reality, we do not have such abrupt changes in the distribution. Donolato [48] used a Gaussian model instead. The shape in his model was still a sphere, but now, the distribution varies according to a Gaussian distribution. Following [133], Donolato wrote the expression in x - z plane when the beam is located at $x = x'$ as follows.

$$h(x - x', z) = \frac{1.14}{2\pi\sigma^2} \exp\left(-\frac{(x - x')^2 + (z - z')^2}{2\sigma^2}\right) \quad (6.1)$$

where z' and σ are related to the electron penetration range by

$$z' = 0.3R \quad (6.2)$$

$$\sigma = R/\sqrt{15} \quad (6.3)$$

The term (x', z') can be considered as the centre of mass of the generation volume, while σ is the standard deviation of the Gaussian distribution.

Cohn and Caledonia [116], however, showed that the shape of the generation volume is not perfectly a sphere. It is rather in the shape of a tear-drop

or a pear-shape. This 3-D pear-shape generation volume was modeled by Donolato in [134] as follows

$$g(r, z; R) = \frac{\Lambda(z/R)}{2\pi R\sigma^2(z, R)} \exp\left(-\frac{r^2}{2\sigma^2(z, R)}\right) \quad (6.4)$$

In the thesis, we use $g(r, z)$ for a 3-D generation volume distribution, and $h(x, z)$ for a 2-D distribution. In this model, the standard deviation σ is no longer a constant as the case of the sphere Gaussian generation volume. Rather, it is a function of depth (z) and electron range (R). This contributes to the pear-shape geometry of the generation volume. The expression for this standard deviation is [134]

$$\sigma^2(z, R) = 0.36d^2 + 0.11z^3/R \quad (6.5)$$

where d is the beam diameter.

The term $\Lambda(z/R)$ is a function describing the distribution along the z axis, and is given by Everhart and Hoff in terms of a polynomial [8]. This polynomial function can be written as

$$\Lambda(\xi) = \begin{cases} 0.6 + 6.21\xi - 12.4\xi^2 + 5.69\xi^3; & 0 \leq \xi \leq 1.1, \\ 0; & \xi > 1.1 \end{cases} \quad (6.6)$$

and $\xi = z/R$.

One year later, Donolato and Venturi used the same model but with a different function $\Lambda(z/R)$ [109]. The reason was for simplicity in the calculation. In that paper, they used the expression by Fitting *et al.* [133]

$$\Lambda(\xi) = 1.14 \exp[-7.5(z/R - 0.3)^2] \quad (6.7)$$

In 1996, Bonard *et al.* used a different model that is based on experimental results [113]. The generation volume was characterized using a multi-quantum well structure. The model, however, examined only AlGaAs materials. Parish and Russel [111] generalized this model for all materials. The distribution can be written as

$$h(x, z) = \frac{1}{2\sqrt{\pi}\sigma_x\sigma_z^3} \exp\left(-\frac{x^2}{\sigma_x^2}\right) z^2 \exp\left(-\frac{z}{\sigma_z}\right) \quad (6.8)$$

where σ_x is the lateral electron range and σ_z is the depth electron range. These are functions of the materials 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 as follows.

$$h(x, z) = k(x)j(z) \quad (6.9)$$

$$k(x) = A \exp(-x^2/\sigma_x^2) \quad (6.10)$$

$$j(z) = Bz^2 \exp(-z/\sigma_z) \quad (6.11)$$

where A and B are constants. These expressions can be fitted separately in the x and z axes into Monte Carlo data. The data, however, must first be integrated along the other axes. For example, in order to obtain the σ_x parameter, the data of a 3-D generation volume distribution must be integrated along the y and the z axis.

The function $k(x)$ can be linearized as

$$\ln[k(x)] = \ln(A) - \frac{x^2}{\sigma_x^2} \quad (6.12)$$

while the function $j(z)$ as

$$\ln[j(z)] - 2 \ln(z) = \ln(B) - \frac{z}{\sigma_z} \quad (6.13)$$

These two functions can be fitted into the data. The advantage of this model is that it is customizable since the parameters are obtained from the fitting of the Monte Carlo data. The disadvantage is that we need to run a Monte Carlo simulation first before we can use the expression.

We will try to compare some of these models in the following section. A preferred model will then be chosen that will give closer EBIC profile in the region near to the collectors. This is because the EBIC profile near to the collectors is affected much by the generation volume.

6.3 Method

The three generation volume models that have pear-shape geometry were compared. The first one is the model that is described by Eqs. (6.4), (6.5), and (6.6), which was proposed by Donolato [134]. This is Gaussian in the x direction, but follows Everhart and Hoff polynomials in the z direction. We denote this as the Donolato model. The second one is the model described by Eqs. (6.4), (6.5), and (6.7), which was proposed by Donolato and Venturi [109]. In this model, the distribution along the z direction is another Gaussian centred at $\bar{z} = 0.3R$. We denote this model as the Donolato-Venturi. The last model is the one proposed by Bonard *et al.*, and used by Parish and Russel [111, 113].

The structure was a p-n junction with a normal-collector configuration,

and the material was Silicon. A density of 2.33 g/cm^3 was used in the calculation. The depletion layer's edges were set at $0.3 \text{ }\mu\text{m}$, with the metallurgical junction located at $x = 0$. The diffusion length was set to $3 \text{ }\mu\text{m}$, and for simplicity, the top surface was assumed to have a zero surface recombination velocity. The profile was computed from $x = 0$ to $x = 0.5 \text{ }\mu\text{m}$, with a spacing of $\Delta x = 0.01 \text{ }\mu\text{m}$.

In order to compute the EBIC profile, we need the expressions for the charge collection probability as well as the generation volume data or the generation volume models. In the first following section, we discuss the generation volume data from the Monte Carlo simulation. Then, we also discuss the computation of the three generation volume models: the Donolato model, the Donolato-Venturi model, and the Bonard *et al.* model. After these, we discuss the computation of the profile including its first and second derivative.

6.3.1 EBIC Profile using the Monte Carlo Data

The EBIC profiles from the three models were compared with the EBIC profile using data from the Monte Carlo simulation. The Monte Carlo simulation has been described in more detail in Chapter 5. For the analysis in this chapter, we used 3 keV beam energy with 10 nm beam radius. The same physical models were used. The energy distribution on the x - z plane was then obtained and stored as a matrix.

The matrix was then convoluted with the charge collection probability as given in Eqs. (4.8) and (4.9). For simplicity, we computed only one

side of the junction. The important feature that we want to compare is the profile around the depletion layer's edge. The Matlab code for this computation is given in Appendix C.2. The function takes three input. The first one is the *parameter* input. It consists of information on the location of the depletion layer's edges, diffusion lengths, and the surface recombination velocities of the regions. The second input is the *beam position*. The third one is a parameter that takes the *filename* of the matrix storing the energy distribution obtained from the Monte Carlo simulation.

6.3.2 EBIC profiles using the Mathematical Models

The EBIC profiles from the three generation volume models were computed numerically. Since the charge collection probability that is available is in the x - z plane, we need to project the 3-D distribution of Donolato's models into the x - z plane. This can be done by integrating Eq. (6.4) with respect to the y axis.

$$h(x, z) = \int_{-\infty}^{\infty} g(x, y, z) dy \quad (6.14)$$

This results in

$$h(x, z) = \frac{\Lambda(z/R)}{\sqrt{2\pi}\sigma R} \exp\left(-\frac{x^2}{2\sigma^2}\right) \quad (6.15)$$

In the above equation both σ and R have a dimension of a unit length, while the other terms are unit-less. Therefore, we can see that the unit of $h(x, z)$ is ehp/(unit area). Substituting Eq. (6.6) into Eq. (6.15) results in the Donolato model. On the other hand, substituting Eq. (6.7) into Eq. (6.15) results in the Donolato-Venturi model.

The value of R is required in the computation. This electron penetration range, R , can be calculated as discussed in Chapter 5. For simplicity, the electron range was computed using Eq. (5.1) which is quite accurate for Si. Moreover, the calculation of the parameter σ , as given in Eq. (6.5), requires the value of the beam diameter. The value used was 20 nm beam diameter, or 10 nm beam radius.

The Bonard *et al.* model, on the hand, requires fitting Eqs. (6.10) and (6.11) into the data from the Monte Carlo simulation. In the fitting process of $k(x)$, the data was integrated along the z axis. On the other hand, in the fitting of $j(z)$, the data was integrated along the x axis. The linearized functions (Eqs. (6.12) and (6.13)) were fitted into the data. For Si with 3 keV beam energy and 10 nm beam radius, we obtained

$$\sigma_x = 5.7811 \times 10^{-2} \mu\text{m} \quad (6.16)$$

$$\sigma_z = 1.6077 \times 10^{-2} \mu\text{m} \quad (6.17)$$

These mathematical models were then convoluted with the charge collection probability to give the EBIC profile.

The computation for the EBIC profile was the same as that in Section 4.3.2. The EBIC profiles were computed as a convolution of the generation volume distribution with the charge collection probability. In other words, the EBIC profiles were computed from Eqs. (4.8) and (4.9), and with the corresponding generation volume models. The Matlab code is given in Appendix C.

The differences of the profiles near the depletion layer's edges were found to be easily analysed when they are plotted in their first or second derivatives with respect to the x axis. The first and the second derivatives were taken from the natural logarithmic of the EBIC profile. In the computation of the first derivative, we used

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} \quad (6.18)$$

where h is the distance between the points. This centred difference formula is second order accurate [88]. On the other hand, the second derivative was computed using a centred difference formula as follows

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \quad (6.19)$$

6.4 Results

Fig. 6.1 shows the EBIC profile in a semi-logarithmic plot. The differences among the models cannot be easily observed. Therefore, we need to analyse the first and the second derivative plots. They are given in Figs. 6.2 and 6.3. It can be seen that the profile of the Donolato Model is close to the Donolato-Venturi Model. On the other hand, Bonard *et al.* model is quite close to the Monte Carlo data, though some slight difference can be observed in the second derivative plot.

Another observation is that the profiles using the Donolato and the Donolato-Venturi models change more rapidly than the other two. This can be seen clearly from Fig. 6.2. A similar indication can also be seen in

Figure 6.1: EBIC profiles comparison. The beam energy is 3 keV and the beam radius is 10 nm.

Figure 6.2: First derivative EBIC profiles comparison. The beam energy is 3 keV and the beam radius is 10 nm.

Figure 6.3: Second derivative EBIC profiles comparison. Second derivative EBIC profiles comparison. The beam energy is 3 keV and the beam radius is 10 nm.

the second derivative plot (Fig. 6.3). The second derivative plots seem to show qualitatively the lateral dimension of the generation volumes.

6.5 Discussion

The results show that the Bonard *et al.* model gives a closer EBIC profile to the one from the Monte Carlo simulation. In the region around the edge of the depletion layer, Bonard *et al.* model changes less rapidly compared to the Donolato and the Donolato-Venturi models. The second derivative plots show that this could be due to the lateral dimension of the generation volume model.

We can also plot the contour of the energy ionization of the three models as well as the data from the Monte Carlo simulation. Fig. 6.4 shows the

Figure 6.4: Contours of generation volume in the x - z plane. (a) Distribution from Monte Carlo data, (b) the Donolato model, (c) the Bonard *et al.*, (d) the Donolato-Venturi model. The scales of x - z plane are in nm and the intensity is in eV.

contour of energy ionization among the models. It can be seen that the Donolato and the Donolato-Venturi model is very close to one another. The later has a slightly larger lateral dimension. These two, however, have a much smaller lateral dimension compared to the Monte Carlo. Bonard *et al.* model has about the same lateral dimension as the Monte Carlo. However, the contour of the Bonard *et al.* model seems to show some differences in the shape of its distribution compared to the Monte Carlo simulation.

The Monte Carlo distribution seems to drop rather fast as it moves away from the beam axis. The distribution then decreases slower. The Bonard *et al.*, on the hand, drops with an approximately constant rate. This can be seen from the gradation of the contour. The lateral size of the Bonard *et al.* model, however, is about the same as that of the Monte Carlo simulation.

The EBIC profiles also give this same conclusion. The profile using the Bonard *et al.* model fits better with the one from the Monte Carlo data. The second derivative plots (Fig. 6.3) also show that the Monte Carlo data has a higher peak and drops faster in the beginning. Since in this thesis, the model is used for EBIC profile analysis, we would choose the model that gives a better EBIC profile agreement with the EBIC profile obtained from the Monte Carlo data. In other words, we would choose the Bonard *et al.* model. The good agreement is, of course, due to the fitting from Monte Carlo simulations. However, an analytical expression is still a benefit. The Bonard *et al.* model gives this analytical expression.

It is interesting to note that, in the first derivative plot, all models intersect at the depletion layer's edge. Even though, they have different lateral dimensions, the three models have the same value at the depletion layer's

edge. This is confirmed by the plot of the second derivative. The minimum of all the models are located at the depletion layer's edge.

This gives some alternative ways to obtain a depletion layer's edge location. In other words, besides the technique developed in Chapter 4, we can also obtain the depletion layer's edges from the minimum of the second derivative plots, or the intersection points of the first derivative plots. The intersection point of the first derivative plots can be obtained only when the size of the generation volume differs. This can be obtained by changing the beam energy. The difficulty in using the minimum of the second derivative plots is that the EBIC measurement usually contains noise. And this noise is amplified in the first and in the second derivative plots. The approach of using the intersection of the first derivative is more probable. The measurement, however, must ensure that the size of the generation volume is still smaller than the width of the depletion layer. Due to scope limitation, these techniques cannot be investigated further in this thesis.

6.6 Conclusion

This chapter discussed the generation volume model to be used to compute the EBIC profile, particularly for region near to the collectors. A brief survey of the available generation volume model was given. Three pear-shape distribution models were then compared with respect to the data from the Monte Carlo simulation. The three distributions are the Donolato model, the Donolato-Venturi model, and the Bonard *et al.* model.

It was shown that the EBIC profile using the Bonard *et al.* model fits

well with the profile obtained from the Monte Carlo simulation. The plots of the contour show that this model has a lateral dimension of about the same as that obtained from the Monte Carlo data. The shape of the distribution, however, is slightly different. This difference can be observed clearly in the second derivative of the EBIC profile. The other two models' lateral dimensions are smaller than the one from the Monte Carlo data. This gives a more rapid change in the first derivative plots. Therefore, since the Bonard *et al.* model gives a better EBIC profile agreement, we choose to use it for the EBIC profile computation in this thesis.

The first and second derivative plots also open up the possibilities of obtaining the edges of the depletion layer. It was qualitatively shown that the minimum of the second derivative plot is located at the depletion layer's edge. Moreover, when the size of the generation volume varies, the plots of the first derivative intersect at the depletion layer's edge. The analysis and validation of these alternative techniques are beyond the scope of the current thesis.

Chapter 7

Generalized Diffusion Length Measurement Technique from Any Values of Junction Depths

7.1 Introduction

The previous chapters deal with analysis on the EBIC technique for the conventional collector configurations with semi-infinite dimension. In this chapter, we are interested in generalizing the available technique to be used for extracting diffusion lengths from any values of junction depth. Thus, vertical dimension of the collector is no longer assumed to be infinitely large. Moreover, a new boundary condition is introduced by the horizontal part of the junction well.

One of the most commonly used configurations for diffusion length measurements is the normal-collector configuration (Fig. 7.1). The induced

Figure 7.1: Normal-collector configuration.

current was derived in [25, 38] for the case of zero surface recombination velocity as

$$I = k \exp(-x/L) \quad (7.1)$$

Taking the natural logarithm of the above equation gives

$$\ln(I) = \ln k - \frac{x}{L} \quad (7.2)$$

It is shown in Eq. (7.1) that the minority carrier diffusion length can be determined from the negative reciprocal of the slope. This equation, however, is only valid for the zero surface recombination velocity. For an infinite surface recombination velocity, Berz and Kuiken gave the induced current as follows [38].

$$I = kx^{-0.5} \exp(-x/L) \quad (7.3)$$

And taking the natural logarithm to give

$$\ln \left(\frac{I}{x^{-0.5}} \right) = \ln k - \frac{x}{L} \quad (7.4)$$

This equation is only valid for very large surface recombination velocities. Some sample preparations must be done to ensure the recombination at the surface to be very large. Ong *et al.* [36] generalized Eqs. (7.1) and (7.3) to make the method applicable for any values of surface recombination velocities by introducing the following empirical equation.

$$I = kx^\alpha \exp(-x/L) \quad (7.5)$$

Taking the natural logarithm gives

$$\ln \left(\frac{I}{x^\alpha} \right) = \ln k - \frac{x}{L} \quad (7.6)$$

where α (alpha) is a fitting parameter. The range of values for the fitting parameter alpha is from 0 to -0.5 depending on the actual values of the surface recombination velocities. This method was found to be applicable to the planar-collector configuration as well, but with a different range of the alpha parameter values [58].

In practice, however, a p-n junction is normally fabricated as a diffused junction. This is especially so for planar devices. This configuration is shown in Fig. 7.2. In this configuration, the junction has a finite depth, and therefore, another boundary condition must be introduced to take into account the collection of carriers at the bottom of the junction. The literature review has been given in Section 1.3.4.

This chapter proposes a method of extracting the diffusion lengths accurately from any values of the junction depths and surface recombination

Figure 7.2: EBIC measurement in a diffused junction.

velocities. It will be shown later that Eq. (7.5) can be generalized to take into account the junction depths of the collector. Thus, a simple and accurate method of extracting the diffusion lengths can be obtained for diffused junctions. This method can be used with any values of the junction depths and surface recombination velocities.

7.2 Theory

7.2.1 Boundary Conditions

It was shown in [36] that the diffusion lengths can be extracted accurately from a normal-collector configuration for any values of surface recombination velocities. The diffusion lengths are obtained from the negative reciprocal slope of Eq. (7.6). Comparing Fig. 7.1 with Fig. 7.2, the normal-collector configuration can be thought of as a diffused junction with an infinite junc-

tion depth.

For this infinite junction depth, the steady-state diffusion equation must satisfy at least two boundary conditions [48]

$$q = 0 \text{ at } x = 0 \quad (7.7)$$

$$\frac{dq}{dz} = sq \text{ at } z = 0 \quad (7.8)$$

where q is the minority carrier concentration, and $s = v_s/D$ is the surface recombination velocity. The x axis is taken from the junction, and the z axis is taken from the top surface.

The first boundary condition comes from the fact that the built-in electric field at the collecting junction sweeps away all minority carriers reaching the junction. The second boundary condition is simply from the definition of the surface recombination velocity. The minority carriers recombine at the surface. In this case, the concentration gradient of the minority carriers at the surface is proportional to the surface recombination velocity as well as the concentration at that surface.

For the case of a finite junction depth, another boundary condition must be introduced to take into account the collection at the bottom of the junction. This is given by

$$q = 0 \text{ at } z = h \text{ and } x < 0 \quad (7.9)$$

where h is the depth of the junction, and $x < 0$ is used to indicate the location of the diffused junction in Fig. 7.2.

Figure 7.3: Planar-collector configuration.

Before we can modify Eq. (7.5) to take into account the finite junction depth, it is useful to study the case when the junction depth is very small and close to the surface. In this case, the boundary condition can be written as

$$q = 0 \text{ at } z \approx 0 \text{ and } x < 0 \quad (7.10)$$

The above condition is the same as the boundary condition of a planar-collector configuration (Fig. 7.3) where the Schottky barrier is located at the surface ($z = 0$ and $x < 0$) [53, 54].

Therefore, it can be concluded at this point in time that the infinite junction depth has the same boundary condition as the normal-collector configuration, while the shallow junction depth has the same boundary condition as the planar-collector configuration.

It is important to note that Eq. (7.5) holds true for both configurations,

that is for the normal-collector [36] as well as the planar-collector configuration [58]. In the case of the normal-collector, the alpha parameter ranges from 0 to -0.5. On the other hand, the alpha parameter ranges from -0.5 to -1.5 for the case of the planar-collector configuration. In both configurations, the alpha parameter is a function of the surface recombination velocity, the normalized beam distance from the collector, and the normalized depth of the generation volume. The dependence of the alpha parameter on these three factors has been given in Chapter 3 and [135].

7.2.2 Generalized Model

The finite junction depth can be taken into account in Eq. (7.5) by rewriting it as

$$I = k_1 x^\gamma \exp(-x/L) \quad (7.11)$$

where γ (gamma) and k_1 are the new fitting parameters replacing the alpha parameter and the constant k in Eq. (7.5). The change of symbol is intended to indicate that the new parameters are also affected by the depth of the junction. In other words, the parameter gamma is a function of the alpha parameter as well as the depth of the junction, i.e. $\gamma = f(\alpha, h)$.

The values of the gamma parameter can be estimated easily for the case of the zero surface recombination velocity. Comparing with the normal-collector configuration, it can be expected that the value is close to zero for the infinite junction depth. On the other hand, comparing with the planar-collector configuration, the value can be expected to be about -0.5 for the case of a very shallow junction depth. By comparing the gamma parameter

with the alpha parameter in Eq. (7.5), it is expected that the effect of the surface recombination velocity is to make the gamma values more negative [59]. Therefore, the following equation can be fitted into the EBIC data in order to extract the diffusion lengths.

$$\ln \left(\frac{I}{x^\gamma} \right) = \ln k_1 - \frac{x}{L} \quad (7.12)$$

7.2.3 Physical Explanation

The physics behind Eq. (7.11) can be explained as follows. For simplicity, the case of zero surface recombination velocity will be considered first. The case for finite surface recombination velocities can be easily explained after that.

When the junction depth is very large, the configuration simplifies to that of the normal-collector configuration, and the gamma values are close to zero. Substituting gamma equals to zero into Eq. (7.12) results in (7.2). The logarithmic plot of the induced current is a straight line with a slope of $-1/L$.

The induced current given in Eq. (7.2) will be reduced due to either recombination at the surface or, for the case of the finite junction depth, to more recombinations of carriers as they diffuse further to the bottom part of the junction. As the junction depth reduces, more carriers diffuse to the bottom part of the junction instead of being collected at the vertical part. Since the distance to reach the bottom part of the junction is longer than the vertical junction, more recombinations take place. Thus, the induced current is reduced.

This reduction in the induced current causes the profile to be no longer exponential. The logarithmic plot is no longer a straight line but rather concave upward and is below the straight line given by Eq. (7.2). It will be shown later that Eq. (7.12) fits well with this concave curve. In this equation, the parameter γ determines how concave the curve is. This is the same as the case for the α parameter [135].

In summary, as the junction depth reduces, more recombinations take place before being collected at the bottom part of the junction. Thus, the induced current decreases, and the logarithmic plot is concave upward. This results in the γ parameter being more negative. The effect of finite surface recombination velocities is to reduce the induced current even further, and therefore, the γ parameter is expected to be more negative when the recombination at the surface is present.

The assumption used in developing the model follows [84] and [85]. First, it is assumed that the diffused junction has a sharp corner. In other words, the diffused junction has a geometry of an L-shape. Second, the diffused junction is assumed to be isolated. This means that there are no competing junctions near the beam positions. The last assumption also implies that the ohmic contact locations are far enough from the beam positions so as not to affect the induced current profile.

7.3 Verification

The verification of theories of this nature has traditionally been done by experimental means. However, there are some drawbacks with this method.

The first is that there is a question of how accurate the fabrication process is able to control the parameters of the material. The second is the magnitude of errors, which might be introduced into the experiment. The third and the most significant drawback is that there is a limit to which the material parameters can be varied.

To overcome these drawbacks, a two-dimensional (2-D) computer simulation, MEDICI, was used to verify the proposed method. The device structure was created according to the configuration shown in Fig. 7.2. An abrupt junction with a sharp edge was used in the simulation. A fine grid of $0.1 \mu\text{m}$ was used along the surface as well as at the junction. This is to accommodate accurate computations for minority carriers recombining at the surface as well as those collected at the junction.

The generation volume implemented in the MEDICI is an extended generation volume, which is the same as the one used in [63]. The beam energy was set to 8 keV. This value results in a $0.75 \mu\text{m}$ electron penetration range (R) with a centre of mass ($\bar{z}$) at $0.31 \mu\text{m}$ from the surface. The beam current was set to 1.5 nA following [63] and the generation rate was computed as shown in Appendix D.6. The detail for implementing the extended generation volume in MEDICI can also be found in Appendix D.6.

The minority carrier diffusion lengths were set to $3 \mu\text{m}$ for both the p and n regions. The minority carrier diffusion lengths were set by specifying the carrier lifetimes. The values of the carrier lifetime were calculated from

$$\tau = L^2/D \tag{7.13}$$

where L is the minority carrier diffusion length in centimeters, and D is the

diffusivity in square centimeters per second. The diffusivity in the simulation depends on the doping concentration. A uniform doping concentration of $1 \times 10^{18} \text{ cm}^{-3}$ for both p and n regions were specified. Specifying the lifetime affects the Shockley-Read-Hall recombination, which in turn affects the carrier-concentration distribution inside of the device. Once the carrier concentration is known, the device simulator will compute the corresponding current density. The details of the implementation of the generation volume, the setting of the minority carrier diffusion-length value, as well as the EBIC simulation using MEDICI can be found in [63], [91], and Appendix D.

The first set of the simulations dealt with zero surface recombination velocity. The variable that was varied was the depth of the junction. The values of the junction depth (h) were chosen to be the same as those in [85]. The h/z ratios are 200, 100, 25, 20, 15, 10, 5, 2, 1, and 0. For the last ratio, the simulation used $h/z = 0.3$ to approximate zero ratio.

The line scans were done at the region outside of the diffused junction. This means that the extracted diffusion length is for the minority carrier electron. The scanning range started from $x/L = 2$ and ended at $x/L = 11$ to satisfy the requirement given in Chapter 3 or in [135]. Eq. (7.11) was fitted into the data from each line scan using linear regression theory described in Chapter 2. The fitting process gave the gamma parameter.

The second set of simulations used the same structures and varied the surface recombination velocities from 10 to $1 \times 10^7 \text{ cm}^2/\text{s}$. There were eight different surface recombination velocity values used in the simulations. The same procedure was applied to obtain the diffusion lengths for the data in the second set.

Figure 7.4: EBIC profile for the case of $h/z = 10$ and zero surface recombination velocity.

7.4 Results

An example of the semi-logarithmic plot of the induced current is shown in Fig. 7.4. The maximum peak indicates the location of the vertical junction. The sudden changes at the two ends of the profile are caused by the ohmic contacts. The minority carrier diffusion length for the p region is obtained by fitting Eq. (7.11) into the profile at the right hand side of the junction.

Table 7.1 shows the extracted diffusion lengths for different junction depths for the case of zero surface recombination velocity. The extracted diffusion lengths have a maximum error of about 3%. For very large junction depths, the gamma values are close to zero. The values become more negative as the junction depths decrease.

Table 7.1: Extracted Diffusion Lengths for Any Values of Junction Depths with Zero Surface Recombination Velocity.

h/z	Extracted L (μm)	Error (%)	γ
200	3.005	0.17	-0.0118
100	3.055	1.83	-0.0501
25	2.909	-3.03	-0.0567
20	2.917	-2.77	-0.1251
15	2.934	-2.20	-0.2148
10	2.952	-1.60	-0.2958
5	2.969	-1.03	-0.3655
2	2.975	-0.83	-0.3876
1	2.976	-0.80	-0.3883
≈ 0	2.975	-0.83	-0.3850

Figure 7.5: Errors for various values of normalized surface recombination velocities ($S = v_s L/D$) and junction depths.

Figure 7.6: Gamma-parameter variation with the surface recombination velocity for $h/z = 10$.

The errors are slightly increased when the surface recombination velocity is taken into account. For any surface recombination velocities, the maximum error for the extracted diffusion lengths is about 7%. This is shown in Fig. 7.5. The gamma values become more negative as the surface recombination velocities increase for a fixed value of junction depth. This can be seen from Fig. 7.6.

The maximum errors for both the zero and the finite surface recombination velocities were found to be around $h/z = 25$. This was found to be due to the mesh in the simulation. When the junction is located around $h/z = 25$, the meshing of the simulation faced difficulty in putting fine grid spacing around the junction as well as at the top surface within the available given nodes. Figs 7.7 and 7.8 show the simulation grid for $h/z = 10$ and

Figure 7.7: MEDICI structure for $h/z = 10$. The green region is an n-type and the yellow region is a p-type.

Figure 7.8: MEDICI structure for $h/z = 25$. The green region is an n-type and the yellow region is a p-type.

$h/z = 25$ respectively. It can be seen that the grid is rather sparse for the case of $h/z = 25$.

7.5 Discussion

The shape of the EBIC profile shown in Fig. 7.4 is similar to the experimental results in [136] and the theoretical calculation in [85]. Inside the diffused junction, the EBIC profile is limited by the current collected at the horizontal junction, which is a near horizontal line in Fig. 7.4. The peak at $45\text{ }\mu\text{m}$ shows the maximum collection at the vertical junction. Outside the diffused junction, the profile behaves as described in the theory and in [85].

The results show that the minority carrier diffusion lengths can be extracted for any values of junction depths and surface recombination velocities. The accuracy of the method was proven to be reasonably high for the given diffusion length value.

The results in Table 7.1 suggest that the fitting-parameter γ depends on the depth of the junction. The values of the γ parameter become more negative as the junction depths decrease. This result agrees with the theory. This is because more recombinations occur before reaching the bottom part of the junction. Thus, the induced current reduces, and the semi-logarithmic plot of the profile becomes more concave. A more concave plot results in a more negative γ value.

The value of the γ parameter for a very large h/z ratio is close to zero. In this case, the configuration is similar to a normal-collector configuration. On the other hand, the γ value is around -0.4 for the case

Figure 7.9: Gamma values as functions of junction depths and surface recombination velocities.

of a very small h/z ratio. In this case, the configuration is more similar to the planar-collector configuration. Thus, the gamma values can be used to approximate the depth of the junction.

Besides being a function of the junction depth, the gamma parameter is also a function of the alpha parameter, which depends on the surface recombination velocity. For a given junction depth, the variation in the gamma values with respect to the surface recombination velocities follows that of the alpha parameter in [36, 59, 135].

Fig. 7.9 shows the gamma values as a function of the h/z and S . The plot is logarithmic in the x and y axis. It can be seen that the shape in both the x and the y axis follows a sigmoidal distribution. The minimum value is around -1.4, which is obtained when the junction depth is very shallow and the surface recombination velocity is very large. On the other hand, the

maximum is around 0, which is obtained when the junction depth is very large and the surface recombination velocity is very small.

7.6 Conclusion

This chapter provides a generalized method of extracting the minority carrier diffusion lengths from a diffused junction. It has been shown that the proposed method is able to extract the diffusion lengths accurately for any values of junction depths and surface recombination velocities.

A fitting parameter, called the gamma parameter, was used to take into account the depth of the junction. The gamma parameter is a function of the alpha parameter, which depends on the surface recombination velocity, as well as the depth of the junction.

The gamma values become more negative as the junction depth decreases. At a fixed junction depths, the gamma value decrease as the surface recombination velocity increases. The physical explanation for the variation in the gamma values due to the junction depth and the surface recombination velocity was discussed. A more detailed study of how the alpha parameter and the junction depth affect the gamma values should be done in the future.

Chapter 8

Charge Collection from within a Junction Well

8.1 Introduction

This chapter derives analytical expressions for the charge collection profiles due to the bombardment of electron beams for the case of an L-shaped and a U-shaped collectors. The vast applications of EBIC have arisen from the availability of the analytical equations of the EBIC profile. The two most commonly used collector configurations for the EBIC measurements are the normal-collector configuration and the planar-collector configuration (Fig. 8.1). For these two configurations, analytical expressions for the EBIC profiles are available in the literature.

In planar technology, many devices are fabricated with finite p-n junction depths as shown in Figs. 8.2 and 8.3. Therefore, when one uses the available expressions from the normal-collector or the planar-collector configurations,

Figure 8.1: (a) The normal-collector configuration, and (b) the planar-collector configuration.

Figure 8.2: L-shape geometry of a diffused junction.

Figure 8.3: U-shape geometry of a diffused junction.

some assumptions must be made. For example when one uses the expression for the normal-collector configuration, the junction is assumed to be infinitely deep and the generation source is located near to the surface. Similarly, when one uses the expression for the planar-collector configuration, the junction is assumed to be very narrow.

Several works have been done to study the charge collection from a finite junction depth (Section 1.3.4). A thorough analysis of the EBIC profile from a sharp L-shape geometry was done by Soukup and Ekstrand [85]. The analytical expressions were derived for collections from both the inside and outside of the junction well. The expressions, however, involve non-elementary functions such as the Bessel functions. The previous chapter discussed the case when the beam scans outside of the junction well. This chapter deals with the case when the beam scans within the junction well. It will be shown later that EBIC expressions containing only elementary functions can be found for the case when the beam scans inside of the junction well.

The EBIC expression provided by Soukup and Ekstrand is valid when the collections occur at two collecting junctions. They are the horizontal and the vertical junctions as shown in Fig. 8.2. For this case, the width of the collecting region was assumed to be infinitely wide. In other words, the charge collection by the horizontal junction is from zero to infinity. In today's devices, most junctions have a finite width. Moreover, the shape of the junction is no longer L-shaped, but rather, a U-shaped as shown in Fig. 8.3. Currently, we have not found any EBIC expressions available for the case of finite width and finite junction depth collection. The availability of an

analytical expression would help to enhance the study of charge collection in today's devices where the dimensions of the junction can no longer be assumed to be infinite.

The present chapter provides the analytical EBIC expressions when the generation source is located *within* the well region. Two cases will be considered: the L-shaped geometry junction, and the U-shaped geometry junction. The effects of certain parameters, such as the junction depth, the junction width, diffusion lengths, as well as the depth of the generation source will be analysed.

8.2 Derivations

We will first derive the analytical expression for the case of the L-shape geometry. The Green's function method is used for this purpose. The expression for the case of the U-shape geometry will similarly be derived using the Green's function. For the case of the U-shape geometry, we start the derivation in a slightly different manner, by applying the reciprocity theorem [137–139].

8.2.1 Expression for the L-shape Geometry

Let us formulate the mathematical problem for a point generation source EBIC expression. The expression for the EBIC profile is simply the convolution of the point generation source expression with the generation volume distribution.

For the L-shape geometry, the current collected from the two sides of the

junction can be written as [48]

$$Q(x', z') = D \left\{ \int_0^h \frac{\partial G(x, z|x', z')}{\partial x} \Big|_{x=0} dz - \int_0^d \frac{\partial G(x, z|x', z')}{\partial z} \Big|_{z=h} dx \right\} \quad (8.1)$$

where D is the diffusion constant, G is the Green's function of the problem, h is the junction depth, and d is the junction width. This expression simply means that the charge collection current due to a point source located at (x', z') is the sum of the integration of the concentration gradient at the two sides of the junction. The Green's function of the problem is also the solution of the minority carrier concentration due to a point source. The minority carrier concentration profile must satisfies the continuity equation, which in 2-D can be written as [140]

$$\frac{\partial^2 q(x, z)}{\partial x^2} + \frac{\partial^2 q(x, z)}{\partial z^2} - \lambda^2 q(x, z) = -\frac{h(x - x', z - z')}{D} \quad (8.2)$$

where q is the concentration of the minority charge carrier, which in this case is assumed to be holes. In the above equation, $\lambda = 1/L = 1/\sqrt{D\tau}$, where L is the diffusion length and is related to the lifetime τ as given. The right hand side term, $h(x, z)$, is the projection of the generation volume distribution onto the $x - z$ plane. According to the theory, the Green's function also satisfies the continuity equation [141]. However, the source is a delta function located at (x', z') . Therefore, the Green's function is basically the solution of the carrier concentration due to a point source located at (x', z') . This can be written as

$$\begin{aligned} \frac{\partial^2 G(x, z|x', z')}{\partial x^2} + \frac{\partial^2 G(x, z|x', z')}{\partial z^2} \\ - \lambda^2 G(x, z|x', z') = -\frac{\delta(x - x')\delta(z - z')}{D} \end{aligned} \quad (8.3)$$

The Green's function must also satisfy the same boundary conditions as that of the concentration q . For simplicity, we assume that the boundary at $x = d$ satisfies the Neumann boundary condition. In other words, the boundary acts so as to make the concentration gradient at that boundary equals to zero. These same boundary conditions are valid for the case when the surface has zero surface recombination velocity. Furthermore, we assume that the ohmic contact at the top surface spans throughout the well without short circuiting the p-n junction. This simplification allows us to use a homogenous boundary condition at the top surface. Then, the concentration is assumed to be zero at the junction. This means that all minority carriers arriving at the junction are assumed to be collected and transported to the other side. Therefore, we can write the boundary conditions for the Green's function as follows.

$$G = 0, \text{ for } x = 0 \text{ and } 0 \leq z \leq h \quad (8.4)$$

$$\frac{\partial G}{\partial x} = 0, \text{ for } x = d \text{ and } 0 \leq z \leq h \quad (8.5)$$

$$G = 0, \text{ for } z = 0 \text{ and } 0 \leq x \leq d \quad (8.6)$$

$$G = 0, \text{ for } z = h \text{ and } 0 \leq x \leq d \quad (8.7)$$

The details of the calculation of the Green's function are given in Appendix B. In this chapter, only the end result is presented. The solution is given in Eqs. (B.18) and (B.19), i.e.

$$G_I(x, z|x', z') \quad (8.8)$$

$$= \sum_{n=1,3,5,\dots}^{\infty} \frac{2 \sin(p_n x)}{d D \mu_n h \sinh(\mu_n h)} \sinh(\mu_n (h - z')) \sin(p_n x) \sinh(\mu_n z)$$

$$G_{II}(x, z|x', z') \quad (8.9)$$

$$= \sum_{n=1,3,5,\dots}^{\infty} \frac{2 \sin(p_n x)}{d D \mu_n h \sinh(\mu_n h)} \sinh(\mu_n z') \sin(p_n x) \sinh(\mu_n (h - z))$$

where $G_I(x, z|x', z')$ and $G_{II}(x, z|x', z')$ are the Green's functions for region I and II respectively. Region I is the case of $0 \leq z \leq z'$, and region II is $z' \leq z \leq h$, and $n = 1, 3, 5, \dots$ to infinity. In the above expressions,

$$p_n = \frac{n\pi}{2d} \quad (8.10)$$

$$\mu_n = (p_n^2 + \lambda^2)^{1/2} \quad (8.11)$$

Eqs. (8.8) and (8.9) can then be substituted into Eq. (8.1) to give the EBIC profile for the point generation source in the L-shape geometry. The result is shown below.

$$\begin{aligned} Q(x', z') &= \sum_n^{\infty} \frac{2 \sin(p_n x')}{d \sinh(\mu_n h)} \left\{ \frac{p_n}{\mu_n^2} [\sinh(\mu_n (h - z')) (\cosh(\mu_n z') - 1) \right. \\ &\quad \left. + \sinh(\mu_n z') (\cosh(\mu_n (h - z')) - 1)] - \frac{\sinh(\mu_n z')}{p_n} \right\} \end{aligned} \quad (8.12)$$

It can be seen that the expression contains only elementary functions. The above equation can be computed numerically to give the charge collection profile for the case where the beam scans inside of the junction well.

8.2.2 Expression for the U-shape Geometry

To derive the EBIC profile for this U-shape geometry, we begin by utilizing the reciprocity theorem [137–139]. The previous approach starts from the continuity equation of the carrier concentration (i.e. q). The charge collection probability expression is then obtained from the integration of the concentration gradient (i.e. gradient of G) along the collectors. According to the reciprocity theorem, the solution for the charge collection probability expression can be obtained from the continuity equation of the charge collection probability itself (i.e. Q). Therefore, the expression for the carrier concentration need not be obtained. This theorem states that the charge collection current also satisfies the *homogeneous* continuity equation, that is

$$\frac{\partial^2 Q(x', z')}{\partial x^2} + \frac{\partial^2 Q(x', z')}{\partial z^2} - \lambda^2 Q(x', z') = 0 \quad (8.13)$$

and for the case of U-shape geometry, it also satisfies the following boundary conditions

$$Q = 1, \text{ for } x = 0 \text{ and } 0 \leq z \leq h \quad (8.14)$$

$$Q = 1, \text{ for } x = d \text{ and } 0 \leq z \leq h \quad (8.15)$$

$$Q = 0, \text{ for } z = 0 \text{ and } 0 \leq x \leq d \quad (8.16)$$

$$Q = 1, \text{ for } z = h \text{ and } 0 \leq x \leq d \quad (8.17)$$

These conditions are obvious from the physical configuration. When the beam is located at the ohmic contact, the collection is zero (8.16). On the other hand, when the beam is located at the three junction sides, the collection is unity. Solving Eq. (8.13) gives the expression for the charge collection for the case of the U-shape geometry. Therefore, the expression for the minority carrier need not be computed beforehand as in the previous case. This theorem simplifies the derivation of the charge collection profile for certain geometries.

However, in this thesis, we use the method of Green's function and so indirectly prove that the solution is the same as when we derived the expression starting from the continuity equation for the minority carrier concentration, which is the case of the L-shape geometry. It was shown in [140] that the solution of the homogeneous problem with the inhomogeneous boundary conditions, such as what we have, can be expressed as

$$Q(x', z') = \oint Q_s \frac{\partial G}{\partial \mathbf{n}} \cdot d\mathbf{A} \quad (8.18)$$

where Q_s is the value at the surface, and the gradient of G is outward normal to the surface. This expression means that the current collected is simply obtained by multiplying the charge collection at the boundary with the gradient of the Green's function in the direction normal to the boundary. In this case, the Green's function also satisfies the homogeneous continuity equation, that is

$$\frac{\partial^2 G(x, z|x', z')}{\partial x^2} + \frac{\partial^2 G(x, z|x', z')}{\partial z^2} - \lambda^2 G(x, z|x', z') = 0 \quad (8.19)$$

and homogeneous boundary conditions

$$G = 0, \text{ for } x = 0 \text{ and } 0 \leq z \leq h \quad (8.20)$$

$$G = 0, \text{ for } x = d \text{ and } 0 \leq z \leq h \quad (8.21)$$

$$G = 0, \text{ for } z = 0 \text{ and } 0 \leq x \leq d \quad (8.22)$$

$$G = 0, \text{ for } z = h \text{ and } 0 \leq x \leq d \quad (8.23)$$

A similar Green's function as that for the L-shape geometry can be obtained for the case of the U-shape geometry. It can be seen that only one boundary condition changes from the previous case (compare with boundary conditions (8.4) to (8.7), particularly compare (8.5) with (8.21)). And to satisfy this new boundary condition, the same function $\sin(p_n x)$ (refer to (B.4)) can be used to satisfy the two boundaries at $x = 0$ and $x = d$. However, the eigenvalues must now change to satisfy $G = 0$ at $x = d$, or in other words, $\sin(p_n x) = 0$, and therefore,

$$p_n = \frac{n\pi}{d} \quad (8.24)$$

where $n = 1, 2, 3, \dots$ to infinity. Thus, the Green's function satisfying Eq. (8.19) and boundary conditions (8.4) to (8.7). is

$$G_I(x, z|x', z') \quad (8.25)$$

$$= \sum_n \frac{2 \sin(p_n x)}{d \mu_n h \sinh(\mu_n h)} \sinh(\mu_n (h - z')) \sin(p_n x) \sinh(\mu_n z)$$

$$G_{II}(x, z|x', z') \quad (8.26)$$

$$= \sum_n \frac{2 \sin(p_n x)}{d \mu_n h \sinh(\mu_n h)} \sinh(\mu_n z') \sin(p_n x) \sinh(\mu_n (h - z))$$

By using the values of the boundary conditions (8.14) to (8.17), Eq. (8.18) can be expanded into

$$\begin{aligned}
 Q(x', z') &= \left\{ \int_0^h \frac{\partial G(x, z|x', z')}{\partial x} \Big|_{x=0} dz - \int_0^d \frac{\partial G(x, z|x', z')}{\partial z} \Big|_{z=h} dx \right. \\
 &\quad \left. - \int_0^h \frac{\partial G(x, z|x', z')}{\partial x} \Big|_{x=d} dz \right\} \quad (8.27)
 \end{aligned}$$

which is similar to Eq. (8.1), but with an additional collecting junction term. Note also that if we compare Eqs. (8.25) and (8.26) with Eqs. (8.8) and (8.9), the diffusivity term D is missing from the nominators of (8.25) and (8.26). This is because the Green's function satisfies the homogeneous equation (8.19). The solution, however, still gives the correct answer because the term D also does not appear in Eq. (8.27). In the previous solution, the D term cancels out. Thus, the reciprocity theorem is shown to be valid. Substituting the Green's function into Eq. (8.27) gives

$$\begin{aligned}
 Q(x', z') &= \sum_{n=1}^{\infty} \frac{2 \sin(p_n x') (1 - (-1)^n)}{d \sinh(\mu_n h)} \left\{ \frac{p_n}{\mu_n^2} [\sinh(\mu_n (h - z')) (\cosh(\mu_n z') - 1) \right. \\
 &\quad \left. + \sinh(\mu_n z') (\cosh(\mu_n (h - z')) - 1)] + \frac{\sinh(\mu_n z')}{p_n} \right\} \quad (8.28)
 \end{aligned}$$

This expression can be evaluated numerically to give the charge collection due to a point source for the case of the U-shape geometry.

Eqs. (8.12) and (8.28) give the profile for a point generation source. In reality, the generation of ehps usually occurs in a finite volume. In this case, the expression for the point source must be convoluted with the distribution of the generation volume.

$$I_N(x', z/R) = \int \int Q(x, z) h(x - x', z/R) dx dz \quad (8.29)$$

where $h(x - x', z/R)$ is the distribution of the generation volume in the x-z plane. This function is also a function of the electron penetration range R , which is determined by the beam energy. The common models for this generation volume usually involve the Gaussian distribution. Discussion on these models has been given in Chapter 6.

8.3 Computation

8.3.1 Numerical Computation

In order to investigate the effects of certain parameters on the EBIC profile, Eqs. (8.12) and (8.28) were evaluated numerically. For the L-shape geometry, the following parameters were investigated: the junction depth (h), the diffusion lengths (L), and the centre of mass of the generation source (z). The profile was computed from $x = 0$ to $x = d$. Since the boundary at $x = d$ is Neumann boundary condition, the effect of the width of the well (d) is not significant. For the case of the U-shape geometry, however, the parameter d was also varied to investigate its effect on the profile.

The junction depth h was set to 1 μm , 3 μm , and 5 μm . The diffusion length L was varied from 2 μm to 7 μm . The values for the depth of the

junction z were 0.3, 0.6, 0.9, 1.2, and 1.5 μm . For the U-shape geometry, additional simulations for the width of the well were done. The widths had values 5, 7, and 9 μm . The Matlab codes for the U-shaped junction well computation can be found in Appendix C.6.

8.3.2 MEDICI Simulations

The computation results from the analytical equation derived in the previous section were verified using the MEDICI 2-D device simulator. The reason for using a simulator is that the parameters investigated can be varied in a precise manner. Structures as shown in Figs. 8.2 and 8.3 were constructed with a fine grid of 0.1 μm located at the junction, the region of the generation source, and regions near the contacts. The doping was uniform for both regions and was set at $1 \times 10^{18} \text{ cm}^{-3}$. The lifetime was set to give the appropriate values of diffusion lengths. In order to approximate a point source generation source, the simulator used a square generation source with 0.2 μm on each side. It has been shown in [91] that this geometry can be used to approximate a round generation source with a radius of 0.1 μm . The generation rate within this area was uniform and was set to 5.22×10^{23} carriers/ cm^3 . The value was calculated using 1.5 nA beam current [63]. The detail implementation in MEDICI can be found in Appendix D.

8.4 Results

Figs. 8.4 to 8.6 show the results for the L-shape geometry, and Figs. 8.7 to 8.10 show the results for the U-shape geometry. The shape of the profile is

Figure 8.4: Effect of junction depth on the EBIC profile for collection from within the L-shape geometry junction. The lines are computed from the analytical equation while the points are from the MEDICI simulation. The parameters are: $L = 5 \mu\text{m}$, $z = 0.3 \mu\text{m}$, $d = 5 \mu\text{m}$.

the same as the experimental results found in [136]. It can also be seen that the results computed from the analytical equation agree with the results from the MEDICI simulator. Figs. 8.11 to 8.13 gives the absolute difference between EBIC profile obtained from MEDICI simulator and that from the analytical equations (we did not show the error for variation in d , since similar conclusion can be obtained from the other three figures). We see that the difference is maximum when it is near the vertical junction. However, the maximum differences are all less than 0.16.

The accuracy seems to be affected by the number of n terms that are summed up in the Eqs. (8.12) and (8.28). In Fig. 8.5 and 8.8, where the plot is in natural logarithmic, the plots from the analytical equation for the case of small diffusion lengths look slightly oscillatory. The cause seems to

Figure 8.5: Effect of diffusion length on the EBIC profile for collection from within the L-shape geometry junction. The lines are computed from the analytical equation while the points are from the MEDICI simulation. The parameters are: $h = 5 \mu\text{m}$, $z = 0.3 \mu\text{m}$, $d = 5 \mu\text{m}$.

Figure 8.6: Effect of the depth of the generation source on the EBIC profile for collection from within the L-shape geometry junction. The lines are computed from the analytical equation while the points are from the MEDICI simulation. The parameters are: $L = 5 \mu\text{m}$, $h = 5 \mu\text{m}$, $d = 5 \mu\text{m}$.

Figure 8.7: Effect of junction depth on the EBIC profile for collection from within the U-shape geometry junction. The lines are computed from the analytical equation while the points are from the MEDICI simulation. The parameters are: $L = 5 \mu\text{m}$, $z = 0.3 \mu\text{m}$, $d = 5 \mu\text{m}$.

Figure 8.8: Effect of diffusion length on the EBIC profile for collection from within the U-shape geometry junction. The lines are computed from the analytical equation while the points are from the MEDICI simulation. The parameters are: $h = 5 \mu\text{m}$, $z = 0.3 \mu\text{m}$, $d = 5 \mu\text{m}$.

Figure 8.9: Effect of the depth of the generation source on the EBIC profile for collection from within the U-shape geometry junction. The lines are computed from the analytical equation while the points are from the MEDICI simulation. The parameters are: $L = 5 \mu\text{m}$, $h = 5 \mu\text{m}$, $d = 5 \mu\text{m}$.

Figure 8.10: Effect of the width of the junction on the EBIC profile for collection from within the U-shape geometry junction. The lines are computed from the analytical equation while the points are from the MEDICI simulation. The parameters are: $L = 5 \mu\text{m}$, $z = 0.3 \mu\text{m}$, $h = 5 \mu\text{m}$.

Figure 8.11: Absolute difference between EBIC profile from MEDICI simulation and analytical equations when varying the depth of junction.

Figure 8.12: Absolute difference between EBIC profile from MEDICI simulation and analytical equations when varying the diffusion length of the material.

Figure 8.13: Absolute difference between EBIC profile from MEDICI simulation and analytical equations when varying the depth of the generation volume.

come from the denominator term $\sinh(\mu_n h)$, which tend to go to infinity. This causes the series to converge prematurely. As the value of the diffusion length is reduced, the term λ and, therefore, μ_n increases. For large values of h and μ_n , the hyperbolic sine term would go to infinity very quickly and, therefore, for a given precision, the number of the n terms that can be summed up will be limited. This accuracy can be improved by using higher precisions in the computation.

Another observations is that in Figs. 8.6 and 8.9, for the case of $h = 1 \mu\text{m}$, the computed results from the analytical equation is rather low compared to the results from the MEDICI simulator. This could be due to the effect of the finite generation source in MEDICI. This effect is more pronounced when the generation source is near the collecting junction. The generation source in MEDICI has a dimension of $0.2 \mu\text{m}$, and therefore, is

comparable to the value of h .

The finite generation volume in MEDICI causes a shift in the centre of mass of the generation source which is supposed to represent a point generation source. In order to explain this, let us consider the EBIC value at x distance away from the vertical collectors. In this consideration, it is assumed that the contribution due to the vertical junctions are negligible. According to [48], the collection can be approximated as

$$Q(z') \approx \frac{\sinh(\lambda z')}{\sinh[\lambda(h - z')]} \quad (8.30)$$

It can be seen that at $z' = 0$, the collection probability is zero, while at $z' = h$, the collection probability is unity. The finite dimension of the generation source causes a different contribution between the top of the source with the bottom of the source. At the top, the collection probability can be written as (c.f. 8.30)

$$Q_t = \frac{\sinh[\lambda(z' - \Delta z)]}{\sinh[\lambda(h - (z' - \Delta z))]} \quad (8.31)$$

where Δz is half the side of the generation source in MEDICI, i.e. $0.1 \mu\text{m}$.

The collection probability at the bottom is

$$Q_b = \frac{\sinh[\lambda(z' + \Delta z)]}{\sinh[\lambda(h - (z' + \Delta z))]} \quad (8.32)$$

It can be seen that $Q_b > Q_t$ for all values of z . Therefore, the effective centre of mass of the point source is actually below the middle point between the top and bottom edges of the generation volume used in the simulation. The new centre of mass can be calculated from

$$z'_m = \frac{\int_{z'-\Delta z}^{z'+\Delta z} zQ(z)dz}{\int_{z'-\Delta z}^{z'+\Delta z} Q(z)dz} \quad (8.33)$$

where z'_m is the new centre of mass for the MEDICI generation source, and $Q(z)$ can be approximated from Eq. (8.30) for the case where the beam is far away from the vertical junctions. For the case of $z' = 0.3 \mu\text{m}$, $L = 5 \mu\text{m}$, and $h = 5 \mu\text{m}$, the new centre of mass was computed to be $z'_m = 0.3122 \mu\text{m}$. The amount of shift is a function of the location of z' . The effect of this shift is not significant for large values of h . However, for small values of h , the shift is more pronounced.

Since the centre of mass shifts down below z' , the curves from the MEDICI simulations would produce current values which are higher than the results from the analytical equations with the point source located at z' . The computational results from the analytical equations, then, should use the values of the shifted centre of mass in order to get the same curves as those from MEDICI. Increasing the z' values used in the computed analytical equations gives higher charge collection probability, and this would coincide with the curve from the MEDICI simulations.

In Figs. 8.5 and 8.8, the results from the analytical equation are found to be lower than the results from MEDICI simulations for small values of diffusion length. This can again be explained from the finite dimension of the MEDICI's generation source. Let us consider again the collection due to a source far away from the vertical junctions. The collection is affected mainly by the distance from the source to the bottom junction, i.e. $(h - z')/L$. The charge collection is related exponentially to this distance. The shift of the centre of mass changes and shortens this distance to $(h - z' - \Delta z')/L$, where $\Delta z' = z'_m - z'$. The actual shift is therefore, $\Delta z'/L$. It can be seen that small values of L causes the effect of this shift to be more pronounced.

Similar observations can also be seen in almost all figures in regions very close to the vertical collectors. However, for this case, the effect is due to the finite *lateral* dimension of the source in MEDICI. The computed results are slightly lower than the one obtained from MEDICI simulations for the regions that are very close to the vertical collectors, i.e. for regions near $x = 0$ for the L-shaped configuration, and regions near $x = 0$ and $x = d$ for the U-shaped configuration. This enables us to understand why the maximum difference shown in Fig. 8.11 to 8.13 occurs at the locations near the vertical junction. The error due to finite size adds up when it approaches the vertical junction. Therefore, the analysis presented previously explains all discrepancies between the analytical equations and the MEDICI simulations.

8.5 Effects of the Parameters

Figs. 8.4 and 8.7 show the effect of changing the junction depth on the EBIC profile. It can be seen that narrow junction depths give higher EBIC profiles. This result agrees with theory since narrower junctions have a higher probability for the charge to be collected. The difference becomes imperceptible as the junction depth becomes comparable to the diffusion length. This is because the changes in the z direction are approximately exponential. In order to see these changes better, the plot should be in logarithmic scale.

Another interesting observation is that the collection is dominated by the bottom junction side as the beam moves further away from the vertical junction sides. If the width is large enough, we would expect the profile to

approach a constant value.

Figs. 8.5 and 8.8, on the other hand, give the plots on the effect of changing the diffusion length values. Larger diffusion lengths result in higher EBIC profiles. This diffusion length value affects the slope of the profile in the logarithmic scale. For the case of the L-shape geometry, if bottom junction is not present, the profile becomes that of the normal-collector configuration, with an infinite surface recombination velocity at the top surface.

The effect is mostly significant for beam distances that are further away from the vertical collecting junctions. However, the change becomes negligible as the diffusion length becomes comparable to the distance between the source and the collecting junction. Therefore, in order to extract the diffusion lengths from these geometries, the values of the diffusion lengths must be smaller than the dimensions of the junction well.

In Figs 8.6 and 8.9, the results show the effect of the depth of the generation source. It can be explained physically that deeper generation sources result in higher EBIC profiles. This is simply because the distance between the generation source and the bottom collecting junction decreases, which results in a higher collection probability. In practice, it is impossible to generate a point source beyond a certain depth inside the material by using electron beam bombardment. The electron beam generates ehps in a volume similar in shape to that of a tear drop [13]. And thus, a convolution such as given by Eq. (8.29) must be used.

Fig. 8.10 shows the effect of the width of the junction well for the case of the U-shape geometry. Besides extending the profile wider, the width also affects the minimum EBIC current value slightly. Wider junctions give

lower values of EBIC minimum. This can be explained by considering the effect of the diffusion length on the recombination of the minority carriers as the width is increased. Larger width increases the distance from the centre of the junction well, where the beams are located, to the vertical collecting junctions. This results in a lower charge collection probability or a lower induced current.

8.6 Conclusion

This chapter provides the analytical equations for the charge collection profiles when the beams scan within the junction wells. Two cases were considered: the L-shaped and the U-shaped geometry junctions. For these two cases, the analytical solutions for a point generation source were derived using the Green's function technique. The case for an extended generation volume can be obtained simply by convolution.

The computation results were verified with a semiconductor device simulation program on a computer to check its accuracy. The results show that the computations give good agreements with the simulations. A discussion of the accuracy of the computations has also been given.

The effects of the parameters were then investigated. The results were explained from a physical point of view by taking into account the diffusion lengths and the geometries of the structure. The analytical equations, together with the analysis presented, would help the development of EBIC techniques in smaller devices.

Chapter 9

Conclusion and Recommendation

The EBIC technique has been widely used for semiconductor material characterizations, particularly for characterizing the minority carrier properties. In this thesis, we have analysed some parameters related to the diffusion length and the surface recombination velocity measurements. A method of determining the edges of the depletion layer has been proposed and analysed. Related to this analysis is the study on the range-energy relationship and the mathematical model for the generation volume distribution. Moreover, a generalized technique was developed for diffusion lengths measurement in non-conventional collector geometry that is more commonly found in today's devices. And lastly, analytical EBIC expressions for the charge collection from within an L-shape and a U-shape p-n junction wells were derived and analysed.

The most common method to extract the diffusion lengths of the material

is the one proposed by Ong *et al.*, which involves a fitting parameter called the alpha parameter. This parameter was thought to be affected only by the surface recombination velocity and not by other parameters such as the beam energy and the diffusion lengths. An expression for the alpha parameter that shows its dependency on other parameters was derived for the normal-collector configuration. It has been shown that the alpha parameter is a function of both the normalized scanning range with respect to the edge of the depletion layer as well as the normalized depth of the generation volume. A correction to the expression for determining the surface recombination velocity from the Normal distribution equation was given. The conditions for accurate measurements were also provided.

It was shown in the discussion that the accuracy of the diffusion lengths extraction is affected by the locations of the depletion layer's edges. This is particularly true for materials with small diffusion lengths. In Chapter 4, a synthesis of the EBIC profile around the junction was given from the physical point of view, considering the interaction of the generation volume as it enters into the depletion layer. This hypothesis profile was verified with a mathematical model that was developed together with computer simulation results. An analysis was done on the first derivative of the profile to study the position where the generation volume starts to enter the depletion layer and affects the profile significantly. For small surface recombination velocities, it was shown that the edge of the depletion layer can be determined quite accurately from the first derivative profile. The lateral dimension of the generation volume must be approximated when using this technique. In this thesis, it is approximated to be 10% of the value of the electron range. In this

way, the width of the depletion layer can be determined from the same line scans data that is used to determine the diffusion lengths. An application of this technique was demonstrated on a GaN LED. The accuracy of the technique seems to be determined by at least two factors. These are the noise which is amplified in the first derivative plot, as well as the approximation for the lateral dimension of the generation volume. The effect of the surface bend bending was not considered in this thesis. This might affect the value extracted, particularly when low beam energy is used in the experiment.

The technique to determine the depletion layer edges requires the knowledge of the value of the electron range. In the EBIC technique, higher resolutions can be obtained by using lower beam energies, which result in lower electron range values. Since no range-energy relationship is available for low beam energy range, some fitted expressions for this relationship were given for beam energy less than 5 keV. The expression is particularly valid for Si and GaN materials. The data for the fitting process were obtained from the Monte Carlo simulation. The electron range value is obtained from the extrapolation of the linear negative slope region of the energy distribution down to the zero of the y axis. The same approach can be used for other materials as well.

The electron range is simply a parameter used to characterize a more complicated interaction of the electron beam and the sample which results in a generation volume. An analytical model for the generation volume distribution is needed for the mathematical model of the EBIC profile around the junction. Chapter 6 deals with the discussion on which models to use. The Bonard *et al.* model was chosen in this thesis since it agrees with the

EBIC profile obtained using the data from the Monte Carlo simulation. In the discussion, some insights were obtained for some alternative approaches that one can use to determine the edges of the depletion layer. The study and implementation of those techniques, however, are beyond the scope of this thesis.

After analysing certain parameters that would affect the diffusion lengths, more attentions are given to the extraction of the diffusion lengths from non-conventional collector geometries. In this case, the diffusion lengths are extracted from a line scan outside of an L-shape p-n junction well. The technique of Ong *et al.* with its alpha parameter was generalized for this geometry. A fitting parameter gamma was introduced as a function of the alpha parameter and the junction depth. It was shown that the method is able to extract diffusion lengths accurately for any values of junction depths and surface recombination velocities.

On the other hand, there had been no analytical expressions of EBIC profiles for the case when the beam scans from within the junction well. Using the method of Green's function and Eigenfunctions expansion, analytical EBIC expressions, containing only elementary functions, were derived for two cases: the L-shaped and the U-shaped junction wells. An analysis was given for the effect of some parameters such as the depth of the junction, the diffusion lengths, the depth of the generation volume, as well as the width of the junction well. The availability of these analytical expressions would enhance the development of EBIC techniques to be used from within the p-n junction collectors which dimensions can no longer be assumed to be infinite.

Further studies can be done on several issues. For the case of the depletion width extraction, some works can be done to reduce the noise of the EBIC profile, particularly in its first derivative plot. Moreover, the approximation of the lateral dimension of the generation volume can be bettered with a more accurate expression. This improvement can also be done by developing a better expression for range-energy expressions. Efforts should be put to unify the range-energy relationships for various materials in the low beam energy range.

In this thesis, the analysis for the depletion layer's edges determination was done mainly from the mathematical model of the EBIC profile around the junction. Further analysis should be done in real experimental setups. Only in this way, the technique can be applied with confidence by the experimentalists. Alternative approaches to determine the edges of the depletion layer using the second derivative as well as varying the beam energies as hinted in the discussion of Chapter 6 can also be studied further. Developing mathematical models as well as doing real experimental setups is important to study the two alternative approaches using the intersections of the first derivative plots under different generation volume sizes and using the minimum of the second derivative plots.

It is also important to study the effect of the surface depletion region on the extracted value of the depletion width. This is because when low beam energy is used in the experiment, the generation volume would like completely within the surface depletion region. This might reduce value of the depletion width extracted.

And lastly, further works can be pursued in developing EBIC techniques

to extract the diffusion lengths or the junction depths from within the junction well. This would enable EBIC's applications in today's devices which dimensions tend to scale down. Many areas of research can be done. In this thesis, we only explore the case where the junction wells have sharp edges on the corners. This is not the case in real devices. Moreover, the doping concentration is assumed to be constant. In practice, ion implantation and diffusion create a Gaussian doping concentration. A non-uniform doping concentration creates a non-uniform diffusion length values. Therefore, it is important to study the extraction of non-uniform diffusion length inside of a p-n junction well.

Author's Publications

Journal Papers

Published

1. O. Kurniawan and V. K. S. Ong, "Charge Collection from within a Diffused Junction Well", *IEEE Transaction on Electron Device*, vol. 55, no. 5, pp. 1220, 2008.
2. O. Kurniawan and V. K. S. Ong, "Investigation of range-energy relationships for low energy electron beams in Silicon and Gallium Nitride," *Scanning Journal*, vol. 29, no. 6, pp. 280-286, 2007.
3. G. Moldovan, P. Kazemian, P. R. Edwards, V. K. S. Ong, O. Kurniawan, C. J. Humphreys, "Low-voltage cross-sectional EBIC for characterisation of GaN-based light emitting devices," *Ultramicroscopy*, vol. 107, no. 4-5, pp. 382-389, 2007.
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Appendix A

Derivation of the Exponential Behaviour of EBIC

The solution of the EBIC profile can be solved starting from the diffusion equation of the minority carriers. It is given as

$$\nabla^2 n + g - (1/L^2)n = 0 \quad (\text{A.1})$$

where g is the source and equals to zero in the bulk outside of the source, n is the electron concentration, and L is the minority carrier diffusion length. For the region outside the source, the term g can be omitted. In a spherical coordinate [142, p. 636], the equation can be written as

$$\frac{d^2 n}{dr^2} + \frac{2}{r} \frac{dn}{dr} - \frac{n}{L^2} = 0 \quad (\text{A.2})$$

This differential equation can be solved by substitution. Recall that for the following differential equation

$$y'' + P(r)y' + Q(r)y = 0 \quad (\text{A.3})$$

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can be reduced to

$$z'' + q(r)z = 0 \quad (\text{A.4})$$

where $q(r)$ is given by

$$q(r) = Q(r) - (1/2)P'(r) - (1/4)P^2(r) \quad (\text{A.5})$$

and the solution for y is

$$\ln y = \ln z - (1/2) \int P(r)dr \quad (\text{A.6})$$

Similarly, we can use this substitution to solve the diffusion differential equation. Substituting $Q(r) = 1/L^2$ and $P(r) = 2/r$ and its derivative into Eq. (A.5) gives

$$q(r) = -\frac{1}{L^2} - \frac{1}{2} \left(\frac{-2}{r^2} \right) - \frac{1}{4} \left(\frac{2}{r} \right)^2 \quad (\text{A.7})$$

The second and the third term cancel and only the first remains to give

$$q(r) = -1/L^2 \quad (\text{A.8})$$

Substituting this to Eq. (A.4) gives a new and yet simpler differential equation

$$z'' - (1/L^2)z = 0 \quad (\text{A.9})$$

This equation can be solved easily to give

$$z = C_1 \exp(-r/L) + C_2 \exp(+r/L) \quad (\text{A.10})$$

The solution for n can be solved from Eq. (A.6)

$$\begin{aligned} \ln n &= \ln z - (1/2) \int (2/r)dr \\ \ln n &= \ln z - \ln r = \ln z/r \\ n &= z/r \end{aligned} \quad (\text{A.11})$$

Therefore, the solution for n is

$$n = \frac{C_1}{r} \exp(-r/L) + \frac{C_2}{r} \exp(+r/L) \quad (\text{A.12})$$

This equation, however, still has two unknowns. We can solve for the unknowns by considering the boundary conditions of the problem. The boundary conditions can be formulated as follows. It is assumed that space is infinite. In this way $n \rightarrow 0$ as $r \rightarrow \infty$. To satisfy this, $C_2 = 0$. Next, we consider a point generation source of spherical symmetry. For $r \ll L$, we can write the current density in the materials as

$$J_n = -qD_n \frac{dn}{dr} = \frac{qG}{4\pi r^2} \quad (\text{A.13})$$

where G is the generation rate of a point source. The equation says that the current density of a point source with spherical symmetry is proportional to the concentration gradient of the carriers. Differentiating the solution for n and substituting to the current density equation, we would obtain $C_1 = G/4\pi D_n$. Therefore, the complete solution of the carrier distribution is

$$n = \frac{G}{4\pi r D_n} \exp(-r/L) \quad (\text{A.14})$$

The EBIC profile can be calculated by evaluating the current at the junction. To introduce a boundary condition $n = 0$ at the junction, we can use the method of images by putting an imaginary source with equal but opposite magnitude at $x = -w$, where w is the position of the source from the junction on the positive axis. The current, therefore, is given by

$$I = 2qD \int_0^\infty 2\pi R dR \left. \frac{\partial n}{\partial x} \right|_{x=0} \quad (\text{A.15})$$

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where R is the radius of a circle, and the integration is in cylindrical coordinate. We use the following geometrical relation to transform the axis from the source to the junction.

$$r^2 = R^2 + w^2 \tag{A.16}$$

which simply means that r is the distance from the source to a point in the junction plane, which is the hypotenuse of a right angle triangle, where the legs are the radius from an axis in the junction (R) and the distance between the junction plane and the source (w). Deriving this relation gives $RdR = rdr$ which can be substituted to the current expression. Solving the integration, then, gives

$$I = qG \exp(-w/L) \tag{A.17}$$

where w is the distance of the source from the junction plane.

Appendix B

Calculation of Green's Function

In this section, the details for the derivation of the EBIC profile are given. The aim is to solve Eq. (8.3) with boundary conditions given in (8.4) to (8.7). In order to solve this, the Eigenfunctions expansion is used. The first step is to divide the region into two, where region I lies in $0 \leq z \leq z'$, and region II lies in $z' \leq z \leq h$. Within each region, the Green's function satisfies the homogeneous equation

$$\frac{\partial^2 G(x, z|x', z')}{\partial x^2} + \frac{\partial^2 G(x, z|x', z')}{\partial z^2} - \lambda^2 G(x, z|x', z') = 0 \quad (\text{B.1})$$

To solve this differential equation, a separation of variable is used. Let $G = X(x)Z(z)$, and substituting this into Eq. (B.1) and dividing with XZ gives

$$\frac{X''}{X} + \frac{Z''}{Z} - \lambda^2 = 0 \quad (\text{B.2})$$

where we denote the second derivative of X and Z as X'' and Z'' respectively. It can be seen that this equation can be separated into two ordinary

differential equations (ODEs). The first is

$$\frac{X''}{X} = -p^2 \quad (\text{B.3})$$

where we have chosen the constant to be negative. In this case the solution is in the form of sine and cosine. In order to satisfy the boundary condition (8.4) at $x = 0$, we choose

$$X(x) = \sin(px) \quad (\text{B.4})$$

And to satisfy the second condition at $x = d$ (boundary condition (8.5)), we need to have $\cos(px) = 0$, or

$$p_n = \frac{n\pi}{2d} \quad (\text{B.5})$$

where n is an odd number starting from 1, i.e. $n = 1, 3, 5, \dots$

The second ODE, can be written in the form of

$$Z'' - \mu_n^2(Z) = 0 \quad (\text{B.6})$$

where $\mu_n = (\lambda^2 + p_n^2)^{1/2}$. The solution is in the form of exponential, and to satisfy boundary condition (8.6) at $z = 0$, we can choose for region I,

$$Z_{nI} = \sinh(\mu_n z) \quad (\text{B.7})$$

, while to satisfy the boundary condition (8.7) at $z = h$, we can choose for region II,

$$Z_{nII} = \sinh(\mu_n(h - z)) \quad (\text{B.8})$$

Therefore, the solution can be written as a linear combination of the individual solutions.

$$G_I(x, z|x', z') = \sum_{n=1,3,5,\dots}^{\infty} C_n \sin(p_n x) \sinh(\mu_n z) \quad (\text{B.9})$$

$$G_{II}(x, z|x', z') = \sum_{n=1,3,5,\dots}^{\infty} D_n \sin(p_n x) \sinh(\mu_n(h - z)) \quad (\text{B.10})$$

where C_n and D_n are constants with respect to x and z .

Since the solution must be continuous at $z = z'$, it must satisfy $G_I = G_{II}$, and if we utilize the orthogonality of $\sin(p_n x)$, we can obtain

$$C_n \sinh(\mu_n z') = D_n \sinh(\mu_n(h - z')) \quad (\text{B.11})$$

from which we can define a new constant as follows.

$$E_n \equiv \frac{C_n}{\sinh(\mu_n(h - z'))} = \frac{D_n}{\sinh(\mu_n z')} \quad (\text{B.12})$$

and therefore, we can write the Green's function in (B.9) and (B.10) in terms of E_n .

$$\begin{aligned} G_I(x, z|x', z') &= \sum_{n=1,3,5,\dots}^{\infty} E_n \sinh(\mu_n(h - z')) \sin(p_n x) \sinh(\mu_n z) \end{aligned} \quad (\text{B.13})$$

$$\begin{aligned} G_{II}(x, z|x', z') &= \sum_{n=1,3,5,\dots}^{\infty} E_n \sinh(\mu_n z') \sin(p_n x) \sinh(\mu_n(h - z)) \end{aligned} \quad (\text{B.14})$$

Now we need to obtain the expression for E_n . For simplicity, let's write the Green's function in the form $G = \sum g_n(z, x', z') \sin(p_n x)$. Substituting

this instead into Eq. (8.3), together by multiplying with $\sin(p_n x)$, and then integrating from 0 to d , gives

$$\left\{ -(\mu_n)^2 g_n + \frac{dg_n}{dz^2} \right\} \frac{d}{2} = -\frac{\sin(p_n x') \delta(z - z')}{D} \quad (\text{B.15})$$

The summation results in only one term due to the orthogonality property of $\sin(p_n x)$. Integrating this at a very small interval around $z = z'$ gives

$$\frac{d}{2} \left[\frac{dg_n}{dz} \right]_{z' - \varepsilon}^{z' + \varepsilon} = -\frac{\sin(p_n x)}{D} \quad (\text{B.16})$$

where $\varepsilon \rightarrow 0$. Solving this equation results in the expression for E_n .

$$E_n = \frac{2 \sin(p_n x)}{dD\mu_n h \sinh(\mu_n h)} \quad (\text{B.17})$$

Therefore, the final solution of the Green's function is given by

$$G_I(x, z|x', z') \quad (\text{B.18})$$

$$= \sum_{n=1,3,5,\dots}^{\infty} \frac{2 \sin(p_n x)}{dD\mu_n h \sinh(\mu_n h)} \sinh(\mu_n(h - z')) \sin(p_n x) \sinh(\mu_n z)$$

$$G_{II}(x, z|x', z') \quad (\text{B.19})$$

$$= \sum_{n=1,3,5,\dots}^{\infty} \frac{2 \sin(p_n x)}{dD\mu_n h \sinh(\mu_n h)} \sinh(\mu_n z') \sin(p_n x) \sinh(\mu_n(h - z))$$

The collected current for the L-shaped junction is obtained by substituting this expression into Eq. (8.1). The result is given in Eq. (8.12).

Appendix C

Matlab Codes

C.1 Codes for Fitting an EBIC Profile

```
function y=mfitalpha(x,lncur)
%this function fit ebic into the  $\ln i = \ln k + \alpha \cdot \ln x - x/L$ 
%where x is the distance from the junction

%check whether lncur is a column vector
[nr,nc]=size(lncur);
if(nc~=1)
    lncur=lncur';
end

%matrix X
x0=ones(length(x),1);
x1=real(log(x));
```

```
x2=x;
XM=[x0,x1,x2];

%perform QR factorization on X
[q,r]=qr(XM);

%compute vector c1 and c2
c=q'*lncur;
c1=c(1:3);
c2=c(4:length(c));

%compute vector beta
beta=r\c;

%compute the actual values of the parameters
k=exp(beta(1));
alpha=beta(2);
L=-1/beta(3);

%compute the r^2
yprime=beta(1)+beta(2).*x1+beta(3).*x2;
r2=var(yprime)/var(lncur);

%returns the parameters and the coefficient of determination
y=[k;alpha;L;r2];
```

C.2 Codes for Computing EBIC Profiles with Monte Carlo Data

```
function [cdat]=mgetebicmonte(param,beampos,fname)

% fname is the file for the generation volume distribution data file and
% the x-z axis data file, with x in the first column and z in the second
% column
% it must be stored in this way: fname=strvcat('gvdata.dat','xzaxis.dat');
% note that beampos is the beam position with x=0 at the metallurgical
% junction
% e.g. beampos=0.6;
% param is in the form of param=[deplvector,matparam]
% The deplvector should be in the form of deplector=[xl,xr]
% e.g. deplvector=[-0.3,0.3];
% The matparam should be in the form of
% matparam=[difflengthl,surfvel1,difflengthr,surfvelr]
% e.g. matparam=[3,0,3,0]

% this files read the data of Energy distribution in x-z plane and
% compute the EBIC profile
% the Energy distribution in x-z plane data is
% the integrated distribution along the y-axis
% the Energy distribution is stored in "data" variable
% the axis of the x and z plane is read and stored into
% the "xg" and "zg" var.
```

```

% The format for the x-z plane data must be as follows
% the rows represent the z axis data, and the cols
% represent the x axis data.
% the beam position is at the centre of the x axis data.
% the format for the x and z axis values must be as follows
% the first column is the values for x,
% while the second one is for z.
% the two column is separated by a tab or space.

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Reading the Energy distribution data, the data in one row is
% the data along the x axis,
% while the data in one column is the data along the z axis

datafname=deblank(fname(1,:)); % read the x-z plane data filename
axisfname=deblank(fname(2,:)); % read the axis value filename
[data]=dlmread(datafname);      % read the x-z plane data into a matrix

% Reading the values of the x and z axis, the first columns is x, and
% second column is z axis

[xg,zg]=textread(axisfname,'%f %f');

% Calculate the Integrated rate, it must be equal to one

```

```
% if not equals to one, then normalize it to one
% The "totalnorm" must be equal to one

total=sum(sum(data));
datanorm=data./total;
totalnorm=sum(sum(datanorm)); % this value must be equal to one

% change the axis to microns
% comment this part if the data is in microns already
x0axis=xg*1e-3;
z0axis=zg*1e-3;

% beam position

xbeam=beampos;

% preparing the matrix for the total current

% set the location of the depletion width,
% the metallurgical junction is assumed at x=0
deplvector=param(1:2);
x0l=deplvector(1); % the location of the depletion edge on the right
x0r=deplvector(2); % the location of the depletion edge on the left

% set the diffusion length
```

```
matparam=param(3:6);
difflengthl=matparam(1);
surfvell=matparam(2);
difflengthr=matparam(3);
surfvelr=matparam(4);

% shift the generation volume to xb
xbshifted=(x0axis+xbeam)';

% plot the surface of the generation rates
% mesh(xbm,zgm,datanorm);

% the most left position of the generation volume
xbl=xbshifted(1);

% the most right position of the generation volume
xbr=xbshifted(length(x0axis));

% Starting the Convolution
% the matrix to store the convoluted value
im=zeros(length(z0axis),length(x0axis));

il=0;
ic=0;
ir=0;
xint=0;
```

```

% If the generation volume is totally outside
if (xbl>x0r || xbr<x0l)

    for col=1:1:length(xbshifted)
        for row=1:1:length(z0axis)
            if(xbl>x0r)
                Lp=difflengthr;
                sp=surfvelr;
                xint=x0r;
            elseif (xbr<x0l)
                Lp=difflengthl;
                sp=surfvell;
                xint=x0l;
            end
            im(row,col)=datanorm(row,col)*mgetQ(xbshifted(col)- \
xint,z0axis(row),Lp,sp);
        end
    end

% If the generation volume is totally inside
elseif (xbr<=x0r && xbl>=x0l)

    % then multiply the gen rate with unity
    im=datanorm*1;

% if it is in between
elseif ((xbl<=x0r && xbr>x0r) || (xbr>=x0l && xbl<x0l))

```

```
% locate the portion where the genrate is inside
midentify=zeros(length(x0axis),1);

for n=1:1:length(xbshifted)
    % If inside, mark as 1
    if (xbshifted(n)<=x0r && xbshifted(n)>=x0l)
        midentify(n)=1;
    else
        % If outside, mark as 0
        midentify(n)=0;
    end
end

% find the vector index of the border, last data for inside
position=find(midentify);
idborderl=position(1);
idborderr=position(length(position));

% For inside, calculate the convolution by multiplying with unity
for col=idborderl:1:idborderr
    for row=1:1:length(z0axis)
        im(row,col)=datanorm(row,col)*1;
    end
end
```



```

% For outside, calculate the convolution by multiplying with Q
if (xbr > x0r )
    for col=(idborderr+1):1:length(xbshifted)
        for row=1:1:length(z0axis)
            im(row,col)=datanorm(row,col)*mgetQ(xbshifted(col)- \
x0r,z0axis(row),difflengthr,surfvelr);
        end
    end
end
if (xbl < x0l)
    for col=1:1:(idborderl-1)
        for row=1:1:length(z0axis)
            im(row,col)=datanorm(row,col)*mgetQ(xbshifted(col)- \
x0l,z0axis(row),difflengthl,surfvell);
        end
    end
end
end

itotal=sum(sum(im)); % sum the convoluted value

cdat=itotal';

```

C.3 Codes for Computing EBIC Profiles with Donolato Model

C.3.1 Function for EBIC Profiles

[illegible]

```
xbeam=beampos;

% extract the left and right edge of the depletion layer
deplvector=param(1:2);
xl=deplvector(1);
xr=deplvector(2);

% extract the material parameter, the diffusion lengths and
% surface recombination velocity for the left and right region
matparam=param(3:6);
diffll=matparam(1);
svl=matparam(2);
diffflr=matparam(3);
svr=matparam(4);

% extract the beam parameter, electron range and beam diameter
Rp=beamparam(1);
dbeam=beamparam(2);

% set the beam position to xb(row)
xbeam=beampos;

% store the material parameter to global variable to be passed on
Lp=diffll;
sp=svl;
xedge=xl;
```

```

% calculate the ebic profile on the left of the depletion layer
il=0;
ic=0;
ir=0;
xint=0;

xbl=(xbeam-2*Rp);
xbr=(xbeam+2*Rp);
if(xbl<x1)
    if(xbr<x1)
        xint=xbr;
    else
        xint=x1;
    end
    il=dblquad(@(x,z) funcur(x,z,xbeam,Rp,Lp,sp,xedge),xbl,xint,0,2*Rp);
end

% calculate the ebic profile inside of the depletion layer

ic=dblquad(@(x,z) mgeth(x,z,xbeam,Rp,dbeam),x1,xr,0,1.2*Rp);

% store the material parameter to global variable to be passed on
Lp=diffflr;
sp=svr;
xedge=xr;

```

```

% calculate the ebic profile on the right of the depletion layer
if(xbr>xr)
    if(xbl>xr)
        xint=xbl;
    else
        xint=xr;
    end
    ir=dblquad(@(x,z) funcur(x,z,xbeam,Rp,dbeam,Lp,sp,xedge),xint,xbr,0,2*Rf)
end

% sum all the current
itotal=il+ic+ir;

%find the maximum current
xbeam=0;
imax=dblquad(@(x,z) mgeth(x,z,xbeam,Rp,dbeam),-1.2*Rp,1.2*Rp,0,1.2*Rp);

% normalized the current profile
cdat=itotal./imax;
function y=funcur(x,z,xbeam,Rp,dbeam,Lp,sp,xedge)

xdj=x-xedge;
for i=1:length(x)
    for j=1:length(z)
        y(j,i)=mgeth(x(i),z(j),xbeam,Rp,dbeam).*mgetQ(xdj(i),z(j),Lp,sp);
    end
end

```

```

    end
end

```

C.3.2 Function for Charge Collection

```

function y=mgetQ(xbm,zgm,L,s)
% function to compute Q
% version 1.0
    if (s==0)
        spart=0;
    else
        % instead of integrating to infinity, transform the equation
        % with the following substitution k=t/(1-t), and so
        % the integration is from 0 to -1
        for n=1:length(xbm) %to handle in the case that xbm is a vector
            spart(n)=-2.*s./pi.*quad(@t fs2(t,L,s,xbm(n),zgm),0,-1+eps);
        end
    end
end;

y=exp(-abs(xbm)./L)+spart;

function y=fs2(t,Lp,sp,xp,zp)
    y=(t./(1+t))./(mu((t./(1+t)),Lp).^2.*(mu((t./(1+t)),Lp)+sp)).* \
exp(-mu((t./(1+t)),Lp).*zp).*sin((t./(1+t)).*abs(xp)).*(-1./(t+1).^2);

```

```
function y=mu(k,L)
    y=sqrt(k.^2+(1/L).^2);
```

C.3.3 Function for Generation Volume Distribution

```
function y=mgeth(x,z,xbeam,Rp,dbeam)
%this generation volume model use Donolato model with
% everhart and hoff in the z direction and exponential in the x direction.
xprime=x-xbeam;
n=length(x);
m=length(z);
for i=1:n
    for j=1:m
        mresult(j,i)=funte(z(j),Rp)/(Rp*sqrt(2*pi)*sigma(z(j),Rp,dbeam))* \
exp(-xprime(i)^2/(2*sigma(z(j),Rp,dbeam)^2));
    end
end

%total=sum(sum(mresult));
y=mresult;
%y=mresult./total;

function y=funte(z,r)
rat=z./r;
if(rat>1.1)
```

```

        y=0;
    else
        y=0.6+6.21.*rat-12.4.*rat.^2+5.69.*rat.^3;
    end

```

```

function y=sigma(z,r,d)

```

```

y=sqrt(0.36.*d.^2+0.11*z.^3./r);

```

C.4 Codes for Bonard Generation Volume

```

function y=mgethbonard(x,z,xbeam,px,pz)

```

```

% generation volume projected into the x-z plane from

```

```

A=px(1);

```

```

B=pz(1);

```

```

sigmax=px(2);

```

```

sigmaz=pz(2);

```

```

xprime=x-xbeam;

```

```

n=length(x);

```

```

m=length(z);

```

```

for i=1:n

```

```

    for j=1:m

```

```

        mresult(j,i)=(1./(2.*sqrt(pi).*sigmax.*sigmaz.*3)).* \

```



```

exp(-xprime(i).^2./sigmax.^2).*z(j).^2.*exp(-z(j)./sigmaz);
    end
end

%total=sum(sum(mresult));
y=mresult;
%y=mresult./total;

```

C.5 Codes for Smoothing Filter

```

function g=SavGol(f,nl,nr,M)
% function to smooth using Savitsky-Golay filter
% g is the returned smooth data
% f is the data to be smoothed
% nl is the number of point on the left of the data to be averaged
% nr is the number of point on the right of the data to be averaged
% M is the degree of polynomial to be used

A=ones(nl+nr+1,M+1);
for j = M:-1:1,
    A(:,j)=[-nl:nr]' .* A(:,j+1);
end

[Q,R]=qr(A);
c=Q(:,M+1)/R(M+1,M+1);

```

```
n=length(f);  
g=filter(c(nl+nr+1:-1:1),1,f);  
g(1:nl)=f(1:nl);  
g(nl+1:n-nr)=g(nl+nr+1:n);  
g(n-nr+1:n)=f(n-nr+1:n);
```

C.6 Codes to Compute U-shaped EBIC Profile

```
function y=mgetQushape2(x,z,L,d,h)  
%sum up 600 terms  
NTERMS=600;  
  
total=0;  
result=0;  
n=1;  
while (n<=NTERMS)  
totalold=total;  
result=funget(x,z,L,d,h,n);  
total=total+result;  
n=n+1;  
end
```

```
y=total;
```

```
function y=funpn(n,d)
% function to compute the eigenvalues
y=n*pi/d;
```

```
function y=funmun(la,p)
% to be called by funget function
y=sqrt(la.^2+p.^2);
```

```
function y=funget(x,z,L,d,h,n)
% function to compute the term inside the sum
pn=funpn(n,d);
lambda=1/L;
mun=funmun(lambda,pn);
f11=(d.*sinh(mun.*h));
if (isfinite(f11))
    f1=(2.*sin(pn.*x))./f11;
    f2=sinh(mun.*z);
    f3=(pn./mun.^2);
    f4=sinh(mun.*(h-z)).*(cosh(mun.*z)-1);
    f5=f2.*(cosh(mun.*(h-z))-1);
    f0=(1-(-1).^n);
    y=f1.*f0.*(f3.*(f4+f5)+(f2./pn));
else
```

```
y=0;  
end;
```

Appendix D

MEDICI Simulations Codes

D.1 Introduction

This chapter gives example of MEDICI input files used in this thesis. It is not meant to be a rigorous explanation on MEDICI or its physical models. Details on MEDICI statements and its physical models can be found in [143].

D.2 Device Structure

The simulation of EBIC using MEDICI starts with a construction of the device structure. For accurate results, simulation mesh is important, and fine grid spacing should be put in the regions of interest. In most of the simulations in this thesis, the regions of interest are located at the collectors, which either a p-n junction or a Schottky barrier, and the surface where the carriers recombine due to the surface recombination velocity. Fig. D.1 shows the input file of MEDICI device structure.

```
title structure for lshape junction simulation with l=5,d=5,h=5
mesh out.file=MDSTR555
x.mesh width=10 h1=0.1
y.mesh depth=10 h1=0.1

eliminate columns x.max=4 y.min=1
eliminate columns x.min=4 y.min=6

electrode name=anode top x.min=5.2
electrode name=cathode top x.max=4.5

region silicon

profile p-type n.peak=1e18 x.min=5 y.max=5 uniform
profile n-type n.peak=1e18 x.max=5 uniform
profile n-type n.peak=1e18 x.min=5 y.min=5 uniform

regrid doping ratio=2 logarithmic out.file=MDSTR555R

plot.2d grid fill scale
```

Figure D.1: Input file for a MEDICI device structure.

The structure starts by defining the mesh in the x and y direction. In MEDICI, the zero axis of x is located at the left most of the device, while the zero axis of the y axis is located at the top most of the device. After the mesh, the locations of the electrodes must be specified. In all of the simulations in this thesis, two electrodes were used. One is on the p-side while the other is on the n-side. It is also important to define the material used in the simulation. This is done using the keyword *region* to set the material for each region of the device. In the example, all region is defined as Silicon. The next important thing to do is to define the doping concentration using the keyword *profile*. In all of the simulations in this thesis, uniform doping was used.

D.3 Surface Recombination Velocity

The surface recombination velocity in MEDICI can be defined between two region of materials using the keyword *interface*. In order to do this, we must first define a very thin oxide layer on top of the surface where the surface recombination velocity is to be defined. A very thin oxide layer always exist in Silicon when it is put in room temperature. An example of this is shown below.

```
interface region={topsurf,nregion} x.min=0 x.max=5 s.n=1e5 s.p=1e7
```

The statement defines both the electrons and the holes the surface recombination velocities at the interface of *topsurf* and *nregion* regions from $x = 0$ to $x = 5 \mu\text{m}$. The surface recombination velocities were set to $1 \times 10^5 \text{ cm/s}$ and $1 \times 10^7 \text{ cm/s}$ for electrons and holes respectively.

D.4 I-V Characteristics Simulations

Once the device structure is done, I-V characteristic simulation was usually done to make sure that the p-n junction works fine. In every simulation, the physical models and the numerical methods must be specified. The input file for this I-V simulation was given in Fig. D.2.

```

title I-V simulation for MDSTR555
mesh in.file=MDSTR555R

models conmob consrh
material silicon taun0=8.043e-7 taup0=1.138e-6

symbolic gummel carriers=0
solve

log out.file=iv555.log

symbolic newton carriers=2
solve electrode=anode vstep=0.1 nsteps=30

plot.1d in.file=iv555.log x.axis=v(anode) y.axis=i(anode) y.log

```

Figure D.2: MEDICI input file for I-V simulations.

The physical model is specified with the statement *models*. In the simulation of Fig. D.2, *conmob* and *consrh* are used, which refers to the concentration dependent mobility and concentration dependent lifetime. This means that the mobilities of the carriers are determined from the doping concentrations. The lifetimes of the carriers are modeled using the SRH recombination, which is the dominant recombination process in Silicon. This lifetime is also affected by the doping concentration.

The numerical computation is solved using the Newton method with two

carriers in the calculation. Newton method calculates four coupled physical equations described by the simulation. This computation is rather slow and takes time. In order to have a good initial guess, the computation starts with Gummel method with zero carriers.

D.5 EBIC simulations

The EBIC phenomena are simulated using the statement *photogen*. This statement generates electron-hole pairs due to light illumination. Since the simulator assumes that it is due to light illumination, it does not take into account the excess electrons that come from the beam. This causes inaccuracy in the simulation. Nevertheless, the effect of beam current can be easily taken into account since the amount is constant throughout the line scans. Fig. D.3 shows the input file for the EBIC line scans.

In this example, the generation volume is a square with $0.2 \mu\text{m}$ on each side. The generation rate was specified from the parameter A1 in the *photogen* statement. The code for implementing an extended generation volume is given below. Wu gave another implementation in his thesis [92] which worth consideration.

The diffusion lengths of the material are set using the statement *material*, through the concentration dependent lifetime *taun0* and *taup0*. The dependence of this lifetime on the concentration can be found in [143]. The lifetime for electrons is computed from

$$\tau_n(x, y) = \frac{\text{TAUN0}}{1 + N_{\text{total}}(x, y)/\text{NSRHN}} \quad (\text{D.1})$$

```

title ebic simulation for MDSTR555
mesh in.file=MDSTR555R

models conmob consrh
material silicon taun0=8.043e-7 taup0=1.138e-6

symbolic gummel carriers=0
solve

symbolic newton carriers=2

assign name=NSTEPS n.value=100
assign name=YT n.value=0.2
assign name=YB n.value=0.4
log out.file=ebic555.log

loop steps=@NSTEPS
  assign name=XPOS n.value=0.1 delta=0.1
  extract name=XL expressi=@XPOS-0.1 now
  extract name=XR expressi=@XPOS+0.1 now
  photogen x.min=@XL x.max=@XR y.min=@YT y.max=@YB a1=5.22e23 uniform
  solve
  extract name=CUR expressi=@i(cathode) now
  echo "EBIC at xpos = "@XPOS" is "@CUR
1.end

```

Figure D.3: MEDICI input file for EBIC simulation. The beam scans along the top surface.

where N_{total} is the total impurity concentration, and NSRHN is a constant and equal to $5 \times 10^{16} \text{ cm}^{-3}$. The diffusion length is, then, related to the lifetime according to

$$L = \sqrt{\tau D} \quad (\text{D.2})$$

where D is the diffusivity or the diffusion constant. The value for the diffusion constant is determined from the mobility following the Einstein's rela-

tion.

$$D = \frac{kT}{q} \mu \quad (\text{D.3})$$

where kT/q at room temperature is a constant with values of about 0.0259 eV. When using the *conmob* model, the mobility depends on the concentration. The dependency can be found in [143].

D.6 Extended Generation Volume

As mentioned briefly in the previous section, the electron-hole pairs generation is simulated using the command *photogen* in MEDICI. The generation rate equation is computed by the simulator as follows.

$$G(l, r, t) = L(l)R(r)T(t) \quad (\text{D.4})$$

where $L(l)$ is the length dependence, $R(r)$ is the radial dependence, and $T(t)$ is the time dependence functions. In all the simulations in this thesis, the time dependence is uniform, or in other words constant generation rate. The path of the photogeneration rate is specified as shown in Fig. D.4.

The radial dependence is

$$R(r) = \begin{cases} \exp \left[- \left(\frac{r}{\text{R.CHAR}} \right)^2 \right] & \text{R.CHAR} > 0 \\ 0 & \text{R.CHAR} = 0 \end{cases} \quad (\text{D.5})$$

while the length dependence has the following form

$$\begin{aligned} L(l) = & A1 + A2.l + A3.\exp(A4.l) \\ & + k[C1(C2 + C3.l)^{C4} + L_f(l)] \end{aligned} \quad (\text{D.6})$$

Figure D.4: Specification of Photogeneration Path, taken from [143].

For a uniform generation rate, it is convenient to specify it through A1. For a more complex generation rate distribution, we can specify them using the parameter $L_f(l)$. This represents a table of generation rate as a function of l which is specified from a file. The file is taken by using the parameter *IN.FILE* in the *photogen* statement. The file must contain at least two columns. The first is the distance and the second is the generation rate in cm^3/s . If the parameter *RD.CHAR* is specified in the *photogen* statement, then the value of the radial dependence (*R.CHAR*) is read from the third column of the file.

The most needed information is the beam energy. Once the beam energy is known, we must determine which generation volume model we want to use. A discussion on generation volume models is given in Chapter 6. An example of using the Bonard *et al.* model is given as follows.

Let's assume that the beam energy used in the simulation is 3 keV with Si as its material. Substituting to Eq. (5.1) gives the value of about 0.12

μm for the electron penetration range. Chapter 6 shows that the linear regression for this value of beam energy in Si gives the following parameter for the Bonard *et al.* model.

$$\sigma_x = 5.7811 \times 10^{-2} \mu\text{m} \quad (\text{D.7})$$

$$\sigma_z = 1.6077 \times 10^{-2} \mu\text{m} \quad (\text{D.8})$$

where the distribution can be described as

$$h(x, z) = \frac{1}{2\sqrt{\pi}\sigma_x\sigma_z^3} \exp\left(-\frac{x^2}{\sigma_x^2}\right) z^2 \exp\left(-\frac{z}{\sigma_z}\right) \quad (\text{D.9})$$

Matlab code in Appendix C.4 can be used to compute Eq. (D.9) numerically the generation volume distribution in the x - z plane. Comparing with the MEDICI *photogen* model, the distribution can be rewritten as follows

$$h(x, z) = \left[\frac{1}{2\sqrt{\pi}\sigma_x\sigma_z^3} z^2 \exp\left(-\frac{z}{\sigma_z}\right) \right] \left[\exp\left(-\frac{x^2}{\sigma_x^2}\right) \right] \quad (\text{D.10})$$

where the first square bracket gives the length dependence, and the second square bracket gives the radial dependence. For the Bonard *et al.* model, therefore, the value of R.CHAR is a constant and is given by $\text{R.CHAR} = \sigma_x = 5.7811 \times 10^{-2} \mu\text{m}$. The calculation of the length dependence, on the other hand, requires an assumption. If we assume that the distribution is about constant within each $0.01 \mu\text{m}$, then, the length dependence can be computed from the first square bracket for each z values with interval $0.01 \mu\text{m}$. The computation can be done from $z = 0$ down to about $z \approx 1.1R$ [8].

Eq. (D.10) gives the normalized distribution. In other words, the total generation is unity. This distribution is to be multiplied with the total

```

# example of input file for medici
# z (um).      ehps/s/vol
# this header lines should not be in the
# actual file
0.01.  4.5062E+26
0.02.  9.6768E+26
0.03.  1.1689E+27
0.04.  1.1156E+27
0.05.  9.3586E+26
0.06.  7.2350E+26
0.07.  5.2869E+26
0.08.  3.7072E+26
0.09.  2.5190E+26
0.1.   1.6696E+26
0.11.  1.0846E+26
0.12.  6.9294E+25
0.13.  4.3660E+25

```

Figure D.5: Example of input file "mygenrate.dat" for *photogen* statement with extended generation volume.

generation rate. For one ampere of beam current, the ehps generated can be calculated from

$$G = \frac{E_b(1 - f)}{E_i} \quad (\text{D.11})$$

where f is the fraction due to backscattering, E_b is the beam energy, and E_i is the energy required to produce one ehps. For Silicon, $f = 0.08$ and $E_i = 3.62$ eV [13]. Therefore, the total current generated is

$$I_{\max} = G I_b \quad (\text{D.12})$$

The total number of ehps generated, therefore,

$$g = \frac{I_{\max}}{q} \text{ ehps/s} \quad (\text{D.13})$$

where q is the elementary charge 1.6×10^{-19} C.

The unit of the first square bracket in Eq. (D.10) is per unit area. Therefore, the multiplication of Eq. (D.13) and the first square bracket in Eq. (D.10) gives the unit of ehp/s/(unit area). Since the generation rate in MEDICI is to be given as the rate over a unit volume, we need to divide this with a unit length along the z axis of MEDICI simulator, i.e. 1×10^{-4} cm (note that the default axis in MEDICI is in microns while the generation rate is in cm). An example of calculation with 3 keV beam energy and 1.5 nA beam current is given in Fig. D.5. The MEDICI statement to simulate this ehps generation when the beam is at $x = 5 \mu\text{m}$ is

```
extract name=MAXR expressi=1.1*4e-2*3**(1.75)/2.33 now
photogen x.start=5 x.end=5 y.end=@MAXR
+ in.file=mygenrate.dat r.char=5.7811e-2
```

where MAXR is a variable to store the maximum range. The contour is given in Fig. D.6. The statement assumes that the lateral electron range is constant for all values of z . This is true for Bonard *et al.* model. The assumption is not valid when the Donolato model or the Donolato-Venturi model is used. For these two models, the variable RD.CHAR must be set true and the lateral electron range is put in the third column of the generation data file.

The MEDICI simulation also gave the location of maximum generation. In the above example, the simulator gave the maximum generation range located at $\bar{z} = 0.03$. With the computed value $R = 0.117 \mu\text{m}$, the peak generation rate is about $\bar{z} = 0.26R$, which is about the value of the expected centre of mass of a generation volume (i.e. $\bar{z} = 0.3R$) [35, 48]. The total

Figure D.6: Contour of MEDICI generation volume with 3 keV beam energy using Bonard *et al.* model.

generation rate reported by the simulator was $1.196\text{E-}6 \text{ A}/\mu\text{m}$. The unit is per $1 \mu\text{m}$ because MEDICI is a 2-D simulator. The theoretical maximum current can be computed from Eq. (D.12), which gives the value $1.1436\text{E-}6 \text{ A}$. The error was less than 5%.