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MODELING THE EBIC MEASUREMENTS OF DIFFUSION LENGTHS AND THE RECOMBINATION CONTRAST AT EXTENDED DEFECTS

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Résumé - Une description alternative, basée sur le concept de probabilité de collecte, est proposée pour l'interprétation d'expériences typiques réalisées par la technique du courant induit par faisceau d'électrons (EBIC) associée au microscope électronique à balayage. On montre que la distribution $\varphi(r)$ de cette probabilité dans l'échantillon obéit à une équation de diffusion homogène et que le courant induit résulte de l'excitation des propriétés de l'échantillon par la fonction de génération du faisceau électronique. L'objectif des expériences EBIC est de déterminer les paramètres essentiels caractérisant le semiconducteur ou le défaut, dont φ dépend. Différentes méthodes d'accès à cette information sont discutées et quelques nouvelles possibilités sont présentées.

Abstract - An alternative description is proposed of typical experiments that are performed with the electron beam induced current (EBIC) technique of the scanning electron microscope, on the basis of the notion of charge-collection probability. It is shown that the distribution $\varphi(r)$ of this probability in the specimen obeys a homogeneous diffusion equation, and the induced current results from probing this sample property with the generation function of the electron beam. EBIC experiments aim at determining the essential semiconductor or defect parameters upon which φ is dependent. Different methods of recovering this information are discussed and some new possibilities are presented.

1 - INTRODUCTION

The electron beam induced current (EBIC) technique of the scanning electron microscope (SEM) has been used extensively to characterize semiconductor materials and devices; review articles on the principles and applications of EBIC are available /1-3/.

This paper aims at demonstrating that different EBIC experiments can be given a common phenomenological description using the notion of charge collection probability, i.e. the probability that an injected minority carrier will be collected by the junction contact and thus contributes to the induced current. The concept of one-dimensional charge collection probability has been used by Possin and Kirkpatrick /4/ to analyze quantitatively EBIC measurements on planar p-n junctions. Here this notion will be generalized to three dimensions and moreover, it will be shown that the charge-collection probability distribution in a given structure can be calculated directly by solving a homogeneous diffusion equation, even in the presence of defects. The induced current can then be described as the result of probing this local property of a device with the generation volume of the SEM electron beam.

As observed in /4/, the charge-collection probability distribution contains all information about the motion of minority carriers that can be obtained by the EBIC technique. Therefore characterizing quantitatively a semiconductor structure by EBIC means recovering this distribution (or the essential parameters upon which it is dependent), under the assumption that the probe function of the electron beam (i.e. the spatial distribution of the generation) is known. Typical methods used to perform this reconstruction and new possibilities are discussed, making reference to specific experiments for clarity of the discussion.

2 - THE CHARGE COLLECTION PROBABILITY

The usual way of describing an EBIC experiment follows the sequence of physical processes that occur in the semiconductor sample as a result of the electron bombardment, i.e.:

Fig.1 - The two equivalent descriptions of charge collection. (a): through the density $p(r)$ of beam-injected minority carriers; (b): by the charge collection probability $\phi(r)$.

- a) the generation of electron-hole pairs by the electron beam
- b) the transport of beam-generated minority carriers
- c) the collection of minority carriers by the junction.

The process a) is described by introducing the generation function $g(r)$ [$\text{cm}^{-3} \text{s}^{-1}$], which gives the generation rate of pairs per unit volume at the position r in the sample. A number of analytical approximations of this function have been used, to simplify the analytical treatment of the problem b) /1/, the simplest generation model being that of the point source; Monte-Carlo simulations of $g(r)$ have also been employed /5,6/. The generation of carriers with spatial rate $g(r)$ brings about a steady-state concentration $p(r)$ [cm^{-3}] of excess minority carriers. The two functions are connected by the diffusion equation:

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

where D and τ are the diffusion coefficient and lifetime of minority carriers, respectively; τ may depend on r if the sample is not homogeneous or contains localized defects. To specify uniquely p for a given g , we must add to Eq.(1) suitable boundary conditions. For instance, in the idealized case illustrated in Fig.1a (semi-infinite semiconductor, with the surface as collector), the boundary conditions are:

$$p(r) = 0 \quad \text{at } z=0; \quad p(r) = 0 \quad r \rightarrow \infty \quad (2)$$

Once the solution of Eq.(1) with (2) has been determined (step b)), the collected particle current I [s^{-1}] is calculated by integrating over the collection plane $z=0$ the density of the diffusion current (step c)):

$$I = D \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left. \frac{\partial p}{\partial z} \right|_{z=0} dx dy \quad (3)$$

The resulting expression for I is /7/:

$$I = \int_0^{\infty} \exp(-z/L) g_1(z) dz \quad (4)$$

where $L = (D\tau)^{\frac{1}{2}}$ is the minority-carrier diffusion length, and

$$g_1(z) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} g(\underline{r}) \, dx \, dy \quad (5)$$

is the depth distribution of the generation. Equation (4) shows that I can be expressed through two one-variable functions: $\exp(-z/L)$, which is related to a specimen property (L), and $g_1(z)$ which describes the external generation. Therefore, one might wonder whether it was really necessary to calculate first the three-dimensional distribution $p(\underline{r})$ to obtain Eq.(4). Actually the calculation of $p(\underline{r})$ can be avoided by introducing the function $\varphi(\underline{r})$ which represents the charge collection probability at the point $\underline{r}$.

On the basis of a reciprocity theorem for charge collection /8/, it has been shown that $\varphi(\underline{r})$ obeys the homogeneous version of Eq.(1):

$$\nabla^2 \varphi(\underline{r}) - \frac{1}{\tau} \varphi(\underline{r}) = 0 \quad (6)$$

with the boundary conditions

$$\varphi(\underline{r}) = 1 \quad \text{at } z=0; \quad \varphi(\underline{r}) = 0 \quad r \rightarrow \infty. \quad (7)$$

Equations (6), (7) involve only device properties and not those of the generation, and also take into account the symmetry of the sample. In fact, it is easy to see that the solution to Eqs.(6), (7) is the simple one-variable function

$$\varphi(z) = \exp(-z/L) \quad (8)$$

The independence of φ of x, y is a consequence of the translational symmetry of the structure of Fig.1a along these directions. The induced current I is then obtained by multiplying the generation rate at a depth z by the corresponding charge collection probability and integrating over z ; this leads again to Eq.(4). The presence of a depletion layer, where all generated carriers are assumed to be collected, can be taken into account simply by specifying that $\varphi = 1$ within the depleted region. In the more general case of a specimen where $\varphi = \varphi(\underline{r})$, Eq.(4) becomes:

$$I(\underline{t}) = \int_V \varphi(\underline{r}) g(\underline{r}-\underline{t}) \, dV = \int_0^\infty \varphi * g \, dz \quad (9)$$

where $\underline{t} \equiv (x_0, y_0)$ is the vector describing the beam position in the xy plane and the symbol $*$ denotes the two-dimensional convolution.

The alternative picture of charge collection following from Eq.(9) is represented schematically in Fig.1b and includes the two following steps of the modeling:

- a1) the distribution of the charge collection probability in the specimen
- b1) the sampling of this distribution with the beam probe.

This formulation corresponds closely to the theory of image formation in scanning microscopes /9/; it may simplify both the analytical calculations, as just shown in a particular case, and the numerical treatment of the charge collection problem in configurations of low symmetry. In fact, the homogeneous Eq.(4) is well suited to numerical solution; once $\varphi(\underline{r})$ has been calculated over a suitable grid, the value of I for different $g(\underline{r})$ (either known analytically or through Monte Carlo simulation) can be computed by using the discretized version of Eq.(9).

3 - THE CHARGE COLLECTION EFFICIENCY

Having outlined how the beam-induced current can be conveniently computed, let us consider the inverse problem i.e. how from EBIC measurements, through proper modeling, information can be gained on electrical properties of the material/device under investigation.

Here the simple one-dimensional case of a Schottky diode irradiated with a stationary electron beam will be examined (Fig.2). From Eq.(9), with $\underline{t} = 0$, and writing more explicitly $g_1(z) = g_0 h(z, E)$, where g_0 [s^{-1}] is the total generation rate and $h(z, E)$ is the normalized one-dimensional generation function, we have

$$I(E) = g_0 \int_0^\infty \varphi(z) h(z, E) \, dz \quad (10)$$

It is convenient to introduce the charge collection efficiency of the device $\eta(E) = I(E)/g_0$ /2,4/, i.e. the fraction of the injected carrier that is collected and gives rise to the

Fig.2 - Schematic representation of charge collection efficiency measurements on a Schottky diode.

induced current. A measurement of $\eta(E)$ for different values of E yields the data from which information about $\varphi(z)$ is obtained [4,11,12].

It is convenient to rewrite Eq.(10) using in place of E the primary electron range R , which for a given material is a known function of E . Thus η and φ will be expressed as functions of variables with the same physical dimension (that of a length); moreover, this substitution allows exploiting the empirical result [10] that $h(z, E(R))$ is only dependent upon z/R and not on z and R separately. Hence Eq.(10) becomes [4]:

$$\eta(R) = \frac{1}{R} \int_0^{\infty} \varphi(z) \Delta(z/R) dz \quad (11)$$

where $\Delta(z/R)$ is a universal function independent of the beam energy [10]. If we were able to probe the device with a point source of carriers, the measured collection efficiency would equal the collection probability at the source position. Since experimentally we can only probe the sample with an extended source, we measure a smeared version of $\varphi(z)$, i.e. $\eta(R)$.

The method most frequently used to recover information about φ (in particular to determine the value of the bulk diffusion length L of the semiconductor) from $\eta(E)$ data assumes the form of φ to be known a priori in terms of a small number of device parameters; the values of these parameters are then found by fitting the theoretical expressions obtained from Eq.(11) to experiment [4,11,12]. Typical parameters for a Schottky diode are the thickness h of the metallization, the width W of the depletion layer and L . For the purpose of determining L , however, it is not necessary to fit the whole $\eta(R)$ profile, but only its high energy part, which is more sensitive to the value of L [2,11]. An approximate expression for $\eta(R)$ valid in the limit of $R \gg h + W$ has been proposed recently [13]:

$$\eta(R) \simeq \exp(W/L) \eta_0(R/L) \quad (12)$$

where η_0 is the collection efficiency of an ideal Schottky barrier with $h=W=0$.

The method of the model function is useful as long as the form assumed for φ is known to describe adequately the device and the number of parameters involved is small.

There are relevant practical cases, however, where these conditions are not met; this happens, for instance, with the Schottky structure of Fig.2 if layers with enhanced recombination (and generally unknown width and position) are present in the device. In this case a direct method of recovering φ from $\eta(R)$ without any assumption about the form of φ appears desirable. This is possible in principle, since Eq.(11) is an integral equation which has a unique solution for a given $\eta(R)$ and a known Δ [4]. When Δ is a polynomial of the variable $\xi = z/R$, as in the approximation by Everhart and Hoff [10], an explicit solution for

Fig.3 - Schematic illustration of collection efficiency measurements on bevels for depth profiling of the diffusion length. The actual value of α is about 3° .

φ of Eq.(11) can be found and has the form /14/:

$$\varphi(R) = F(R, \eta, \eta', \eta'') \quad (13)$$

where η' and η'' are the first and second derivative of $\eta(R)$, respectively. The application of Eq.(13) to practical cases, however, requires evaluating reliably η' and η'' from actual noisy experimental data, and has not yet been attempted.

Another situation where it is difficult to give a priori the form of φ occurs when L is depth-dependent, i.e. when $L=L(z)$, for instance as result of gettering treatments. The reconstruction of the relevant function $L(z)$ is made easier, if the experimental arrangement of Fig.3 is used, i.e. if η is measured at a fixed beam energy at different positions on a Schottky diode fabricated on the sample after angle beveling. This makes it possible to probe the semiconductor at different depths with a fixed generation volume, whereas in energy-dependent measurements of η different depths are reached by changing the extension of the generation region. Sampling a variable property, as $L(z)$, with a fixed probe is expected to yield better chance of recovering directly this property.

In fact, if $\eta(z)$ is the value of the collection efficiency when the beam is at a distance $x=z/\sin\alpha$ from the bevel edge (α is the bevel angle), it is possible to give a simple relation between $L(z)$ and $\eta(z)$ in the ideal case of negligible thickness of the depletion layer /15/:

$$L(z+a/2) \simeq f(z)/\sqrt{1+f'(z)} \quad (14)$$

where

$$f(z) = -a/\ln \eta(z) \quad (15)$$

a being the average generation depth. The presence of the derivative in Eq.(14) sharpens up the smooth experimental $\eta(z)$ profile to yield $L(z)$ (Fig.4). The advantage of performing the measurements at a fixed beam energy is also reflected in the form of Eq.(14), which involves the first derivative of η only, and not the second one as in Eq.(13).

The modeling of experiments that involve a two-dimensional distribution of φ (e.g. the analysis of EBIC scans obtained on a cross-section of a p-n junction) is obviously more difficult and further approximations must be introduced to limit the complexity of the discussion. Some methods and problems of the two-dimensional case are discussed in /16/.

4 - THE EBIC CONTRAST OF DEFECTS

Equation (6) for the charge-collection probability also holds if τ is position-dependent, and therefore can be used to describe charge collection in the presence of semiconductor defects. By representing a defect as a region F where the lifetime τ' (supposed constant

Fig.4 - Computer simulated collection efficiency profile $\eta(z)$ for a hypothetical diffusion length profile (continuous line). The reconstructed diffusion length profile (dots) has been calculated using Eqs. (14), (15).

within F) is smaller than the bulk lifetime τ /7/, we obtain from Eq.(6)

$$\nabla^2 \varphi(\underline{r}) - (\gamma/D) e(\underline{r}) \varphi(\underline{r}) - 1/L^2 \varphi(\underline{r}) = 0 \quad (16)$$

where $\gamma = (1/\tau'' - 1/\tau)$ and $e(\underline{r}) = 1$ inside F and vanishes elsewhere; the boundary conditions are still those of Eq.(7).

The factor γ [s^{-1}] represents the recombination strength of the defect. Equation (16) can be solved approximately by treating the term containing γ as a perturbation and writing $\varphi = \varphi_0 + \varphi_1$, where φ_0 is the solution to Eq.(16) in absence of the defect (see Eq.(8)), and φ_1 is a (small) deviation from φ_0 produced by the presence of the defect; the approximate solution is /16/:

$$\varphi(\underline{r}) = \varphi_0 + \varphi_1 = \exp(-z/L) - \gamma \int_F \exp(-z'/L) G(\underline{r}, \underline{r}') dV' \quad (17)$$

where G is the Green's function of Eq.(6) that vanishes at the surface. The second term in Eq.(17) represents the decrease of the charge collection probability in the device due to the presence of the defect. This produces a decrease of the EBIC current, which can be calculated from Eq.(9) to be

$$I^* = \int_0^\infty g * \varphi_1 dz \quad (18)$$

The corresponding image contrast is given by

$$i^*(\underline{t}) = \frac{I^*}{I_0} = \frac{\gamma}{I_0} \int_0^\infty dz \left\{ g * \int_F \exp(-z'/L) G(\underline{r}, \underline{r}') dV' \right\} \quad (19)$$

where I_0 is the background current and has the expression already given in Eq.(4). It is not difficult to check that Eq.(19) reproduces the expression derived previously /7/ starting from the solution of the diffusion equation for $p(\underline{r})$.

The two approaches to the defect contrast calculation correspond to different but equivalent descriptions of charge collection, as in Sec.2. According to the former model /7/, the presence of a defect modifies the distribution $p(\underline{r})$ of the beam-injected minority carriers (in a way that is dependent on the beam-defect distance) and hence the induced current through a reduction of the gradient of p at the charge-collecting surface. In the present

approach, a defect reduces in its surroundings the probability that a generated carrier reaches the junction (i.e. ϕ); the induced current is the result of sampling ϕ with the generation volume, and therefore is lower when the beam is near the defect. The formulation of the problem in terms of charge collection probability does not simplify, in general, the expression of the image contrast, since the presence of a defect breaks the symmetry of the original device. For defects of special shape, however, the defect-device configuration may retain some symmetry and the introduction of ϕ will allow some simplification of the treatment.

Eq.(19) has been generally used to determine γ from EBIC measurements by computing $i^*_{\max}$, i.e. the maximum contrast, and comparing this value to the experimental one. There is, however, a further characteristic property of $i^*(\underline{r})=i^*(x_0, y_0)$ that can be used advantageously for the same purpose, i.e., its integral over the image plane:

$$V = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} i^*(x_0, y_0) dx_0 dy_0 \quad (20)$$

If i^* is plotted on the z axis as a function of x_0, y_0 the quantity $V [\text{cm}^2]$ represents a volume, which describes the overall influence of the defect on the image contrast. Substituting Eq.(19) into Eq.(20) and taking into account that $G(\underline{r}, \underline{r}') = G(x-x', y-y', z, z')$, since the structure of Fig.1, in absence of the defect, has translational invariance along x, y , we obtain:

$$V = \frac{\gamma}{I_0} \int_0^\infty dz h(z) \left\{ \int_F \exp(-z'/L) G_1(z, z') dV' \right\} \quad (21)$$

where G_1 is the one-dimensional Green's function resulting from the integration of G with respect to x, y . The evaluation of the integral in large brackets requires actually an integration with respect to z' only, since the function to be integrated over F depends only on this variable. Equation (21) shows that, for a given defect geometry, V can be calculated in terms of the one-variable functions h and G_1 , whereas the evaluation of $i^*_{\max}$ would involve the three-variable functions g and G .

The evaluation of V from an experimental image does not require much additional effort, if a digital acquisition system is connected to the SEM, and greatly simplifies the calculations required to recover γ from EBIC contrast data. An example of the use of an integral property of the EBIC image (the area of the contrast profile) to evaluate the recombination strength of dislocations has been reported in /17/.

To illustrate another useful property of V , let us consider a straight semi-infinite dislocation tilted by an angle α from the normal to the sample surface (the z axis). In this case $dV' = (\sigma/\cos \alpha) dz'$, σ being the cross-section of the recombination cylinder associated with the dislocation; the product $\gamma_d = \gamma \sigma [\text{cm}^2 \text{ s}^{-1}]$ can be called line recombination velocity of the dislocation. Hence Eq.(21) becomes

$$V = (1/\cos \alpha) \frac{\gamma_d}{I_0} \int_0^\infty dz h(z) \int_0^\infty \exp(-z'/L) G_1(z, z') dz' \quad (22)$$

which gives, in particular, the relation

$$V(\alpha) = V(0)/\cos \alpha \quad (23)$$

between the value of V of a straight dislocation tilted by α from the z axis and that of a perpendicular dislocation with the same γ_d . Therefore, for this defect, a deviation from the normal incidence changes the maximum contrast and lowers the symmetry of the EBIC image, but leaves the product $V \cdot \cos \alpha$ unaffected. This property can be useful to compare the activity of approximately straight dislocations with different, but known, inclination angles with respect to the surface.

5 - DISCUSSION AND CONCLUSIONS

The description of steady-state EBIC experiments in terms of charge-collection probability offers some formal and computational advantages, but relies on the same physical approximations used previously /7/. Thus, for instance, the model assumes low injection conditions, where $\phi(\underline{r})$ can be calculated independently of $g(\underline{r})$. Injection-dependent effects (both in the bulk /18/ and at defects /19,20/) can be described by taking into account that the probe

function $g(r)$ can modify the pre-existent distribution of the charge-collection probability, so that the calculation steps a1) and b1) of Sec.2 would no longer be independent.

The present discussion of the defect contrast uses the first order (linear) approximation of ϕ in the presence of a defect. Higher order approximations to the contrast have been developed by Pasemann /21/ for a straight dislocation parallel to the surface, and an exact calculation has been given for a plane grain boundary perpendicular to the sample surface /22/. These treatments, while allowing a more accurate determination of the strength of highly recombining defects, produce a non-linear contrast function (i.e. i^* is not proportional to γ) and therefore the advantages related to linearity are lost. The subject of EBIC contrast modeling has been reviewed recently by Jakubowicz /23/.

Further extensions of the linear model have also been considered. Thus Joy and Pimentel /24/ and Sieber /25/ have described recombination at a dislocation partially lying in the depletion region, where carrier motion is not longer purely diffusive, by attributing to the dislocation an effective radius (and hence a recombination strength γ_d) dependent on the depth position (or, equivalently, on the electric field) in the depletion layer. Wilshaw and Booker /20/ have specified in γ_d , which has been introduced in Sec.4 on a purely phenomenological basis, its dependence on the temperature and injection level by modeling additionally the underlying microscopical recombination process.

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