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Analytical model for the quantum-confined Stark effect including electric field screening by non-equilibrium carriers

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We have derived an analytical approximation for the energy levels in a symmetric quantum well applicable in a wide range of the electric field variation. Suppression of the quantum-confined Stark effect due to the electric field screening by non-equilibrium carriers is considered self-consistently within the perturbation theory. Theoretical predictions are compared with available observations. Specific features of the quantum-confined Stark effect in light-emitting diode heterostructures are discussed.

1 Introduction

Quantum-confined Stark effect (QCSE), i.e. a red shift of the band-to-band transition energy caused by a strong electric field in a quantum well (QW), is an essential feature of III-nitride heterostructures where the built-in field may be as high as 1–3 MV/cm due to the spontaneous polarization and piezoeffect [1]. The QCSE is known to be sensitive to the non-equilibrium carriers in the QW, which may screen effectively the electric field being at high concentrations [2–4]. In addition, the QCSE manifestation in the photoluminescence (PL) or electroluminescence (EL) spectra is not straightforward because of its interplay with the carrier localization caused by composition/doping fluctuations in InGaN layers frequently used as active regions in light-emitting diodes (LEDs) and laser diodes [2]. Thus, a deeper understanding of the QCSE is required to access its impact on the spectral position and stability of the emission line in III-nitride optoelectronic devices.

A conventional approach to predict the Stark shift of the transition energy is based on a self-consistent solution of the Poisson and Schrödinger equations [5]. In this paper, we suggest and validate an analytical approach to the QCSE accounting for the electric field screening by non-equilibrium carriers.

2 Theory

Consider first a symmetric single quantum well with the width d and infinitely high barriers under external electric field F applied. The sheet electron and hole concentrations in the QW are assumed to be equal to each other that corresponds, for instance, to a high excitation level. We also suppose the ground electron and hole states to be predominantly occupied that is valid, in particular, for sufficiently narrow QWs typical of III-nitride heterostructures.

Using the first-order perturbation theory for calculating the charge density response to the electric field and the Poisson equation for coupling the charge density and electric potential variation, we can

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find a self-consistent approximation for the screening field induced by the ground-state carriers. In turn, this allows estimating the shifts of the ground-state energy levels induced by the electric field as

$$E_{\mathrm{e,h}} - E^0_{\mathrm{e,h}} = \frac{512 m_{\mathrm{e,h}} e^2 F^2 d^4}{243 \pi^6 \hbar^2 \chi^2}, \qquad E^0_{\mathrm{e,h}} = \frac{\pi^2 \hbar^2}{2 m_{\mathrm{e,h}} d^2}, \tag{1}$$

where e is the electron charge, and $m_{\mathrm{e,h}}$ and $E^0_{\mathrm{e,h}}$ are the carrier effective mass and ground-state energy at zero electric field. The subscripts "e" and "h" denote electrons and holes, respectively. The factor χ describes the electric field screening by the carriers in the QW. It is found to depend on the sheet carrier concentration n as

$$\chi = 1 + \frac{n}{n_{\mathrm{scr}}}, \qquad n_{\mathrm{scr}} = \frac{27\,\pi^3 \varepsilon \hbar^2}{80\, e^2 d^3 (m_{\mathrm{e}} + m_{\mathrm{h}})}. \tag{2}$$

Here, ε is the dielectric constant of the material assumed to be the same for the well and the barriers and n_{scr} is the 2D concentration of the electron–hole pairs providing four-fold suppression of the Stark shift. Equations (1), (2) show, in particular, that the magnitude of the ground-state energy shift decreases dramatically with the QW width.

A formal criterion of the perturbation theory applicability is $\langle \Psi \,|\, eFx \,|\, \Psi \rangle \ll E^0_{\mathrm{e,h}}$, where $\Psi = \sqrt{\frac{2}{d}} \sin \frac{\pi x}{d}$ is unperturbed wave function. Hence, the above analysis is valid for a low electric field, such as $F \ll 15 E^0_{\mathrm{e,h}}/ed$. For nitride heterostructures, typical values of the well width and the electric field are 2–4 nm and 1–3 MV/cm, respectively. The electric field is always "low" for electrons, but may be "high" for holes because of a higher effective mass.

3 Finite barrier height

In the case of a QW with a finite barrier height U_0, we suppose the potential to be constant outside the well, as shown in Fig. 1a. It allows us to avoid difficulties arising from the electron–hole tunneling from the well. Moreover, this approximation is quite applicable to nitride structures, where the spontaneous polarization and piezoeffect induce a built-in electric field mainly inside QWs.

We have found that the above analysis can be extended to the case of the finite barrier height by simple substituting the well width d in Eqs. (1), (2) by an effective width $d_{\mathrm{eff}} = d + C\hbar/\sqrt{2mU_0}$. Here, C is

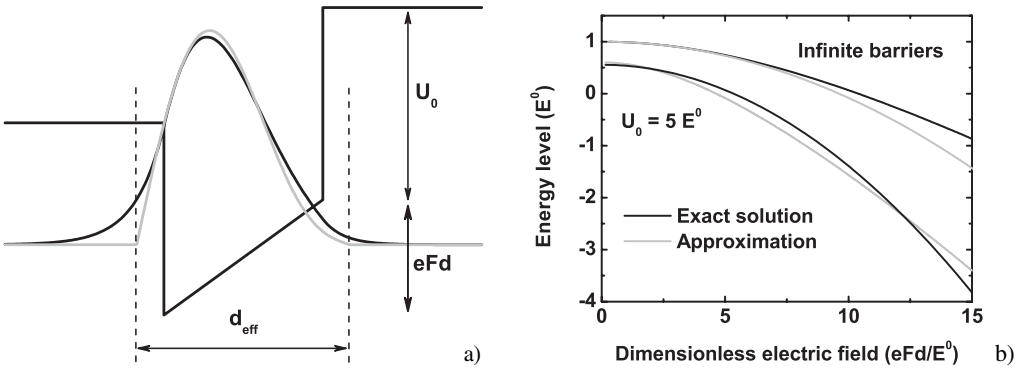

Fig. 1 (a) Potential profile for $U_0 = 5E^0$ and $eFd = 3E^0$. Wave functions obtained by the exact solution to the Schrödinger equation and from the perturbation theory within the approximation of effective well width are shown by the black and grey lines, respectively. (b) Ground energy level as a function of electric field for different barrier height. Black and grey lines represent the exact solution and the perturbation theory (1), respectively.

a fitting parameter that has been found to be of 2.4. Enlarging of the well width accounts for the electron–hole penetration into the barriers. Figure 1b shows the electron ground energy level as a function of electric field for negligible carrier concentration. The analytical approximation (1) is compared with the numerical solution to the Schrödinger equation. It is seen that the approximation (1) works well for electric fields as high as $10E^0_{e,h}/ed$. The suggested effective-well-width approach is found to be applicable for the barrier heights $U_0 > 3E^0$ and, therefore, it can be used for typical III-nitride QWs.

4 Comparison with PL data

The suggested model provides a clear parametric dependence of the Stark shift upon the QW parameters (width and barrier height), carrier concentration, and external electric field. Estimation of the latter parameter, however, is a non-trivial task because the electric field depends not only on the polarization charges at the QW interfaces, but also on the degree of strain relaxation via piezoeffect contribution, the barrier doping via additional space-charge region formation, the p–n junction via the built-in electric field, and the bias applied [3, 6]. Thus, a careful pre-analysis is required to identify factors affecting the total electric field in a well.

For illustration, we apply our model to the PL data reported in [4] for 3 nm InGaN/12 nm GaN multiple-quantum well (MQW). A zero-bias band diagram of the structure plotted in Fig. 2a shows that the most of the QWs are located out of the p–n junction space-charge region, providing a major contribution to PL since the rest of the wells are depleted with carriers. In this case, the electric field in the well can be estimated as $F = (4\pi\sigma/\varepsilon)\cdot(d_b/(d_w + d_b))$, where σ is the interface charge accounting for contributions of both spontaneous polarization and piezoeffect.

The predicted and measured PL peak wavelength as a function of the carrier concentration are compared in Fig. 2. As the indium composition in the MQW was not reported in [4], we have chosen its value to fit the peak wavelength at a low carrier concentration. The carrier concentration has been assumed to be proportional to the measured excitation power. It is seen from Fig. 2 that the analytical expressions (1)–(2) predict quite accurately the magnitude and behavior of the Stark shift in the whole range of the excitation power variation.

5 Stark shift in LED emission

In an LED active region, the electric field generally consists of the p–n junction field and the field induced by the QW interface polarization charges. If the n-region is followed by the p-region in the [1] direction, which is typical of a Ga-faced LED structure, the polarization field is oppositely directed to the p–n

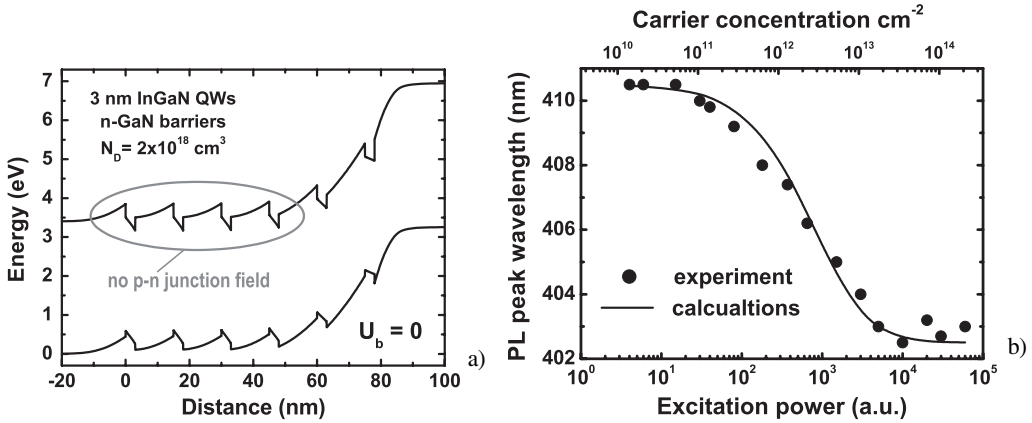

Fig. 2 (a) Equilibrium band diagram of the structure [4], (b) PL peak wavelength vs. the excitation power density (circles) and calculated band-to-band transition energy as a function of carrier concentration (line).

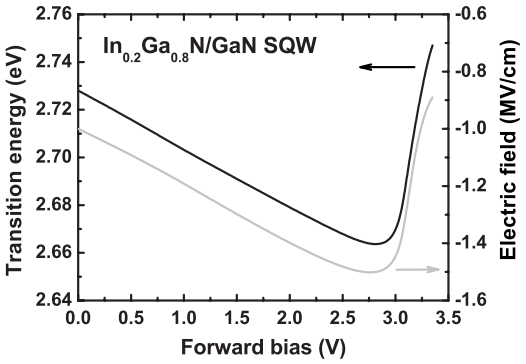

Fig. 3 Calculated electric field in the quantum well (grey line) and band-to-band transition energy (black line) as a function of bias for $In_{0.2}Ga_{0.8}N$/GaN SQW structure. The doping level is chosen 3×10^{18} cm^{-3} for both n- and p-emitters.

junction one. In an $In_{0.2}Ga_{0.8}N$/GaN QW of a typical blue LED structure doped with donors and acceptors up to $1-5 \times 10^{18}$ cm^{-3}, the polarization field normally exceeds the p–n junction one, and the total electric field in the QW is directed from p- to n-region. A small forward bias narrows the depletion region and, hence, reduces the p–n junction field, which results in a red shift of the PL peak wavelength. At a larger bias, the carriers injected into the QW start to screen the polarization field, providing a blue shift of the PL and EL spectra. Thus, the luminescence peak is predicted to exhibit a non-monotonic dependence on the bias applied. In contrast, the polarization and p–n junction fields in a N-faced LED structure are co-directed. Therefore, the total electric field in a QW decreases monotonically with bias, leading to a strong blue shift of the emission spectrum.

Figure 3 shows the variation of the electric field and band-to-band transition energy in an $In_{0.2}Ga_{0.8}N$/GaN SQW with forward bias, computed by a commercial SiLENSe package [7]. A similar non-monotonic dependence of the PL peak energy has been recently observed in InGaN/GaN MQW structure [3]. Authors attribute such a behaviour to the filling of local In-rich regions by the injected carriers. However, the discussed variation of the total electric field in QW with the bias also takes place in MQW structures. So we would suggest that the non-monotonic dependence of PL peak position is controlled by the interplay between the increase of the electric field due to narrowing of the depletion region and the electric field screening by the injected carriers.

6 Summary

We have suggested the analytical model providing a parametric dependence of the Stark shift on the QW parameters, carrier concentrations, and the electric field applied. The magnitude of the Stark shift is found to rise dramatically with the QW thickness, while the electron–hole concentration necessary for effective suppression of the QCSE falls down. Theoretically predicted shift of the PL peak wavelength with the excitation power is consistent with experimental data. A competition between the polarization and p–n junction fields in combination with the screening of the total electric field by non-equilibrium carriers may explain the observed non-monotonic Stark shift dependence on the bias applied to an LED structure.

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