

ELECTRONIC STRUCTURES OF SILICON QUANTUM DOTS AS
NANOCLUSTERS FOR SINGLE-ELECTRON TRANSISTORS

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A project report submitted in fulfillment
of the requirements for the award of the degree of
Master of Science (Physics)

Faculty of Science
Universiti Teknologi Malaysia

AUGUST 2008

Specially dedicated to my beloved parents, sisters, brother, brother-in-laws and my little nephews. Thanks for setting me on the path towards intellectual pursuits and giving me absolute support along the way

ACKNOWLEDGEMENTS

I would like to express my gratitude to all those who gave me the possibility to complete this thesis. First of all, I would like to express my sincerest appreciation to my supervisor, Assoc. Prof. Dr. Ahmad Radzi Mat Isa, and my co-supervisor, Prof. Dr. Karsono Ahmad Dasuki. I am deeply indebted to them who gave me guidance, advices, stimulating suggestions and encouragement throughout the completing of this research and thesis.

I would also like to thank Mr. Mohd Khalid Kasmin who helped me a lot in setting up the Linux parallel-computing cluster. Without his advices and suggestions, this thesis wouldn't be completed smoothly. My further appreciation dedicated to my group members, especially Muniroh who supported, assisted me in my research. Not forgetting this project members: Prof. Samsudi, Prof Yusof, Prof Zulkifli, Dr Sabar, Puan Khatijah, Dr. Uda, Puan Rosnita, Imam Sumpono, Qiao jie, Keng Boo, Wai Woon, Hishamuddin, Zunaidah, Shahrizar and Magen who have all contributed towards the success of this project.

Last but not least, I am very grateful to all my family members for giving me their greatest support, guidance and love all along my way up to now, that form courage in me to face every problem in the difficult times during this research.

ABSTRACT

Nanostructures such as quantum dot and nanocluster have occupied the centre of scientific interest because of their unique electronic nature. In this research, the electronic structures of silicon quantum dot were studied. The quantum dot was homologized with nanocluster since there is no strict distinction between these two nanostructures. The simulations in this research were carried out by using VASP (Vienna Ab-Initio Software Package) which utilizes the method of density functional theory and plane wave basis set. In order to speed up the computational time, parallelization was implemented on VASP. First, silicon clusters with surface passivated by hydrogen, Si_nH_m were simulated and the density of states (DOS) as well as bandstructure for each cluster was yielded. From the DOS graphs, discrete spectrum was observed instead of bulk-like continuous DOS which is the evolution from bulk to nano-size. Bandstructure graphs also showed the discrete energy level in consistence with the discrete energy spectrum from DOS. It was found that the bandgap for hydrogenated silicon clusters increases with the decrease in size. Bare silicon clusters, Si_n were also simulated from 1 to 15 number of silicon atom (n). Optimization was performed to obtain the ground state structure. The bandgaps for the ground state silicon clusters do not show a decreasing trend with the increment of cluster size as that of hydrogenated silicon cluster. The electronic structures of optimized clusters are affected by the surface orientation of the clusters. A comparison of the bandgap values for Si_nH_m and Si_n was made. Finally, the current-voltage (I-V) characteristic and conductance-voltage spectrum (G-V) of single-electron transistor (SET) were studied with a simple toy model. These transport properties have shown the relativity of the electronic structure and the electron transport, where the conductance gap increases with the energy difference between Fermi level of the gold lead and the nearest molecular energy level of silicon cluster.

ABSTRAK

Nanostruktur seperti bintik kuantum dan nano kluster telah menjadi matlamat kajian dalam bidang sains disebabkan sifat elektronik semulajadinya. Dalam kajian ini, struktur elektronik bintik kuantum silikon telah dikaji. Bintik kuantum telah dianggap sama dengan nano kluster, oleh kerana tiada perbezaan yang ketara antara kedua-dua nanostruktur ini. Simulasi kajian telah dijalankan dengan menggunakan perisian VASP (*Vienna Ab-Initio Software Package*) yang menggunakan teori fungsian ketumpatan dan set basis gelombang satah. Untuk menyingkatkan masa pengiraan, keselarisan telah dilaksanakan ke atas VASP. Simulasi ke atas kluster silikon yang permukaannya dipasifkan dengan hidrogen, Si_nH_m telah dilakukan dan ketumpatan keadaan dengan struktur jalur telah diperolehi. Daripada graf ketumpatan keadaan, spektrum diskrit telah didapati. Perubahan ketumpatan keadaan daripada selanjut bagi struktur pukal ke diskrit spektrum bagi nanostruktur merupakan evolusi nano. Jalur struktur juga menunjukkan aras tenaga diskret yang selaras dengan spektrum diskrit daripada ketumpatan keadaan. Jurang jalur untuk silikon terhidrogenasi telah didapati semakin mengurang semasa saiz kluster meningkat. Simulasi ke atas kluster silikon tulen (tak terhidrogenasi), Si_n yang mempunyai bilangan atom (n) dari 1 ke 15 juga dilakukan. Pengoptimuman dilakukan untuk mendapatkan struktur keadaan dasar. Jurang jalur bagi struktur keadaan dasar kluster-kluster itu tidak mempunyai aliran yang menurun dengan peningkatan saiz kluster seperti yang berlaku pada kluster silikon terhidrogenasi. Struktur elektronik kluster-kluster optimum dipengaruhi oleh orientasi permukaan kluster. Perbandingan nilai jurang jalur bagi Si_nH_m dan Si_n dilakukan. Akhirnya, ciri arus-voltan (I-V) dan konduktans-voltan (G-V) bagi transistor elektron tunggal dikaji dengan menggunakan satu model yang mudah. Sifat-sifat pengangkutan elektron itu menunjukkan perkaitan antara struktur elektronik dengan pengangkutan elektron, di mana jurang konduktans semakin bertambah apabila perbezaan tenaga antara aras Fermi elektrod emas dengan aras tenaga molekular yang paling dekat bertambah.

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LIST OF ABBREVIATIONS

SET	-	Single-electron transistor
RTD	-	Resonant tunneling diodes
QCA	-	Quantum cellular automata
ATLAS	-	Automatically Tuned Linear Algebra Software
BLAS	-	Basic Linear Algebra Subprograms
BO	-	Born Oppenheimer
BP	-	Becke-Perdew
BSSE	-	Basis set superposition error
CC	-	Coupled cluster theory
CG	-	Conjugate gradient
CI	-	Configuration Interaction
CMOS	-	Complementary metal oxide semiconductor
CMS	-	Computational materials science
CNT	-	Carbon nanotubes
DFT	-	Density functional theory
DIIS	-	Direct inversion in the iterative subspace
DOS	-	Density of states
ETB	-	Empirical tight binding
EPM	-	Empirical pseudopotential method
EMA	-	Effective mass approximation
2DEG	-	Two-dimensional electron gas
FFT	-	Fast-fourier transform
GEA	-	Gradient expansion approximation

GGA	-	Generalized gradient approximation
GTO	-	Gaussian-type orbital
GVB	-	Generalized valence bond
HF	-	Hartree Fock theorem
HK	-	Hohenberg-Kohn
HOMO	-	Highest Occupied Molecular Orbital
HPC	-	High-performance cluster
IFC	-	Intel Fortran Compiler
Intel® MKL	-	Intel Math Kernel Library
KS	-	Kohn-Sham theorem
LCAO	-	Linear combination of atomic orbitals
LDA	-	Local density approximation
LAPACK	-	Linear Algebra PACKage
LM	-	Langreth-Mehl
LSDA	-	Local spin density approximation
LUMO	-	Lowest Unoccupied Molecular Orbital
LYP	-	Lee-Yang-Parr
MCSCF	-	Multi-Configurations Self Consistent Field
MD	-	Molecular dynamics
MGGA	-	Meta-Generalized Gradient Approximation
MOSFET	-	Metal-oxide-semiconductor field-effect transistor
MPI	-	Message Passing Interface
NC-PP	-	Norm-conserving pseudopotential
NFS	-	Network file system
PAW	-	Projected Augmented Wave
PBE	-	Perdew-Burke-Ernzerhof
PES	-	Potential energy surfaces
PP	-	Pseudopotential
PW	-	Plane Wave
PW91	-	Perdew-Wang 1991

RMM	-	Residual minimization scheme
rPBE	-	Revised-Perdew-Burke-Ernzerhof
RPA	-	Random phase approximation
SA	-	Simulated annealing
SCF	-	Self-consistent functional
SSH	-	Secure Shell
STO	-	Slater-type orbitals
US-PP	-	Ultrasoft Vanderbilt pseudopotential
VASP	-	Vienna Ab-Initio Software Package
VWN	-	Vosko-Wilk-Nusair
QMC	-	Quantum Monte Carlo
WF	-	Wavefunction

LIST OF SYMBOLS

C	-	Capacitance
E	-	Energy
E_F	-	Fermi Energy
E_g	-	Energy gap / bandgap
E_n	-	Energy of n th confined state
E_C	-	Charging energy
E_{XC}	-	Exchange-correlation energy
$f(E)$	-	Fermi energy
F	-	Force
$g(E)$	-	Density of states
g	-	Spin-scaling factor
G	-	Capacitance
G	-	Reciprocal lattice vector
h, \hbar	-	Planck's constant
H	-	Hamiltonian
I_{SD}	-	Source-drain current
j_l	-	Spherical Bessel function
$J[n]$	-	Coulomb interaction
k	-	Wavenumber
k_B	-	Boltzmann's constant
L	-	Edge length
\hat{L}	-	Angular momentum operator
m	-	Mass

n	-	Quantum number of state (integer)
N	-	Total number of states
N	-	Number of electron
$n(\vec{r})$	-	Electron density
p	-	Momentum
\hat{P}_r	-	Linear momentum operator
$\tilde{P}_{lm\epsilon}$	-	Projector function
Q	-	Charge
\mathbf{r}, \vec{r}	-	Position vector
r_i	-	Electron spatial coordinates
r_s	-	Wigner-Seitz radius
$R_{nl}(r)$	-	Radial wavefunction
R	-	Radius
R	-	Resistance
R_A	-	Nuclei spatial coordinates
s, t	-	Dimensionless density gradient
t	-	time
T	-	Kinetic energy
T	-	Temperature
$T(E)$	-	Transmission
u_k	-	Bloch function
V	-	Volume
V	-	Potential Energy
V_{DS}	-	Drain-source voltage
V_T	-	Threshold voltage
V_G	-	Gate voltage
$Y_l^m(\theta, \varphi)$	-	Spherical harmonic
Z_A	-	Nuclei charge
λ	-	Wavelength
λ	-	Coupling constant

Ψ	-	Wavefunction
v	-	Velocity
ω	-	Angular frequency
ν	-	Frequency
$\phi(r)$	-	Envelope function
Θ	-	Unit step function
ε	-	Energy
ε_i	-	Single-particle energy level
Γ	-	Tunneling rates
μ	-	Chemical potential
∇	-	Laplacian operator
ξ	-	Spin-polarization
$\tau(\vec{r})$	-	Kinetic energy density
Ω	-	Volume of unit cell
η	-	Voltage division factor
ρ	-	Density matrix
Si	-	Silicon
Si _n	-	Silicon cluster with n silicon atom
Si _n H _m	-	Hydrogenated silicon cluster with n silicon atom and m hydrogen atom
S_N	-	Speedup
E_N	-	Efficiency

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CHAPTER 1

INTRODUCTION

1.1 Nanotechnology and Nanoscience

Nanotechnology and nanoscience had emerged as a very popular and important issue in every field including science (physics, chemistry and biology) and engineering over the decade. This is the trend of technology as many things get smaller and smaller by time and when it exceeds the ability of microtechnology, it comes to nanotechnology. This is the phenomenon of miniaturization which consequently leads to the brand new era of technology with novel concepts and devices.

The word “nano” refers to the size of 10^{-9} meter. One can imagine how small a nanometer is when a human hair with diameter approximately $100\ \mu\text{m}$ is sliced 10^5 times, a bacterial cell is divided 100 times, and ten hydrogen atoms are lined up. Nanoscience is concerned with study of objects which is anywhere from hundreds to tens of nanometer in size, whilst nanotechnology is related to the practical application of materials and devices in the same size range. Nanotechnology is sometimes called molecular manufacturing which is a branch engineering that deals with the design and manufacture of extremely small electronic circuits and mechanical device built at molecular level of matter.

Indeed, the emergence of nanotechnology already happened in the late 19th century when colloidal science started but it is not referred to nanotechnology at the time. In year 1959, Richard Feynman in his talk “There’s Plenty of Room at the Bottom” had firstly mentioned some of the nanotechnology concepts [1]. He described a process by which the ability to manipulate individual atoms and molecules might be developed. In 1947, the term “nanotechnology” was defined by Professor Norio Taniguchi from Tokyo Science University.

When things shrink into nanoscale, quantum effects come into play and classical theory unable to explain what happens in this extremely small size. Hence, the attributes of nanoscale particles are in between the atom and bulk materials. These attributes will vary by size which leads to the ability of material behavior engineering. This revolution have made nanotechnology and nanoscience a very exotic field which still need a lot more efforts in research to open up and reveal its under covered ability.

1.2 Application of Nanotechnology

The advancements in science and technology have allowed the miniaturization of amazingly complex devices. A lot of the nano-devices are being researched widely and intensively, hence its market potential is bright. A portion of it is as yet conceptual, though realization is not an impossible matter. It is worth to point out that nanotechnology has remarkably brought together technologies from physics, biology and chemistry.

1.2.1 Nanoelectronics, Nanocomputing and Nanophotonics

According to Moore's law, the number of transistors on a microprocessor would double periodically approximately every 18 months. Without taking account of the cost, this prediction had indicated that the transistors will be smaller in order to obey the law. To increase the density of transistors on one chip, the size of transistors must be small enough. Nanotechnology can achieve this target and open up the new phase of Moore's law with nanoelectronics and nanocomputing.

Nanocomputing is the use of the structures on the scale of within 100 nanometers to accomplish any of the tasks that modern computers can do. This kind of computing will adopt a new concept of operation, which is quantum principle. Thus, nanocomputing can also be termed as quantum computing. In making computers faster, power consumption and heat dissipation are the problems that need to be concerned. Amazingly, nanotechnology may overcome these problems. There was an analysis with unbelievable outcome: A CPU-scale system containing a million transistors would fit within a 400 nm cube, run at 1 GHz, and consume 60 nanoWatts [2]. A desktop nanocomputer consuming 100 watts of power would process 10^{18} instructions per second. Indubitably, the memory would increase in consistent with the power and speed. The factor that contributes to these distinct abilities is quantum bits or qubits. Classical computers rely on bits, which 1 represent ON state and 0 represent OFF state. Quantum computing consumes the law of quantum mechanics that allow an atom to be arranged in a coherent superposition of states 0 and 1. This means an atom can be in both states at the same time. While N bits can store a single number out of 2^N possibilities, a qubit can store all 2^N number available.

In order to create quantum computers, nanoelectronics are needed. There are plenty of nanoelectronic devices have been proposed, among which are: single-electron transistor (SET), resonant tunneling diodes (RTD), spin transistor, quantum cellular automata (QCA), carbon nanotubes (CNT), ultra-scaled FETs, superlattice

arrays, and molecular electronic devices. The nanostructures that build these nanoelectronics can be categorized into three: quantum well, quantum wires and quantum dots. The operations of these devices are governed by quantum principles. CNT is one of the popular research targets owing to its special attributes, for instance, it is stronger than steel and it can be used in a lot of applications in field of biology, chemistry as well as physics.

Fabricating nanoelectronics could open new way of making nanophotonic devices. Nanophotonic is the manipulation and emission of light includes near field and far field light using nano-scale materials. It could revolutionize the fields of telecommunication, computing as well as sensing. Its applications includes storing data, as switch operating in computers, and converting electrical energy into light of variable wavelength for the purpose of light sources.

1.3 Introduction to Modeling and Simulation

Modeling is the technique of representing a real-world system or phenomenon with a set of mathematical equations or physical model. A computer simulation then attempts to use the models on a computer so that it can be studied to see how the system works. Prediction may be made about the behavior and performance of the system by changing its variables. In this research, nanostructures are the system targets of the modeling and simulation.

Simulation is a useful and important part of modeling nanostructures to gain insight into the attributes of a structure or a whole system with several structures connected. It is a method to predict the behavior transformation for a variable changing before performing a practical experiment. The simulation can then be proven by the results of experiment. This is also a beneficial approach to test the

most optimal and the best performance of a device which is built by those nanostructures before the real fabrication.

Besides, simulation can give detailed theoretical explanation to the phenomenon that could not be explained by experiment solely. Among the examples are the reconstruction of the nanostructures and the occupation of the electrons. With the 3D graphical viewer and animation, we can view the atomic structure models and the process of the structure transformation. With computer simulation done prior to experiment, the mastering of the nanostructures principles is improved and 'trial and error' could be reduced during experiment.

However, there isn't a comprehensive simulator which can take into account every factor that would contribute to the system changes. Many of those only adopt the approximation which is the most optimal and closest to the real system for the representation. For nanostructures, first principle calculation is an appropriate simulation approach for studying the electronic structures and properties. The advantage of this calculation is that, it can be done without any experimental data. However, it could be a massive calculation that consumes a very long time to accomplish.

Computational science becomes an essential tool in modeling and simulation. It is the application of computational and numerical technique to solve large and complex problem, for example, complex mathematics that involved a large number of calculations. Therefore, modeling and simulation are commonly accomplished by the aid computational science and therefore they are always referred to computer modeling and computer simulation. Computational science could be defined as an interdisciplinary approach that uses concepts and skills from the science, computer science and mathematic disciplines to solve complex problems which allow the study of various phenomena. It can be illustrated by Figure 1.1. To improve the performance and speed of large computation, one of the approaches is parallel computing. Parallel computing can reduce the computing time of computational

costly calculations such as first principle calculations mentioned above, where it distributes the calculation to two or more processors or computers.

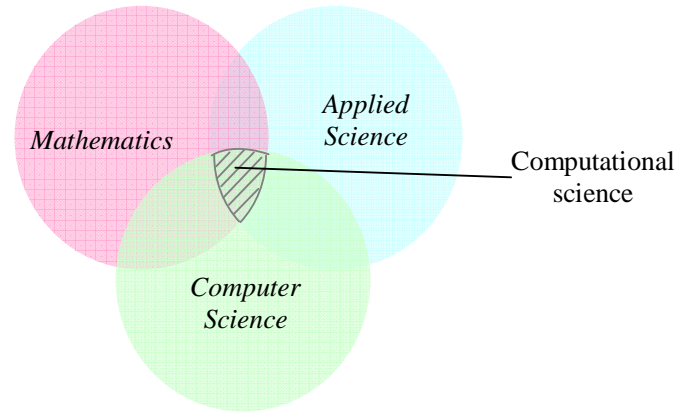


Figure 1.1. Computational science is defined as the intersection of the three disciplines, i.e. computer science, mathematics and applied science.

1.4 Research Objectives

The main interest of this research is to study the electronic structures of silicon quantum dots in the form of clusters. The objectives of this research can be summarized as the following:

- a) to study the electronic structures of quantum dots with variable size and structures.
- b) to study the relation between the bandgap and the size as well as the effect of structure of the quantum dot, and
- c) to study the relation between the electronic structure of the quantum dot and the I-V characteristic of single-electron transistor.

1.5 Scopes of Study

The study scopes of this research are as the following:

- a) Quantum dot is simulated as isolated small range nanocluster.
- b) Silicon is adopted as the material of the quantum dot.
- c) Bandstructure and energy spectrum are studied for the electronic structures of quantum dot.
- d) Density functional theory is used to calculate and simulate the electronic structures of quantum dot.
- e) To build a parallel computing system to speed up the calculation.

1.6 Thesis Overview

Quantum dot is a crucial part in single-electron transistor (SET) that govern the performance of the device. In the next chapter, SET is introduced and its operation principle is discussed. From this chapter, the characteristics of quantum dot in SET could be understood, where the objective of modeling and simulating quantum dot is manifested.

In chapter 3, theory of nanostructures and quantum dot is discussed. The attribute of the evolvement from bulk to nanoscale structure is showed. In this extremely small size, the theory that governs its properties is quantum theory. There are a lot of approaches to simulate the electronic structures of quantum dot. Density

functional theory is a sufficient method in doing this. Its theory is discussed in the next chapter, Chapter 4.

Chapter 5 is discussing the methodology of the simulation. Vienna Ab-initio Software Package which is utilized in this study is introduced. The steps and process of simulation is explained. Following this, Chapter 6 would be results and discussion. Figures and graphs showing the electronic structures of quantum dot are showed, and the results are discussed and interpreted.

Finally Chapter 7 which is the conclusion. Theories and results discussed in the previous chapters are summarized and concluded here. Furthermore, suggestion is given on how to make the simulation work better and more complete.

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