Strain profile and size dependent electronic band structure of GeSn/SiSn quantum dots for optoelectronic application

Tan, Chuan Seng; Bose, Sumanta; Fan, W. J.; Chen, J.; Zhang, D. H.

2014

Bose, S., Fan, W. J., Chen, J., Zhang, D.H., & Tan, C. S. (2014). Strain profile and size dependent electronic band structure of GeSn/SiSn quantum dots for optoelectronic application. 12th International Conference on Fiber Optics and Photonics.

<https://hdl.handle.net/10356/79533>

<https://doi.org/10.1364/PHOTONICS.2014.S4D.5>

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[<http://dx.doi.org/10.1364/PHOTONICS.2014.S4D.5>].

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Paper Title

Date : 14 Dec 2014

Strain Profile and Size Dependent Electronic Band
Structure of GeSn/SiSn Quantum Dots for
Optoelectronic Application

Presenter

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Presentation ID

S4D.3

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Presentation Outline

- **Part 1:**

Background and algorithm of atomistic quantum dot simulation.

- **Part 2:**

*Towards Si photonics: GeSn/SiSn – our system.
Strain, gain & energy profile result*

Part 1:

*Background and algorithm of atomistic
quantum dot simulation.*

What are Quantum Dots ?

“Man-made nanoscale structures in which electrons can be confined in all 3 dimensions”

- Electron energy is quantized -> artificial atoms (coupled QD->molecule)
- Contains a countable number of electrons

Quantum dots are artificial atoms that can be custom designed for a variety of applications

Quantum Dots devices & applications

Laser

Photo-detector/Amplifier

Quantum Computation

Fujitsu
Temperature Independent QD laser
2004

S. J. Xu
Dept. of Physics, University of Hong Kong

World's First Semiconductor Optical Amplifier with Signal Waveform Re-shaping Function at 40Gbps

March 4, 2005

RESEARCH WATCH

World's first 25Gbps data communication using Quantum Dot Laser achieved

By Dario Borghini
00:12 June 4, 2010

FUJITSU

Quantum Information Science is rapidly progressing, and Quantum Dot based optical devices are approaching the market !

M. Usman, Multi-million Atom Electronic Structure Calculation for Quantum Dots, PhD thesis (online nanoHUB)

How Can Theory, Modelling, and Computation Help?

- Why Theory, Modeling and Computation?
  - ✓ Modeling can provide essential insight into the physical data
  - ✓ Obtain information where experimental data is not readily available
  - ✓ Can help experimentalists to design their experiments
- Quantum dots grow in different shapes and sizes
- PL intensity is measured to determine light spectrum
- Experimentalists need to understand the PL spectrum

AFM micrograph of InAs QD

Source:
cqd.eecs.northwestern.edu/research/qdots.php

g

Missing
Physics

Applied Phys. Lett. 78, 3469 (2001)

Atomistic simulation of QDs

Features :

- Calculates eigenstates of arbitrarily structures
- Strain: Valence force field (VFF)

Already used in simulating:

- QDs & Alloyed QDs
- Long range strain effects on QDs
- Effects of wetting layer
- Piezo-electric effects in QDs
- QD nuclear spin interactions
- Impurities in QDs

3D wave-function of QD

Energy States

Absorption /Emission Spectra

Computation Flowchart

Capabilities:

- Arbitrary shape/size of quantum dot
- Long range strain, piezoelectric fields
- Atomistic representation of alloy
- External Electrical/Magnetic fields
- Zincblende/Wurtzite crystals

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Optoelectronic simulation of Quantum Dots for Silicon Photonics

INTO SILICON PHOTONICS

Group IV compatibility with Si CMOS fab

Integration of optical and electronic components onto a single microchip

Providing faster optical data transfer between and within microchips.

CHOICE OF STRUCTURE/MATERIAL

Quantum Dot (QD) based optoelectronic devices: a key enabler in this domain

This work: Self assembled $\text{Ge}_{0.5}\text{Sn}_{0.5}/\text{Si}_{0.5}\text{Sn}_{0.5}$ QDs.

COMPUTATION METHODS

Valence force field (VFF) using Keating potential estimates strain profile

Electronic band structure calculation using 8 band ***k*·*p*** method

STUDY & IMPACT

Strain profile & contour

Energy band structure

QD size effect on the fundamental transition energy.

The effect of tensile strain on the band structure of Ge.

Fig a, Schematic of how the band diagram changes as biaxial tensile strain is applied.

Fig b, Plot of the bandgap energies for the Γ ($E_g(\Gamma)$) and L ($E_g(L)$) bands as a function of tensile strain.

Figure (a) Band structure of bulk Ge, showing a 136 meV difference between direct & indirect BG
(b) the difference between direct & indirect BG can be decreased by tensile strain
(c) the rest of the difference between direct & indirect BG in tensile strained Ge can be compensated by filling electrons into the L valleys via n-type doping.

Our QD geometry: Pyramidal

Our QD geometry: Pyramidal

- ✓ Pyramidal QD grows along $+z$ direction, the base and wetting layer in the x - y plane.
- ✓ QD Height (h) = (6 to 18) $\times a_0$ and base ($2h$) = (12 to 36) $\times a_0$.
- ✓ The entire system's height is $3h$ and the length/width is $4h$.

Fig. 2. 3D schematic of our pyramidal QD

Fig. 3. Top view schematic of our pyramidal QD

Fig. 1. Front view schematic of our pyramidal QD

Valence Force Field Strain Calculation

- ✓ Valence Force Field (VFF) method with Keating potential
- ✓ Calculate the strain energy, E_{strain} expressed in terms of the bond lengths and bond angles as:

$$E_{strain} = \frac{1}{2} \sum_{i(j)} \frac{3\alpha_{i-j}}{8d_{0,i-j}^2} \cdot \left(|x_i - x_j|^2 - d_{0,i-j}^2 \right)^2 + \sum_{i(j)} \frac{3\beta_{i-j-k}}{8d_{0,i-j}d_{0,i-k}} \cdot \left[|x_i - x_j| \cdot |x_i - x_k| + \frac{1}{3} d_{0,i-j} d_{0,i-k} \right]^2$$

x_i is the position vector of the i^{th} atom.

For $i-j$ bond, $d_{0,i-j}$ & $a_{0,i-j}$ are strain free bond length & lattice constant respectively.

α_{i-j} & β_{i-j-k} are bond stretching & bond bending force constant.

E_{strain} is minimized to attain a stable state by allowing each atom to vibrate and settle.

Force on the i^{th} atom is $\mathbf{F}_i = -\nabla_i (E_{strain})$.

Compare final & initial atom position to compute stain profile.

8 band $k.p$ calculation

- ✓ Use the 8 band $k.p$ method to calculate the electronic band structure.
- ✓ 6 band $k.p$ method does not consider the CB-VB interaction.
- ✓ The Hamiltonian for the strained QD can be simply written as

$$[H = H_k + V_{\Gamma}(z) + H_s]$$

- ✓ H_k stands for the kinetic 8-band effective-mass Hamiltonian (incorporating the CB-VB/spin-orbit interaction).
- ✓ $V_{\Gamma}(z)$ accounts for the band offset effects
- ✓ H_s stands for the strain induced Hamiltonian.

Results and Discussion

Strain Profile along [001]

Strain Profile along [010]

Strain Profile along [100]

Strain Profile ϵ_{xx}
in (001) plane, $z=0$

Strain Profile ε_{yy}
in (001) plane, $z=0$

Strain Profile ε_{zz}
in (001) plane, $z=0$

How Strain Changes the Electronic Spectra?

STRAIN

Strain has a very important role in QD energy, gain and optical performance.

Energy Profile

($h/a = 6$)

System: $\text{Ge}_{0.5}\text{Sn}_{0.5}/\text{Si}_{0.5}\text{Sn}_{0.5}$

Gain Profile

($h/a = 6$)

System: $\text{Ge}_{0.5}\text{Sn}_{0.5}/\text{Si}_{0.5}\text{Sn}_{0.5}$

Energy Profile

($h/a = 12$)

System: $\text{Ge}_{0.5}\text{Sn}_{0.5}/\text{Si}_{0.5}\text{Sn}_{0.5}$

Energy Profile

($h/a = 18$)

System: $\text{Ge}_{0.5}\text{Sn}_{0.5}/\text{Si}_{0.5}\text{Sn}_{0.5}$

Gain Profile

($h/a = 18$)

System: $\text{Ge}_{0.5}\text{Sn}_{0.5}/\text{Si}_{0.5}\text{Sn}_{0.5}$

Size dependency of Band Gap of QD (inversely proportional to dimension²)

(h/a)	BG(meV)
6	1079.27
7	891.70
8	667.96
10	538.59
11	521.54
12	511.34
15	451.57
18	414.19

Conclusion

- ✓ Studied GeSn/SiSn QDs for their strain profile and electronic band structure...
- ✓ ...using valence force field method and 8 band $k \cdot p$ method.
- ✓ Strain profile was studied in fair depth for the [001] direction and (001) plane...
- ✓ ...with distinct identification of zones of compressive and tensile strain.
- ✓ Size effect on the fundamental transition energy was studied...
- ✓ ...which is an essential tuning factor in optoelectronic device designs.
- ✓ Selective gain curves was studied.
- ✓ Observed that it predominantly varies inversely with the second power of QD height.

Acknowledgement

W. J. Fan would like to acknowledge the support from MOE Tier 1 funding RG 32/12.

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Thank you !

... for your patience and time...