Modeling Photoluminescence Spatial Mapping of an Isolated Defect under Uniform and Selective Excitation

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***Abstract* — In this work, two different excitation/detection modes, U/L mode and L/L mode for probing an extended defect are compared and discussed. A contrast function is introduced to describe the influence of the defect. We have found that the contrast function not only depends on dimensionality of the system (1-D vs. 2-D), but also depends on the excitation/detection mode. Photoluminescence mapping data using the two modes to study an isolated defect in GaAs are analyzed using our models. The results suggest that the L/L mode can, in principle, offer significantly better spatial resolution than the U/L mode.**

***Index Terms* — extended defect, diffusion, recombination, photoluminescence, steady state, contrast function, modeling.**

I. Introduction

Spatially resolved spectroscopy techniques such as photoluminescence (PL) and cathodoluminescence (CL) are often used to investigate the effect of an individual extended defect on carrier diffusion and recombination. Two distinctly different excitation/detection modes are of particular interest because they are the most common configurations: (1) Uniform illumination/Local detection (U/L mode) and (2) Local excitation/Local detection (L/L mode). For the U/L mode, the sample is illuminated by a large uniform excitation beam and the emission is measured in a spatially resolved manner either imaged with a CCD camera or mapped point-by-point; for the L/L mode, a tightly focused excitation beam is used and the emission is collected from the same excitation site, which is typically accomplished with a confocal optical technique. For the typical CL measurement, it belongs to neither U/L nor L/L, because the emission from all the carriers, including those diffused away from the excitation site, are collected. An alternative to the U/L model is would be the L/U mode, Although the electron excitation beam size in CL could be much smaller than that of a laser beam in PL, the spatial resolution is determined by the carrier diffusion in CL. Superior spatially resolution comparable to the electron beam size can only be achieved for the system with a small carrier diffusion length. Recently we have studied the effect of an extended defect on the carrier diffusion in GaAs using PL in both modes [1,2]. In both cases, the presence of an extended defect (presumably a dislocation) is found to result in a dark region centered at the defect site. However, the effective range of the defect or the size of the affected region is found to vary with the excitation density [1,2], and even non-monotonically in the L/L mode [2]. In the literature, a contrast function C(x) $\propto$ exp(-x/L), where L is the diffusion length, is often used to describe the decay of the emission intensity with distance from the defect center, although it has been pointed out that the decay is actually steeper than this function in a two-dimensional (2-D) model [3]. In the present work, we address two issues: (1) how do we obtain the diffusion length from the experimental data? and (2) how do the two modes compare in terms of the underlying mathematical model and the spatial resolution that can be achieved?

II. Carrier Distribution with One Defect

A. One-dimensional (1-D) problem

We first consider the L/L mode. It is convenient for initial analysis to start with the 1-D case. In steady state, the excess carrier density in the semiconductor is governed by the following 1-D continuity equation:

$$\frac{\partial^2 n(x)}{\partial x^2}-\frac{n(x)}{L^2}+\frac{G\delta(x)}{D}=0 \quad , \qquad (1)$$

where *n(x)* represents the carrier density, *L* is the diffusion length, *D* is the carrier diffusivity, G is the generation rate with the assumption that the excitation profile is a delta function, and L = √(Dτ) with τ being the carrier lifetime. Assuming that an isolated defect at $x_0 > 0$ has an infinite recombination rate, and the excitation is at x = 0, we have these boundary conditions: $n(x_0) = 0$ and $n(\pm\infty) = 0$. The solution of Eq.(1) satisfying these boundary conditions can be shown to be:

$$n(x,x_0)=\begin{cases}\dfrac{1}{2}\dfrac{G\tau[e^{-\frac{x}{L}}-e^{\frac{x}{L}-\frac{2x_0}{L}}]}{L} & (0\le x\le x_0)\\[2ex] \dfrac{1}{2}\dfrac{G\tau[1-e^{-\frac{2x_0}{L}}]e^{\frac{x}{L}}}{L} & (x\le 0)\end{cases} \quad . \qquad (2)$$

Note that letting $x_0 \to \infty$ leads to the solution for the defect-free case, i.e., $n_0 \exp(-|x|/L)$ with $n_0 = G\tau/(2L)$. Following the conventional analysis, the contrast function can be defined as $C(x_0) = [n_0-n(0,x_0)]/n_0$, which describes the relative reduction of the carrier density at the excitation and detection site x = 0 when the defect is at x = x_0. Explicitly,

$$C(x_0) = e^{-\frac{2x_0}{L}} \quad \text{or} \quad \ln C(x_0) = -\frac{2x_0}{L}. \tag{3}$$

Surprisingly, the slope of - $\ln C(x_0)$ vs. x_0 is 2/L, a factor of 2 larger than one might assume intuitively.

For the U/L mode, the steady state solution is simply n = gτ in the absence of defects, where g is the generation rate. Adding a defect is equivalent to introducing a negative generation – Gδ(x), with G = 2Lg at the defect site x = 0. The combined solution is then gτ[1-exp(-|x|/L)], which yields n(0) = 0 and C(x) = exp(-x/L). Clearly, the contrast functions are different for the two excitation/detection modes. The results imply that the effect of the defect is more localized in the L/L mode, which should provide substantially better spatial resolution to distinguish nearby defects.

Although this 1-D problem in the L/L mode have been solved analytically as described above, we introduce an alternative superposition method to solve the same problem because it will be very useful for the more challenging 2-D problem. We note that the effect of the defect can be simulated as an additional negative generation at x_0 with a generation rate of G_D = –G/(2L) exp(-x_0/L), which will yield zero net carrier density at x_0. The contribution of this negative source at the detection site x = 0 would be G_D exp(-x_0/L), exactly the same as the result given above.

B. 2-D Case Without Defect

A 2-D model is appropriate for a relatively thin layer that has nearly uniform carrier density along the growth direction, like the GaInP/GaAs/GaInP double heterostructure used in our recent studies [1,2]. Generally the excitation site is selected at the origin *r* = 0. The diffusion equation in cylindrical coordinates is given as

$$\frac{\partial^2 n(r)}{\partial r^2} + \frac{1}{r}\frac{\partial n(r)}{\partial r} - \frac{n(r)}{L^2} + \frac{G\delta(\vec{r})}{D} = 0 \ , \tag{4}$$

where $\delta(\vec{r})$ is the 2-D delta function. The solution of Eq. (4) is a modified Bessel function $K_0(\xi)$. If we apply the boundary conditions $n(\infty) = 0$ and $2\pi r_0 \frac{dn}{dr}\Big|_{r_0} = \frac{G\tau}{L^2}$ with $r_0 \to 0$. The result is: $n(r) = G\tau/(2\pi L^2)K_0(r/L)$. Though $K_0(r/L)$ is divergent at r = 0, $rK_0(r/L)$ is integrable about r = 0. We can replace $K_0(0)$ with the average of $K_0(r)$ over a small circle of radius ε:

$$\bar{K}_0(0) = \lim_{\varepsilon \to 0} \frac{1}{\pi\varepsilon^2}\int_0^\varepsilon K_0(r) 2\pi r dr \ , \tag{5}$$

which could be understood as having a finite probe size ε. In the PL measurement, it could be the diffraction limit spot size.

C. The Superposition Principle in 2-D Case with Defect

Now we use the superposition principle to derive the carrier distribution with a defect. Firstly the L/L mode is considered and a schematic view of the configuration is shown in Fig. 1.

Suppose that there is an infinitely large plane without defects and the carrier density generated by the laser beam at the center r = 0 is n_0, so at a distance r_0 away from the center, the density drops to ηn_0. Obviously, η is a decay function in the range of $0<\eta<1$. We know that η depends only on the distance r_0, independent of the density at the origin. If a defect with infinite recombination velocity is present at r_0, a negative generation source yielding a density $-\eta n_0$ is needed to ensure that the density at the defect site is zero. Now using the superposition principle, the net density at r = 0 is the superposition of the contributions from the incident light and the negative generation source, which totals $n_0 - \eta^2 n_0$.

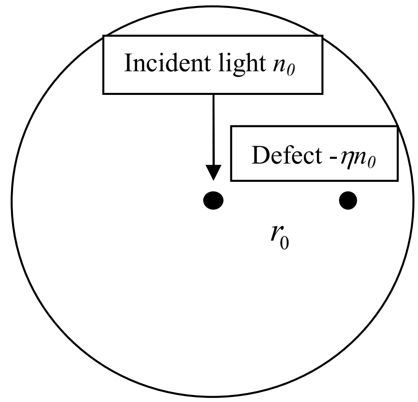


Fig. 1. Schematic illustration of the 2-D model in the L/L mode.

According to the definition of the contrast function,

$$C = \frac{n_0 - (n_0 - \eta^2 n_0)}{n_0} = \eta^2 \cdot$$

So we can conclude that the contrast function *C* in the 2-D case is the square of the decay coefficient, where the decay coefficient η is the ratio of local carrier density to the density at the excitation position. Applying the solution we have, the decay coefficient η is equal to $K_0(r/L)/\bar{K}_0(0)$, so we have

$$C = \eta^2 = \frac{K_0^2(\frac{r}{L})}{\bar{K}_0^2(0)} \ . \tag{6}$$

For the U/L mode, the steady state solution is similar as that in 1-D case. We assume n = $g\tau$ in the absence of defects. At the defect site, the local carrier density is $-\frac{G'}{2\pi D}K_0(\frac{r}{L})$, where G' represents the effective generation rate of the defect. As discussed in 1-D case, a defect is assumed with infinite recombination rate, so we have

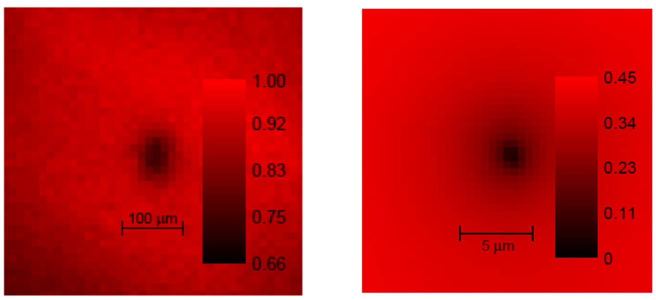
$$\lim_{\varepsilon \to 0}\int_0^\varepsilon -\frac{G'}{2\pi D}K_0(\frac{r}{L}) \cdot \delta(\vec{r}) 2\pi r dr + g\tau = 0 \text{, and}$$

$$G' = 2\pi g L^2 / \bar{K}_0(0) \, .$$

Then the carrier density is $g\tau - \frac{g\tau}{\bar{K}_0(0)} K_0(\frac{r}{L})$, and the contrast function is $K_0(\frac{r}{L}) \Big/ \bar{K}_0(0)$.

We note that these results are similar to what we obtained in the 1-D case, where the contrast function is $\eta = exp(-x_0/L)$ without the defect and $\eta^2 = exp(-2x_0/L)$ with the defect.

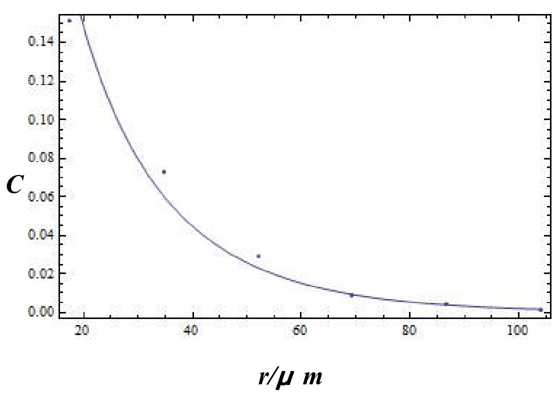
D. Experimental Demonstrations



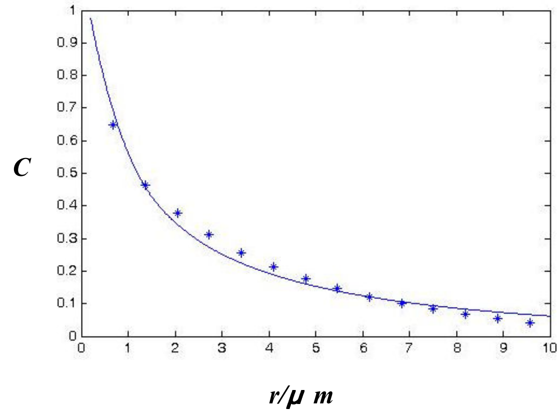
(a)U/L mode (b)L/L mode

Fig. 2. PL images of an isolated dislocation in GaAs using 2 distinct excitation/detection modes

Fig. 2 shows representative examples of PL mapping for an isolated defect in a GaInP/GaAs/GaInP double heterostructure [1-2,4]. While the individual defects analyzed in the independent measurements are different, they were observed on the same sample and may have similar characteristics. We use these maps for a preliminary test of the models.



(a) U/L mode



(b) L/L mode

Fig.3. Variation in contrast with distance from the defect.

The radial contrast profiles deduced from the images are shown in Fig. 3. The contrast results are fitted to $aK_0(\frac{r}{L})$ for the U/L mode and to $bK_0^2(\frac{r}{L})$ for the L/L mode, where a and b are constants. The diffusion lengths deduced from the fits are 22um and 25um, respectively. These two values are rather close, even though the effective range of the defect appears much larger in the U/L mode relative to the L/L mode.

III. Conclusions

In this report, the effect of an isolated extended defect on the carrier recombination and diffusion is modeled for two widely-used excitation/detection modes, and the respective contrast functions are determined. The models are applied to PL mapping images obtained via the two modes. The results confirm that the defect appears much more localized in the L/L mode, indicating that the L/L configuration can give substantially better spatial resolution when PL or CL mapping is used to resolve individual defects.

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