Atomistic Tight Binding Simulations with Real Space Basis Functions: Optical Properties of Multi Million Atom Systems

Prasad Sarangapani*, Yaohua Tan, James Charles, Tarek A. Ameen, Michael Povolotskyi, Tillmann Kubis, and Gerhard Klimeck
School of Electrical and Computer Engineering, Purdue University, West Lafayette-IN, USA
e-mail: psaranga@purdue.edu

INTRODUCTION

Design of optical semiconductor devices require precise control over the frequency of operation. Self-assembled quantum dots can be used to achieve this as their optical response is highly sensitive to the dot dimensions [1]. In literature, often the position operator, used for calculating the optical matrix element, is approximated as a diagonal matrix in TB basis [2]. This approach underestimates the interaction between various orbitals. This work assesses the accuracy of that approximation by comparing it against an explicit form of a position operator derived from atomic orbitals. To capture the absorption spectrum accurately, a tight binding basis derived from DFT *ab-initio* calculations is used [3]. Using atomistic simulations, the present paper investigates the impact of quantum dot size on the optical absorption spectrum using the explicit form of position operator.

DEVICE SIMULATION APPROACH

The quantum dot under consideration is an InAs dot grown on $\mathrm{In_{0.15}Ga_{0.85}As}$ along the [001] direction as shown in Fig (1). Dimensions of the dot are (20nm $\times$ 20nm $\times$ 4.9 nm). A strain reducing capping layer of $\mathrm{In_{0.15}Ga_{0.85}As}$ is grown on top of it. To capture the quantum effects accurately, a 20 band $sp^3d^5s^*$ (including SO-coupling) tight binding (TB) model is employed to solve the Schrödinger's equation. To account for the lattice mismatch, a valence force field strain model [4] is solved on the 10 million atom system over 256 cores using PETSc Newton solver. Then, Schrödinger's equation is solved using the Lanczos method [5] on a smaller electronic domain (dashed box in Fig (1)) consisting of 1 million atoms by redistributing the atoms on these cores. Total simulation time taken for this device is approximately 2.5 hours. The optical matrix elements are calculated using a position operator based on explicit atomic orbitals that takes into account coupling between various tight binding orbitals (Fig (2)) of a particular atom. For example, the coupling between s and p states in Indium is 0.72482 eV and in Arsenic is 0.504095 eV.

RESULTS

Fig (3) indicates energy levels of conduction and valence band states. As the dot dimension is increased, the band gap decreases as the confinement gets weaker. Fig (4) shows the eigenstates of the dot along the x-y plane. When the dot dimension is reduced from 4.9 nm to 3.9 nm there is a significant difference in the valence band states as there is a change in the interaction between s and p states which is evident from Fig (5).

ACKNOWLEDGEMENT

This work was supported by AFRL award No. SUB1122439-001 (AMMTIAC DO 48) to the Network for Computational Nanotechnology at Purdue University.

REFERENCES

[1] Muhammad Usman, et. al. Nanotechnology, IEEE Transactions on, vol. 8, no. 3, May 2009, pp. 330-344
[2] Timothy B. Boykin, et. al. Phys. Rev. B 65, 035202 (2001)
[3] Tan, et. al., Journal of Computational Electronics March 2013, Volume 12, Issue 1, pp. 56-60
[4] Seungwon Lee, et.al., Phys. Rev. B 70, 125307 (2004)
[5] Heath, M. "Computing: An Introductory Survey." (1998).

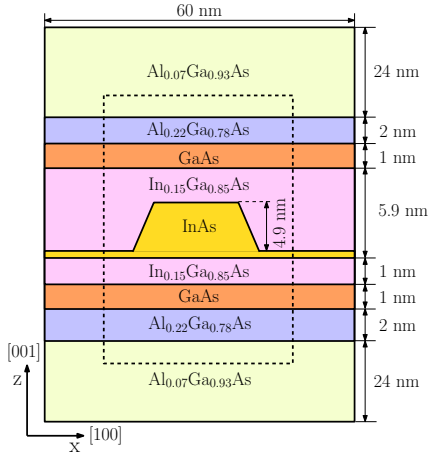
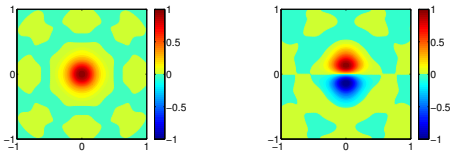
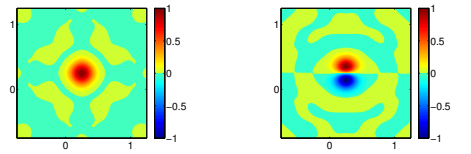


Fig. 1: Quantum dot structure. The dashed box corresponds to the electronic domain on which Schrödinger's equation is solved.



(a) Indium s orbital (b) Indium p_y orbital



(c) Arsenic s orbital (d) Arsenic p_y orbital

Fig. 2: Contour plots of TB basis functions obtained from *ab-initio* calculations for In and As along the x-y plane.

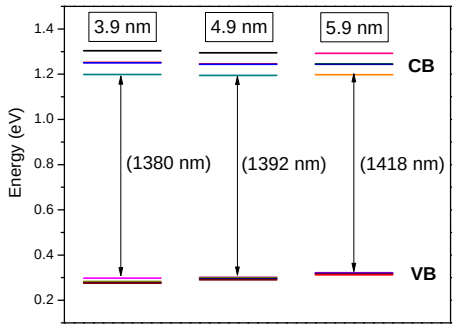
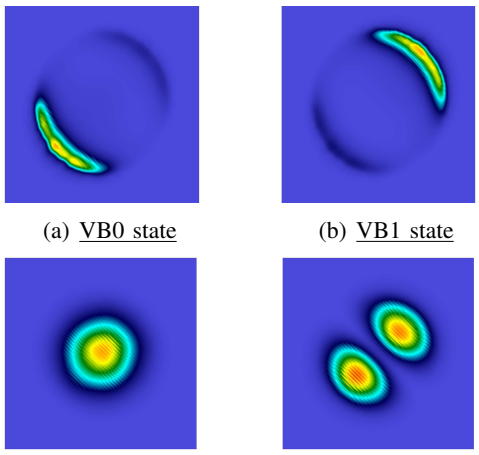


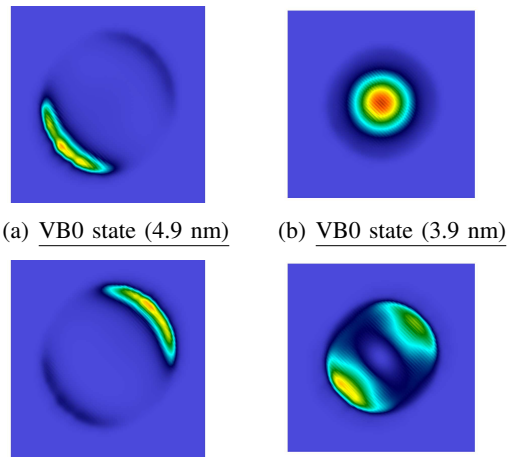
Fig. 3: Eigenstates and optical gap for dots of height 3.9 nm, 4.9 nm and 5.9 nm



(a) VB0 state (b) VB1 state

(c) CB0 state (d) CB1 state

Fig. 4: First two valence and conduction band states along the x-y plane for dot height of 4.9 nm.



(a) VB0 state (4.9 nm) (b) VB0 state (3.9 nm)

(c) VB1 state (4.9 nm) (d) VB1 state (3.9 nm)

Fig. 5: Comparison of first two valence band states along the x-y plane when the dot height is reduced from 4.9 nm to 3.9 nm