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Hydrostatic pressure coefficients of the photoluminescence of InAs/GaAs quantum dots

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Abstract

There is a significant diminution in the hydrostatic pressure coefficients (PCs) of the photoluminescence spectrum for InAs/GaAs quantum dots in comparison with that of bulk binary. We study this phenomenon with the nonlinear elasticity theory. The variation of the lattice and elastic constants plays an important role in the change of PCs, which causes the obvious decrease of the built-in strains of InAs/GaAs quantum dots under the hydrostatic pressure. The decrease will induce the novel change of the energy gap and the electronic confined energy. Finally, the change is shown in the measured small PCs of photoluminescence from quantum dots. Also the calculation reveals that the PCs are sensitive to the sizes of quantum dots because of the change of the electronic confined energy. The smaller the quantum dot is, the stronger the influence of this change on the PCs becomes. This effect gives rise to the increase of PCs when dot size is reduced.

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Keywords: Pressure coefficients; Strain

1. Introduction

A large number of experimental studies of the electronic properties of InAs/GaAs self-assembled quantum dots grown by the Stranski–Krastanov mode have been performed in recent years. Photoluminescence measurement under high hydrostatic pressure has been proved to be an effective tool for exploring the electronic structures and optical transitions in quantum dots. Most of the experimental measured pressure coefficients (PCs) of quantum dots are about 75–90 meV/GPa, 17–30% smaller than that of bulk GaAs [1–5]. They are also smaller than the commonly accepted PC of bulk InAs. In general, it is thought that the PC of InAs/GaAs quantum dots should be between the values of bulk binary. As Paul and Warschauer

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have noted, the pressure coefficients of the zone-center band gaps of the III–V semiconductors are all of the order of 100 meV/GPa [6]. Therefore, the reduced PCs of quantum dots are somewhat surprising. It is interesting to look for the internal cause of the reduced PCs. At present, the phenomenon lacks a firm explanation.

Linear elasticity has been used to predict first-order (linear) effects of pressure, but the striking deduced PCs of quantum dots cannot be explained by this model. It is well known that self-assembled InAs/GaAs quantum dots are characterized by huge built-in strains due to the large difference between the lattice constants of InAs and GaAs. For a strained layer, the elastic constants and the lattice constants may vary independently with pressure, so the nonlinear elasticity theory developed by Frogley et al. is rather suitable to predicting the PCs of photoluminescence from quantum dots [7]. Some authors have used the model to calculate the PCs, but the quantum dot is treated as simple strained well and only the qualitative analysis of energy gap is made in their paper [8]. In order to show clearly the PCs of photoluminescence spectrum from InAs quantum dots, we use the effective mass model and the nonlinear elasticity theory to predict the PCs of energy gap and the confined energy of electrons and holes entirely. We have demonstrated here that the decrease of the built-in strain in InAs dots may be the main reason for the much reduced PCs under the hydrostatic pressure. Also we have revealed that the PCs of InAs quantum dots are sensitive to the dot sizes, which are caused by the change of the confined energy under pressure.

2. Theory

Throughout this Letter, we use a dot model as shown in Fig. 1 with $b = 2a$. The origin of the coordinate system is taken to be at the center of the InAs dot with the z direction being defined as the growth direction. Q is the aspect ratio ($Q = a/h$). As the pressure is applied, the lattice constants of the substrate and quantum dot vary and so, too, do the elastic constants. According to Frogley's model, the lattice constants are

$$a_{l,s}(p) = a_{l,s}\left(1 + \frac{B'P}{B_0}\right)^{-(1/3B')}, \tag{1}$$

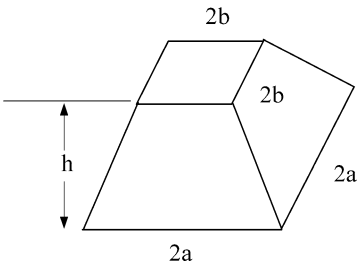

Fig. 1. Schematic representation of the theoretical configuration used in the calculation.

where the subscripts l ans s refer to the strained layer and substrate, respectively. B and B' are the bulk modulus and its pressure derivative. And the elastic constants are

$$C_{ij}(P) = C_{ij} + C'_{ij}P, \tag{2}$$

where the C'_{ij} is the pressure derivatives of the elastic constants ($i = 1, 2, 3,\ \ j = 1, 2, 3$).

Neglecting the small magnitude of exciton binding energy, the relation of the PL peak energy in quantum dots to the pressure is

$$\frac{dE_{\mathrm{PL}}}{dP} = \frac{dE_{\mathrm{Eg}}}{dP} + \frac{dE_{\mathrm{e1}}}{dP} + \frac{dE_{\mathrm{hh1}}}{dP}. \tag{3}$$

So the PC can be written as

$$\mathrm{PC} = \mathrm{PC}_{\mathrm{Eg}} + \mathrm{PC}_{\mathrm{e1}} + \mathrm{PC}_{\mathrm{hh1}}. \tag{4}$$

Taking into account the anisotropy of the elastic properties in cubic crystals, the strain distribution is calculated by means of the Green's function technique [9]. We use an efficient method to calculate the electron and hole energies in quantum dot by expanding the quantum dot states in terms of harmonic-oscillator functions [10].

3. Results and discussion

There is already evidence in the literature of small photoluminescence pressure coefficients in $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{As}$ quantum dots. At the same time, the size dependent of the PCs has been shown in some results. Lyapin et al. have reported the PCs of InAs/GaAs quantum dots, which are 16 nm in lateral size and 1.6 nm in dot height, to be 80(2) meV/GPa [1,2].