Effects of nonlinear elasticity and electromechanical coupling on pressure coefficient of the light emission in group-III nitride quantum structures

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Abstract. We present theoretical studies of the effects of nonlinear elasticity and electromechanical coupling on the pressure coefficients of the light emission, $\frac{dE_E}{dP_{ext}}$, in GaN/AlN and In$_{0.2}$Ga$_{0.8}$N/GaN superlattices with compressively strained quantum wells. We show that effect of the nonlinear elasticity, manifesting itself in pressure dependence of elastic constants, leads to significant reduction of the values of $\frac{dE_E}{dP_{ext}}$ in the considered structures. On the other hand, the effect of the electromechanical coupling, i.e., co-existence of the direct and converse piezoelectric effect, causes increase of the $\frac{dE_E}{dP_{ext}}$ in these structures. However, the contribution to $\frac{dE_E}{dP_{ext}}$, originating from the nonlinear elasticity dominates over the contribution coming from the effect of electromechanical coupling. Interestingly, the influence of the effect of electromechanical coupling on $\frac{dE_E}{dP_{ext}}$ diminishes when the nonlinear elasticity is taken into account.

1. Introduction

In the recent years, optical properties of wurtzite InGaN/GaN and GaN/AlGaN quantum wells (QWs) under hydrostatic pressure have been extensively studied [1-3]. These studies have revealed intriguingly small values of the pressure coefficients of the light emission, $\frac{dE_E}{dP_{ext}}$, in the structures grown along the c-axis. It has been shown that small values $\frac{dE_E}{dP_{ext}}$ originate from the pressure-induced increase of piezoelectric field in these structures [1-3]. However, calculations of $\frac{dE_E}{dP_{ext}}$, based on the linear elastic and piezoelectric theory, have agreed with the experimental results only for GaN/AlGaN QWs with small aluminum concentration [3]. For InGaN/GaN QWs and for GaN/AlGaN QWs with aluminum concentrations larger than 20%, second-order elastic and piezoelectric effects have to be taken into account. First of all, it has been found that the nonlinear piezoelectricity, manifesting itself in dependence of piezoelectric constants on the volume-conserving strain [4], is essential for proper description of the pressure tuning of the built-in electric fields in wurtzite nitride QWs grown along the c-axis [1,2]. This effect is of primary importance for
determination of the $\frac{dE_F}{dP_{ext}}$ in these structures. Recently, the influence of two other second-order electromechanical effects on $\frac{dE_F}{dP_{ext}}$ in nitride QWs has been studied. Namely, it has been shown that the effect of the nonlinear elasticity, originating from the pressure dependence of elastic constants, causes significant reduction of the values of $\frac{dE_F}{dP_{ext}}$ in nitride QWs [5]. On the other hand, the effect of the electromechanical coupling, i.e., co-existence of the direct and converse piezoelectric effect, causes increase of the $\frac{dE_F}{dP_{ext}}$ in these structures [6]. It should be noted, that in [5] and [6], these two effects have been studied assuming the strain dependence of piezoelectric constants of nitrides, i.e., taking into account also the effect of nonlinear piezoelectricity.

In this work, the effects of nonlinear piezoelectricity, nonlinear elasticity and electromechanical coupling on the $\frac{dE_F}{dP_{ext}}$ in nitride quantum structures are studied altogether. We focus on superlattices (SLs) with compressively strained wells and unstrained barriers. The choice of SLs is motivated by the well-defined periodic boundary conditions for the electric fields [6]. We show that the contribution to the $\frac{dE_F}{dP_{ext}}$, originating from the nonlinear elasticity dominates over the contribution coming from the electromechanical coupling effect.

2. Pressure-tuning of strain and electric field in nitride superlattices

Let us indicate all material tensors, fields and parameters by indices ‘$a$’ for the wells and ‘$b$’ for the barriers. Then, one can describe the pressure tuning of the nonzero elements strain tensor and piezoelectric field in a SL with unstrained barriers using the following equations [5,6]

$$\varepsilon_{xx,a}(P_{ext}) = \frac{a_b}{a_a} \left[ 1 + \frac{C_{11,b}(P_b)}{C_{11,a}(P_a)} \frac{C_{13,b}(P_b)}{C_{13,a}(P_a)} \right] P_{ext} - 1$$

$$\varepsilon_{xx,b}(P_{ext}) = \frac{C_{11,b}(P_b) - C_{13,b}(P_b)}{C_{11,a}(P_a) + C_{12,b}(P_b) + C_{33,b}(P_b)} P_{ext}$$

$$\varepsilon_{zz,a} = \frac{-2C_{13,a}(P_a)}{C_{33,a}(P_a)} \varepsilon_{xx,a} + \frac{e_{33,a}}{C_{33,a}(P_a)} E_{zz,a} + \frac{P_{ext}}{C_{33,a}(P_a)} (e_{33,a} E_{zz,a}^{*} - 1)$$

$$E_{zz,a} = E_{zz,a}^{*} + P_{ext} E_{zz,a}^{*}$$

where

$$E_{zz,a}^{*} = \frac{L_b \left[ P_{sp,z,b} + 2 \frac{e_{33,b}}{C_{33,b}(P_b)} \frac{e_{31,b}}{C_{31,b}(P_b)} \right] E_{xx,b} - P_{sp,z,a} - 2 \left[ e_{31,a} - C_{33,a}(P_a) \right] \frac{e_{33,a}}{C_{33,a}(P_a)} E_{xx,a} }{L_a \kappa_a + L_b \kappa_b}$$

$$E_{zz,a}^{*} = \frac{L_b \left[ \frac{e_{33,a}}{C_{33,a}(P_a)} - \frac{e_{33,b}}{C_{33,b}(P_b)} \right] }{L_a \kappa_a + L_b \kappa_b}$$

$$\kappa_a = \lambda_a + \frac{e_{33,a}^2}{C_{33,a}(P_a)}.$$
Formulas for $\varepsilon_{xx,b}$, $E_{zz,b}$, and $\kappa_b$ can be obtained from equations (3) and (4a)-(4d) by changing indices ‘$a$’ and ‘$b$’. In the above equations, $e_{ij}$ are the piezoelectric constants, $C_{ij}(P)$ are the pressure-dependent elastic constants, $P_{ext}$ denotes the external hydrostatic pressure, $L$ is the thickness of the layer, $P$ is the total hydrostatic pressure originating from the external and internal stresses [6].

3. Results and discussion

Using the above model of pressure tuning of the strain and electric field, we compute the electronic states in the SLs as a function of $P_{ext}$ and then calculate $dE_E/dP_{ext}$ [8,9]. We consider GaN/AlN SLs grown on AlN buffers and In$_{0.2}$Ga$_{0.8}$N/GaN SLs grown on GaN buffers. We focus on the SLs with equal widths of wells $L_a$ and barriers $L_b$, since in these structures, the electric fields do not depend on the thickness of the layers (see equations (4a)-(4b)).

![Figure 1](image_url)

Figure 1. The values of $dE_E/dP_{ext}$ for GaN/AlN SLs with $L = L_a = L_b$. Solid lines are added to guide the eyes.

In figures (1) and (2), we show the values of $dE_E/dP_{ext}$ obtained for the considered structures as a function of the common length $L = L_a = L_b$. For each structure, four values of $dE_E/dP_{ext}$ have been calculated. Namely, we have considered the following cases: (i) the effects of nonlinear elasticity and electromechanical coupling are taken into account (full circles), (ii) the effect of nonlinear elasticity is excluded (full squares), (iii) the effect of electromechanical coupling is excluded (empty circles), (iv) both effects of nonlinear elasticity and electromechanical coupling are not taken into account (empty squares). In all the cases, we have taken into account the strain dependence of piezoelectric constants of nitrides, i.e., the nonlinear piezoelectricity.

In both figures (1) and (2), one can see that the values of $dE_E/dP_{ext}$ decrease linearly with $L$. This effect originates from the increase of electric field in the QWs with $P_{ext}$ [5,6]. Let us focus on the contributions to $dE_E/dP_{ext}$ coming from the effects of nonlinear elasticity and electromechanical coupling. The effect of the nonlinear elasticity results in significant reduction of the values of $dE_E/dP_{ext}$ in GaN/AlN and In$_{0.2}$Ga$_{0.8}$N/GaN SLs. The effect of the electromechanical coupling
causes slight increase of $dE_E / dP_{ext}$ in GaN/AlN SLs. For In$_{0.2}$Ga$_{0.8}$N/GaN SLs, this effect is very small (see figure 2). Comparing the differences between full and empty symbols in figure 1, one can also observe that these differences are larger for squares than for circles. This means that the influence of the electromechanical coupling effect on $dE_E / dP_{ext}$ diminishes when the nonlinear elasticity is taken into account.

![Figure 2](image.png)

**Figure 2.** The values of $dE_E / dP_{ext}$ for In$_{0.2}$Ga$_{0.8}$N/GaN SLs with $L = L_u = L_b$. Solid lines are added to guide the eyes.

### 4. Conclusions

We have studied the influence of the effects of nonlinear elasticity and electromechanical coupling on the $dE_E / dP_{ext}$ in nitride SLs. Our calculations have revealed that (i) the effect of the nonlinear elasticity leads to significant reduction of the values of $dE_E / dP_{ext}$ and (ii) the effect of the electromechanical coupling causes increase of $dE_E / dP_{ext}$. The contribution to $dE_E / dP_{ext}$ originating from the nonlinear elasticity dominates over the contribution coming from the electromechanical coupling effect. Interestingly, the influence of the electromechanical coupling effect on $dE_E / dP_{ext}$ diminishes when the nonlinear elasticity is taken into account.

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