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Pressure Dependence of the Light Emission in Zinc-Blende InGaAs/GaAs and InGaN/GaN Quantum Wells

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We present theoretical study of the pressure coefficient of the light emission (dE_E/dP) in compressively strained zinc-blende InGaAs/GaAs and InGaN/GaN quantum wells, grown in a (001) direction. We investigate the contributions to dE_E/dP arising from (i) third-order (nonlinear) elasticity, (ii) nonlinear elasticity, originating from pressure dependence of elastic constants, and (iii) nonlinear dependence of elastic constants on composition in InGaAs and InGaN alloys. The obtained results indicate that the use of nonlinear elasticity is essential for determination of dE_E/dP in the strained InGaAs/GaAs and InGaN/GaN quantum wells, while the inclusion of the nonlinear dependence of elastic constants on composition of InGaAs and InGaN alloys does not improve agreement between the theoretical end experimental values of dE_E/dP in the considered structures.

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1. Introduction

Pressure dependence of the light emission in semiconductor quantum wells (QWs) has been extensively studied in the recent years [1–5]. These studies have revealed that pressure coefficient of the light emission (dE_E/dP) for a QW can be substantially different from the pressure coefficient of the band gap for unstrained bulk material of the same chemical composition. It has been discovered that the magnitude of dE_E/dP in QWs depends significantly on the built-in biaxial strains and piezoelectric fields. Unexpectedly, the linear theory of elasticity and piezoelectricity often failed to predict the values of dE_E/dP in semiconductor QWs, and the nonlinear elastic and piezoelectric effects have been taken into account [1–4].

In this work, we present the results of theoretical study of dE_E/dP in compressively strained zinc-blende InGaAs/GaAs and InGaN/GaN QWs, grown in a (001) direction. In these structures the built-in electric field is not present but the magnitude of dE_E/dP is significantly reduced by the presence of the built-in compressive biaxial strain originating from the lattice misfit between barriers and QWs [1, 4]. The linear theory of elasticity with linear dependence of the second-order elastic constants (C_{ij}) on alloy composition failed to predict this effect [1, 4]. Therefore, we investigate the contributions to dE_E/dP arising from (i) third-order (nonlinear) elasticity, (ii) nonlinear elasticity, originating from pressure dependence of C_{ij}, (iii) nonlinear dependence of C_{ij} on composition in InGaAs and InGaN alloys.

2. Models

In order to study the contributions to dE_E/dP originating from the effects (i) and (ii), we have used two

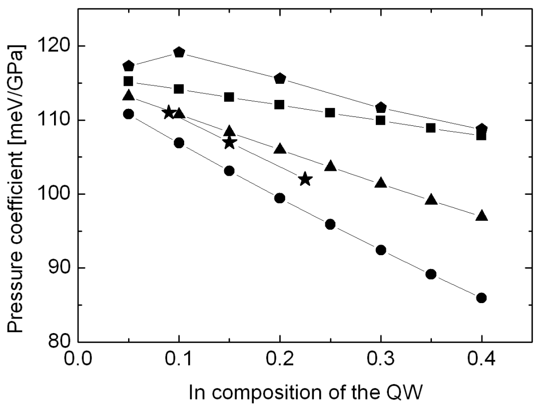

Fig. 1. The values of dE_E/dP for 10 nm InGaAs/GaAs QWs, as a function of In concentration. Stars represent the experimental results (taken from Ref. [1]), squares, triangles, circles, and pentagons correspond to the theoretical results which are obtained using (i) the linear theory of elasticity, (ii) the third-order elasticity theory, (iii) nonlinear elasticity originating from the pressure dependence of the second-order elastic constants, and (iv) the linear theory of elasticity with nonlinear dependence of elastic constants on composition of InGaAs alloys, respectively. Solid lines are added to guide the eye.

models of pressure-tuning of strains in (001)-oriented zinc-blende QWs, which have been presented in detail in Ref. [4]. Using these models, we have calculated the values of dE_E/dP for strained InGaAs/GaAs and InGaN/GaN QWs, assuming linear dependence of the second-order (C_{ij}) and third-order (C_{ijk}) elastic constants on In content in the QWs [4].

To investigate the contribution to dE_E/dP originating from the effect (iii), we have performed *ab initio* calcula-

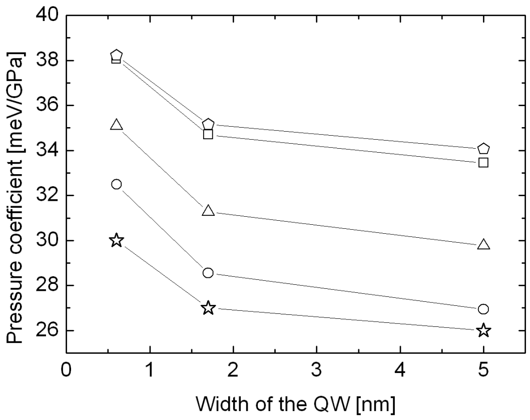

Fig. 2. The values of dE_E/dP for zinc-blende $In_{0.1}Ga_{0.9}N/GaN$ QWs, as a function of QW width. Stars represent the experimental results taken from Ref. [5], squares, triangles, circles, and pentagons correspond to the theoretical results which are obtained using (i) the linear theory of elasticity, (ii) the third-order elasticity theory, (iii) nonlinear elasticity originating from the pressure dependence of the second-order elastic constants, and (iv) the linear theory of elasticity with nonlinear dependence of elastic constants on composition of InGaN alloys, respectively. Solid lines are added to guide the eye.

tions of elastic constants C_{ij} in zinc-blende InGaN alloys. Slightly sub-linear dependence of C_{ij} on In content has been found. In the case of InGaAs alloys, the elastic constants C_{ij} also depend sub-linearly on composition [6]. Then, we have calculated the values of dE_E/dP in the InGaN/GaN and InGaAs/GaAs QWs, assuming linear and sub-linear dependences of C_{ij} on composition of InGaN and InGaAs alloys.

3. Results

The obtained results are shown in Figs. 1 and 2. One can see that the use of third-order elasticity leads to significant reduction of dE_E/dP in both InGaAs/GaAs and InGaN/GaN QWs, in comparison to the values of dE_E/dP obtained by using the linear theory of elasticity [4]. In the case of InGaAs/GaAs QWs, the values of dE_E/dP calculated using third-order elasticity are in reasonable agreement with experimental data taken from Ref. [1]. For zinc-blende InGaN/GaN QWs, better agreement between theoretical and experimental values (taken from Ref. [5]) of dE_E/dP is obtained when instead of third-order elasticity, pressure dependence of C_{ij} is taken into account [4]. On the other hand, we have found that the use of the sub-linear dependence of C_{ij} on composition of InGaN alloys leads to small increase of the dE_E/dP in InGaN/GaN QWs, in comparison to the values of dE_E/dP obtained assuming linear dependence of C_{ij} on In content. Similar effect is found for dE_E/dP in InGaAs/GaAs QWs.

4. Conclusion

In conclusion, we have investigated the contributions to dE_E/dP in strained InGaAs/GaAs and InGaN/GaN QWs arising from the nonlinear elasticity effects and nonlinear dependence of C_{ij} on composition in InGaAs and InGaN alloys. The obtained results indicate that the use of nonlinear elasticity is essential for determination of the values of dE_E/dP in the compressively strained QWs. The inclusion of the nonlinear dependence of C_{ij} on composition of InGaAs and InGaN alloys does not improve agreement between the theoretical end experimental values of dE_E/dP in the considered structures.

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