

ON THE ANALYSIS OF DIFFUSION LENGTH MEASUREMENTS BY SEM

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Abstract—A simpler analysis is given of the diffusion problem related to the scanning electron microscope measurements of bulk diffusion lengths in semiconductors using scanning normal to a p - n junction or a Schottky barrier. The current profile due to a point source is obtained in form of the Fourier transform of an expression containing elementary functions only. It is shown that this form can be readily adapted to include the presence of a back ohmic contact and allows an easier discussion of the case of an extended generation.

1. INTRODUCTION

A widely used method for determining the minority carrier diffusion length in a semiconductor by means of the scanning electron microscope (SEM) relies on the configuration shown in Fig. 1 [1-5]. The sample contains a plane p - n or Schottky barrier junction perpendicular to the free surface and the electron beam of the SEM is scanned over this surface at right angle to the junction. By measuring the steady-state electron beam induced current (EBIC) as a function of the beam-junction distance, current profiles are obtained from which the minority carrier diffusion length and possibly the surface recombination velocity [3-5] are deduced.

Published papers on the theory of such measurements [5-9] generally refer back to the solution of the diffusion problem given by van Roosbroeck [10] for a point source of minority carriers in a semi-infinite sample. In Ref. [10] the boundary conditions are met by the introduction of virtual sources, a method known from the theory of heat conduction [11]. This procedure leads to an expression for the induced current profile $Q(x', z')$ due to a point source at a depth z' , which in principle can be used for studying the current profile with an arbitrary generation. However, this has been done exactly only for a source of negligible lateral extension [5, 9]. More realistic generation schemes, like the uniform sphere or the spherically symmetric Gaussian, have been dealt with either approximately [7] or by numerical methods [12], probably because of the com-

plicated expression of $Q(x', z')$ in terms of integrals of a modified Bessel function.

The present paper proposes an alternative integral representation for $Q(x', z')$ which makes use of elementary functions only. It is shown that this form is convenient both for discussing the case of an extended generation and taking into account the finite sample thickness. The analysis given here has some similarity with that of von Roos [13], since use is made of the Fourier transform method. However, recognition that only a two-dimensional study of the diffusion problem is necessary gives a considerable simplification of the discussion.

2. THE DIFFUSION PROBLEM

We discuss in detail the case where the presence of the back surface of the diode can be neglected, i.e. the sample thickness can be considered infinite [7]. It will be shown shortly that the case of finite sample thickness requires only minor changes in the theory.

The transport of beam-generated minority carriers in the neutral material (for instance, of n -type) is described by a steady-state diffusion equation

$$D\nabla^2 p(\mathbf{r}) - \frac{1}{\tau} p(\mathbf{r}) = -g(\mathbf{r}), \quad (1)$$

where $p(\mathbf{r})$ is the excess hole density at the point $\mathbf{r} = (x, y, z)$, D and τ their diffusion coefficient and lifetime, respectively, and $g(\mathbf{r})$ is the generation rate of electron-hole pairs per unit volume. Usually [5, 7, 13] the solution of eqn (1) is sought, under suitable boundary conditions on the surface and at the junction plane. Once $p(\mathbf{r})$ is known, the collected current is found by integrating the normal gradient of p over the yz plane.

For the purpose of calculating the beam induced current, however, it is actually not necessary to solve the three-dimensional eqn (1). In fact, as observed in [8, 10], the configuration of Fig. 1 has translational invariance along the y axis, in the sense that the contribution to the collected current of any source element does not depend on its y coordinate. Therefore the collected current does

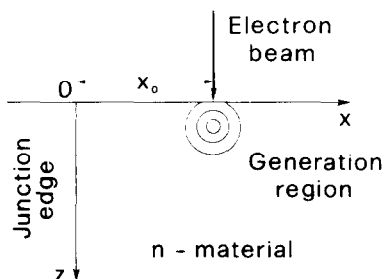


Fig. 1. Schematic diagram of SEM measurements of diffusion lengths.

not depend on the detailed distribution of g along y , but only on the projected generation onto the xz plane

$$h(x, z) = \int_{-\infty}^{\infty} g(x, y, z) dy. \quad (2)$$

Thus we only need to solve the two-dimensional problem

$$D \nabla^2 q(x, z) - \frac{1}{\tau} q(x, z) = -h(x, z), \quad (3)$$

where ∇^2 is now the two-dimensional Laplace operator, with the boundary conditions

$$q = 0 \quad \text{at } x = 0 \quad (4a)$$

$$\frac{\partial q}{\partial z} = sq \quad \text{at } z = 0. \quad (4b)$$

In eqn (4b), $s = v_s/D$, v_s being the surface recombination velocity. Let $G(x, x', z, z')$ be the Green's function for eqn (3), satisfying the boundary conditions (4); the required solution is then given by

$$q(x, z) = \int_0^{\infty} dx' \int_0^{\infty} h(x', z') G(x, x', z, z') dz'. \quad (5)$$

The collected particle current is

$$I = D \int_0^{\infty} \frac{\partial q}{\partial x} \Big|_{x=0} dz = \int_0^{\infty} dx' \int_0^{\infty} h(x', z') Q(x', z') dz', \quad (6)$$

where $Q(x', z')$ represents the fraction of injected minority carriers at (x', z') that flows into the junction, i.e. the carrier collection probability at that point, and is given by

$$Q(x', z') = D \int_0^{\infty} \frac{\partial G}{\partial x} \Big|_{x=0} dz. \quad (7)$$

For a given value of z' , the function $Q(x', z')$ also gives the normalized induced current profile due to a point source at $z = z'$. This function is calculated explicitly in the next Section. The collected current (6) for an extended generation is evaluated in Section 4.

3. THE CARRIER COLLECTION PROBABILITY

The Green's function required for the calculation of the carrier collection probability (7) obeys the equation

$$\frac{\partial^2 G}{\partial x^2} + \frac{\partial^2 G}{\partial z^2} - \lambda^2 G = -\frac{1}{D} \delta(x - x') \delta(z - z') \quad (8)$$

and satisfies the boundary conditions (4). In eqn (8) $\lambda = 1/L$, $L = (D\tau)^{1/2}$ being the minority carrier diffusion length, and δ is the Dirac delta function. A solution of eqn (8) which satisfies the boundary condition (4a) can be written in the form of a Fourier sine transform

$$G(x, z) = \int_0^{\infty} a(k, z) \sin(kx) dk, \quad (9)$$

where the dependence of G and a on x', z' has been omitted for simplicity. Inserting this expansion into eqn (8) and using the integral representation for the delta function (Ref.[14], p. 763)

$$\delta(x - x') = \frac{2}{\pi} \int_0^{\infty} \sin(kx) \sin(kx') dk \quad (10)$$

we are led to the ordinary differential equation for $a(k, z)$

$$\frac{\partial^2 a}{\partial z^2} - (k^2 + \lambda^2) a = -\frac{2}{\pi D} \sin(kx') \delta(z - z'). \quad (11)$$

It is easily seen that the solution of eqn (11) which satisfies the boundary condition (4b) is given by

$$a(k, z) = \frac{1}{\pi D} \frac{\sin(kx')}{\mu} \left\{ \exp[-\mu|z - z'|] + \frac{\mu - s}{\mu + s} \exp[-\mu(z + z')] \right\}, \quad (12)$$

where $\mu = (k^2 + \lambda^2)^{1/2}$. Substitution of this expression in eqn (9) yields the required Green's function. From (7) and (9) we have

$$Q = D \int_0^{\infty} dz \int_0^{\infty} ka(k, z) dk. \quad (13)$$

It is convenient to perform first the integration with respect to z , since

$$\int_0^{\infty} a(k, z) dz = \frac{2}{\pi D} \frac{\sin(kx')}{\mu^2} \left[1 - \frac{s}{\mu + s} \exp(-\mu z') \right]. \quad (14)$$

Hence

$$Q(x', z') = \frac{2}{\pi} \int_0^{\infty} \frac{k}{\mu^2} \left[1 - \frac{s}{\mu + s} \exp(-\mu z') \right] \sin(kx') dk = \frac{2}{\pi} \int_0^{\infty} \Psi(k, z') \sin(kx') dk. \quad (15)$$

This is the required expression for the carrier collection probability, which is seen to be the Fourier sine transform of a function $\Psi(k, z')$ containing elementary functions only. The equivalence between eqn (15) and van Roosbroeck's expression is demonstrated in the Appendix.

Equation (15) may be put in a different form, using the identity (Ref.[15], p. 1150)

$$\frac{2}{\pi} \int_0^{\infty} \frac{k}{k^2 + \lambda^2} \sin(kx') dk = \exp(-\lambda x'). \quad (16)$$

Thus

$$Q(x', z') = \exp(-\lambda x') - \frac{2}{\pi} s \int_0^{\infty} \frac{k}{\mu^2(\mu + s)} \times \exp(-\mu z') \sin(kx') dk. \quad (17)$$

This expression shows clearly that for $s = 0$ the current profile is a simple exponential with decay constant $1/\lambda = L$ for any value of the depth z' of the point generation. The second term on the r.h.s. of eqn (17) represents the influence of the surface on the current collected by the junction; unfortunately, a closed form evaluation of this term was not found.

We are now ready to show how the analysis described above can be adapted to the case of a sample with finite thickness. If d is the distance between the junction edge and the back surface contact, which is assumed to be ohmic, we have an additional boundary condition for eqn (3) and consequently for eqn (8)

$$G = 0 \text{ at } x = d. \quad (18)$$

This condition can be satisfied by replacing the integral in eqn (9) with a sum over the discrete eigenfunctions of the x part of the Laplace operator which vanish both at $x = 0$ and $x = d$. This procedure is just the reverse of that leading to the Fourier integral starting from the Fourier series [14], and yields

$$G(x, z) = \frac{\pi}{d} \sum_{n=1}^{\infty} a(k_n, z) \sin(k_n x); \quad k_n = n\pi/d. \quad (19)$$

Accordingly, the carrier collection probability (15) becomes

$$Q(x', z') = \frac{2}{d} \sum_{n=1}^{\infty} \frac{k_n}{\mu_n^2} \left[1 - \frac{s}{\mu_n + s} \exp(-\mu_n z') \right] \sin(k_n x') \quad (20)$$

where $\mu_n = (k_n^2 + \lambda^2)^{1/2}$. It is not difficult to see that the series (20) represents a simpler expression of eqn (24) of Ref. [13], if the summation of sine functions indicated there is expressed in terms of a series of delta functions by use of the Poisson sum formula (Ref. [14], p. 467). In eqn (20) the term corresponding to $s = 0$ can be calculated explicitly (Ref. [15], p. 40) and separated out, as done for eqn (15); this gives

$$Q(x', z') = \frac{\sinh[\lambda(d - x')]}{\sinh(\lambda d)} - \frac{2}{d} s \sum_{n=1}^{\infty} \frac{k_n}{\mu_n(\mu_n + s)} \exp(-\mu_n z') \sin(k_n x'). \quad (21)$$

This expression is expected to be useful for interpreting diffusion length measurements in samples where L is comparable to d , as in epitaxial layers or solar cells. Equation (21) appears to be a convenient alternative to the series containing modified Bessel functions, which is obtained in this case by the method of virtual sources [16, 17].

4. THE EXTENDED GENERATION

The transport of beam-generated minority carriers can be considered purely diffusive only if the carriers are

generated in the neutral region of the semiconductor. In the case of an extended generation, this requires that the generation volume should lie completely at $x > 0$, i.e. we must assume that x_0 is greater than the lateral extension ϵ of the generation volume. This is not a relevant limitation, since usually data for large values of x_0 are used to evaluate L and s [1–5]. Observing that the form of the generation does not change with beam position, we can write the (projected) generation function as $h(x - x_0, z)$. By eqn (6), inverting the integration order and dropping the prime marks, we have

$$I(x_0) = \int_0^{\infty} dz \int_0^{\infty} Q(x, z) h(x - x_0, z) dx. \quad (22)$$

The integral over x can be extended to $-\infty$, since h will be negligibly small for $x < 0$, and can therefore be put in form of a convolution. The convolved functions are $h(x)$ and the (odd) function of x obtained by allowing negative values of the first argument of Q .

The convolution can be conveniently expressed through the Faltung theorem for Fourier transforms [14]; this yields

$$I(x_0) = \int_0^{\infty} dz \mathcal{F}^{-1}[(2\pi)^{1/2} \tilde{Q}(k, z) \tilde{h}(k, z)], \quad (23)$$

where \mathcal{F} or the tilde denote the Fourier transform. The representation (15) for $Q(x, z)$ shows that

$$\tilde{Q}(k, z) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} Q(x, z) e^{ikx} dx = (2/\pi)^{1/2} i\Psi(k, z). \quad (24)$$

Because of the cylindrical symmetry of the generation about the beam axis, $h(x)$ and consequently $\tilde{h}(k)$ are even functions for any z . Since $\Psi(k)$ is odd, the product $\Psi \cdot \tilde{h}$ is an odd function of k and the inverse Fourier transform of eqn (23) will be a sine transform. Thus

$$I(x_0) = 2(2/\pi)^{1/2} \int_0^{\infty} dz \int_0^{\infty} \Psi(k, z) \tilde{h}(k, z) \sin(kx_0) dk \quad (25)$$

or, reversing the integration order,

$$I(x_0) = 2(2/\pi)^{1/2} \int_0^{\infty} dk \sin(kx_0) \int_0^{\infty} \Psi(k, z) \tilde{h}(k, z) dz. \quad (26)$$

This expression gives the induced current profile for an arbitrary generation, provided that $x_0 > \epsilon$.

To illustrate the consequences of eqn (26) we need to specify the form of $h(x, z)$. We consider here the case of silicon and use as an approximate generation function a three-dimensional Gaussian, as proposed by Fitting *et al.* [18]. Following Ref. [18] we write

$$h(x - x_0, z) = \frac{1.14}{2\pi\sigma^2} \exp \left[-\frac{(x - x_0)^2 + (z - z_0)^2}{2\sigma^2} \right], \quad (27)$$

where z_0 , and σ are related to the primary electron range R by the relations

$$z_0 = 0.3 R, \sigma = R/\sqrt{15}. \quad (28)$$

The factor 1.14 in eqn (17) is a consequence of the normalization to unity of the truncated Gaussian used for representing the depth-dose function. The expression (27) is particularly convenient for the calculations; in fact we have (Ref.[15], p. 1147)

$$\bar{h}(k, z) = \frac{1.14}{2\pi\sigma} \exp \left[\frac{k^2\sigma^2}{2} - \frac{(z - z_0)^2}{2\sigma^2} \right]. \quad (29)$$

Substituting this expression in eqn (26) and performing the integration with respect to z we are led to the final expression for $I(x_0)$

$$I(x_0) = \frac{2}{\pi} \int_0^\infty \frac{k}{\mu^2} \left\{ \exp \left(-\frac{k^2\sigma^2}{2} \right) - 0.57 \exp \left(\frac{\lambda^2\sigma^2}{2} - \mu z_0 \right) \right. \\ \left. \times \frac{s}{\mu + s} \operatorname{erfc} \left[\frac{\sigma}{\sqrt{2}} \left(\mu - \frac{z_0}{\sigma^2} \right) \right] \right\} \sin(kx_0) dk. \quad (30)$$

Since the lateral extension of the generation (27) is $\epsilon = 2\sigma = R/2$, eqn (30) represents the actual induced current profile for $x_0 > R/2$ only. In the case of a sample with finite thickness d , the current profile is obtained from (30) by replacing the integral with a series according to the procedure described in the previous Section. The equivalence between the resulting expression and eqn (23) of Ref.[13] can be verified in the same way as for eqn (20).

The influence of s and R on the behaviour of the function $I(x_0)$ has been studied by performing the integration (30) numerically, using the rational approximation for the error function given in [19]. For $s = 0$, $I(x_0)$ can be expressed in closed form in terms of error functions (see Ref.[15], p. 497); this property is useful for checking the accuracy of the numerical evaluation.

Some representative results are shown in Fig. 2, where the logarithm of the collected current has been plotted as a function of the normalized beam-junction distance x_0/L , for selected values of the ratio R/L and the dimensionless parameter $S = sL$. Figure 2 shows that the current profiles are influenced by the value of the surface recombination velocity, this influence being larger if the beam penetration depth R is small in comparison to the diffusion length L . A pure exponential current decrease (i.e. a straight line in the plot of Fig. 2) is obtained only for $S = 0$: in this case the profile is almost insensitive to the value of R , and the reciprocal slope gives the diffusion length independently of the beam energy. For $S > 0$ the curves can be considered approximately straight only for large values of x_0/L , but the related slope is dependent on S ; this behaviour and the associated problem of extracting the true diffusion length from experimental scans are well known from previous analyses [7, 8].

Figure 2 also shows that an increase of R produces an upward shift of the curves, which is larger for larger

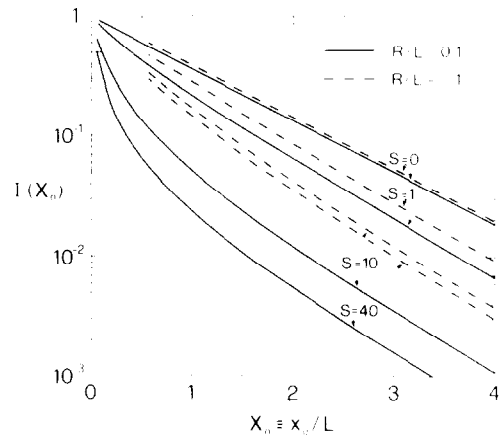


Fig. 2. Normalized collected current vs beam-junction distance for different surface recombination velocities and electron ranges, as calculated from eqn (30).

values of S , but the slope of the (approximately) straight part is practically unaffected by the change of R ; this behaviour is consistent with the experimental observations and calculations of Refs.[5, 12]. However, the value of the slope is still dependent on S , so that it appears that accurate values of L and S can only be obtained by fitting the experimental scans to the theory [5, 12].

5. CONCLUSIONS

This paper gives an analytical description of the determination of semiconductor diffusion lengths by SEM operating in the configuration shown in Fig. 1.

An integral expression has been derived for the carrier collection probability, which is equivalent to that generally used but offers the following advantages: (a) it contains elementary functions only, (b) it can be easily adapted to the case of a sample with finite thickness and (c) it is convenient for discussing the case of an extended generation. Using this expression, the induced current profile due to a three-dimensional Gaussian generation could be expressed through a one-dimensional Fourier transform. This transform has been evaluated numerically for investigating the influence of the dimensions of the generation region on the induced current scans, for different values of the surface recombination velocity.

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APPENDIX

Proof of the equivalence between eqn (15) and van Roosbroeck's expression

Van Roosbroeck's treatment [10] for a point (or line) source at (x', z') leads to the following expression for the carrier collection probability (see e.g. Ref. [7])

$$Q(x', z') = \frac{2}{\pi} \lambda x' \left\{ \int_0^{z'} \frac{K_1[\lambda(x'^2 + z^2)^{1/2}]}{(x'^2 + z^2)^{1/2}} dz + e^{\lambda z'} \int_{z'}^{\infty} \frac{K_1[\lambda(x'^2 + z^2)^{1/2}]}{(x'^2 + z^2)^{1/2}} dz \right\}, \quad (\text{A1})$$

where λ is the reciprocal of the diffusion length and K_1 is the modified Bessel function of the second kind of order one.

Using the identity (Ref. [15], p. 498)

$$\frac{\lambda x'}{(x'^2 + z^2)^{1/2}} K_1[\lambda(x'^2 + z^2)^{1/2}] = \int_0^{\infty} \frac{\exp[-z(k^2 + \lambda^2)^{1/2}]}{(k^2 + \lambda^2)^{1/2}} k \sin(kx') dk \quad (\text{A2})$$

eqn (A1) becomes

$$Q(x', z') = \frac{2}{\pi} \left[\int_0^{z'} dz \int_0^{\infty} \frac{k}{\mu} e^{-\mu z} \sin(kx') dk + e^{\lambda z'} \times \int_{z'}^{\infty} dz e^{-\lambda z} \int_0^{\infty} \frac{k}{\mu} e^{-\mu z} \sin(kx') dk \right], \quad (\text{A3})$$

where $\mu = (k^2 + \lambda^2)^{1/2}$. Inverting the integration order we obtain

$$Q(x', z') = \frac{2}{\pi} \int_0^{\infty} \frac{k}{\mu} \left[\int_0^{z'} e^{-\mu z} dz + e^{\lambda z'} \int_{z'}^{\infty} e^{-(\mu + \lambda)z} dz \right] \sin(kx') dk. \quad (\text{A4})$$

The evaluation of the two integrals with respect to z is straightforward and leads to eqn (15).