Engineering The Optical Transitions of Self-Assembled Quantum Dots

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INTRODUCTION

In this paper, we report a fast effective mass model for accurately calculating the bound states and optical transitions of self-assembled quantum dots. The model include the atomistic strain effects, namely, the strain deformation of the band edges, and strain modification of the effective masses. The explicit inclusion of strain effects in the picture has significantly improved the effective mass model results. For strain calculations, we have found that atomistic strain depend solely on aspect ratio of the quantum dot, and it has been calculated and reported here for a wide range of quantum dot aspect ratios. The deformation theory has been used to include the strain deformation of the band edges. Density function theory has been used to study the effect of strain on the electron and hole effective masses.

THEORETICAL MODEL

The quantum dot is modeled as a 3-dimensional dome shaped finite potential well, the depth of the well is the band offset that can be calculated using deformation potential theory [1],

$$\Delta E_c = CBO - a_c\varepsilon_H,$$

$$\Delta E_{vHH} = VBO + a_v\varepsilon_H + \frac{b}{2}\varepsilon_B,$$

$$\Delta E_{vLH} = VBO + a_v\varepsilon_H - \frac{b}{2}\varepsilon_B,$$

The electron and hole effective masses under strain are calculated using density function theory (DFT) using AtomistixToolKit [2].

For the atomistic strain simulations, harmonic Keating model has been used [3] . The harmonic Keating model treats the interatomic forces as spring forces connecting the atoms together. The relaxed atom positions are obtained by minimizing the energy of the whole structure with respect to individual atom positions. The dimensions of the simulated quantum dot systems are 60 nm x 60 nm x 60 nm and the quantum dot is dome shaped InAs in the middle of GaAs substrate. The strain simulation contains around 10 Million atoms and an atomistic grid is shown in Fig 1. Such large systems are computationally expensive to run strain simulations and require highly scalable computational codes. The code that has been used for our simulations is the Nano Electronic MOdeling tool version 5 NEMO5 [4].

RESULTS

Atomistic strain simulations indicate that lattice strain in the quantum dot depends only on the aspect ratio not on the individual dimensions. As shown in Fig. 2, the magnitude of hydrostatic strain decreases with increasing the diameter to height ratio (D/h), while the magnitude of biaxial strain increases with increasing (D/h). The electron, light hole, and heavy hole effective masses calculated at the different strain components corresponding to the different aspect ratios as indicated in Fig. 3 . To show the impact of including the strain in the effective mass models, we have calculated the optical transition of a dome shaped quantum dot with height of 5 nm and diameter of 20 nm and compared against experimental measurements [5]. The error in calculating the optical transition has been reduced from 25% to 3.7% as shown in Table I.

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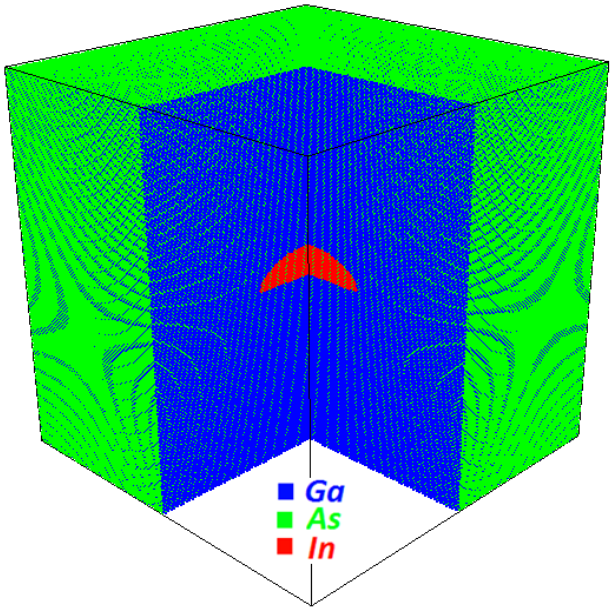

Fig. 1. The atomistic grid of one of the simulated InAs/GaAs quantum dot systems. The quantum dot is a dome with base diameter of 20 nm and height of 5 nm.

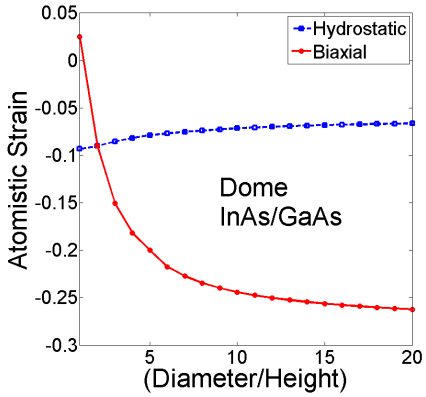

Fig. 2. The atomistic hydrostatic and biaxial strain at different diameter to height ratio (D/H). Strain depend on aspect ratio (D/H) not on individual dimensions. The magnitude of hydrostatic strain decreases with increasing D/h while the magnitude of biaxial strain increases with increasing D/h.

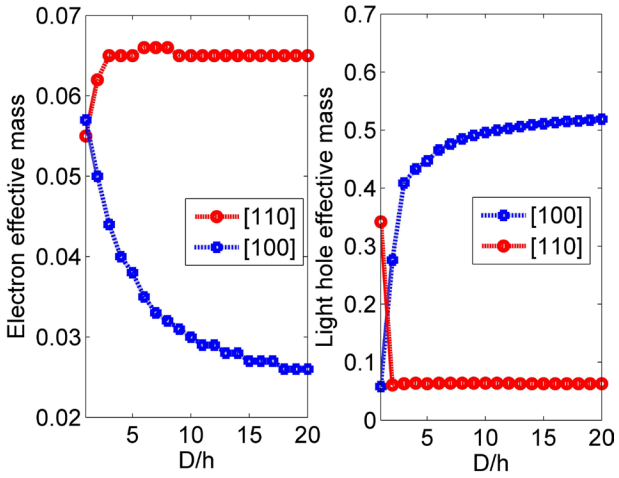

Fig. 3. The electron and light hole effective masses calculated using DFT. The heavy hole effective masses do not change significantly with strain, it is around 0.26 for [100] and 0.32 for [110].

	Without Strain	Including Strain	Experimental
Optical transition	0.7169 eV	1.012 eV	0.976 - 0.93 eV
Error	25%	3.7 %	

TABLE I

CALCULATED OPTICAL TRANSITION VS EXPERIMENTAL MEASUREMENT.

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