DESIGN AND SIMULATION OF SILICON-BASED MICROCAVITIES

A Thesis Proposal

Presented to
The Faculty of Department of Physics
MSU-Iligan Institute of Technology
9200 Iligan City, Philippines

In Partial Fulfillment
of the Requirements for the Degree of
Master of Science in Physics

CHRISTINE MARIE T. CEBLANO
August 2010

BUDGET PROPOSAL

Program Title: Masters of Science in Physics					
Dissertation Title: Design and Simulation of Silicon-based Microcavity					
Source of Fund: ASTHRDP, PCASTRD-DOST	Research and Development Station: MSU-IIT, Iligan City				
Item	1 Year				
	Q1	Q2	Q3	Q4	Total
I. Personal services					
A. Direct Cost					
1. Salaries					
2. Honoraria					
B. Indirect Cost a/					
Sub-Total					
II. Maintenance and Operating Expenses					
A. Direct Cost					
1. Travel(Local and Foreign)					
2. Supplies and Materials					
CPU			20,000		**20,000**
MATLAB & Simulink Student Version R2010a		10,000			**10,000**
Lens (25 -50 focal length)			10,000		**10,000**
Holders			10,000		**10,000**
Lens, Mirror and Post					
Miscellaneous					
Halogen lamp, Stand for Halogen Lamp, dimmer switch, wires, etc.			2,000.		**2,000**
3. Communications					
4. Repair and Maintenance of Facilities					
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6. Transportation and Deliveries Expenses					
7. Utilities Expenses					
8. Training and Scholarship Expenses					
9. Advertising Expenses					
10. Printing and Binding Expenses	2,000	2,000	2,000	4,000	**10,000**
11. Rent Expenses					
12. Representation Expenses					
13. Subscription Expenses					
14. Professional Services					
15. Taxes, Insurance Premiums & Other Fees					
B. Indirect Cost a/					
Sub-Total	**2,000**	**12,000**	**44,000**	**4,000**	**62,000**
Grand Total(PhP)					**62,000**

Submitted by:

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Recommending Approval:

RYAN B. BALILI, Ph. D.
Thesis Adviser

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Graduate Program Coordinator

Department of Physics
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GANTT CHART

" Design and Simulation of Silicon-based Microcavity"

Task	Q1			Q2			Q3			Q4		
Simulate published result												
Measure Reflectivity												
Design and Simulate Si-based Microcavity												
Data Analysis												
Thesis Manuscript writing												

CSM – GS Form 1
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Republic of the Philippines
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ILIGAN INSTITUTE OF TECHNOLOGY
Iligan City

DOST, SEI SCHOLAR

COLLEGE OF SCIENCE AND MATHEMATICS

Date: August 9, 2010

NOMINATION OF MEMBERS OF ADVISORY PANEL

- [ ] DISSERTATION
- [x] THESIS
- [ ] SPECIAL PROJECT

The following graduate faculty members are recommended to compose the Advisory Panel of Mr./Ms. Christine Marie Ceblano in the graduate program leading to the degree Masters of Science in Physics.

	Name	Signature	
1.	Ryan B. Balili, Ph.D		Chairperson/Adviser
2.	Rosario L. Reserva, M.Sc		Member
3.	Florencio P. Recoleto, Jr., Ph.D		Member
4.			Member
5.			Member

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RECOMMENDING APPROVAL:

Salasa A. Nawang, Ph.D
Program Coordinator

APPROVED:

Jinky Bornales, Ph.D
Dean, College of Science and Mathematics

Distribution:
- Panel Members
- Program Coordinator
- College Coordinator
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APPROVAL FOR PROPOSAL HEARING

☐ DISSERTATION
☑ THESIS

As members of the Advisory Panel of Mr./Ms. Christine Marie Ceblano, we recommend approval of the student's application for proposal hearing.

Ryan B. Balili, Ph.D	August 4, 2010
Chairperson	Date
Rosario L. Reserva, M.Sc	August 4, 2010
Member	Date
Florencio D. Recoleto, Jr., Ph.D	August 4, 2010
Member	Date
Member	Date
Member	Date

DATE: August 11, 2010 TIME: 11:30 - 12:30 PLACE: Rm. 130

Recommending Approval:

Salasa A. Nawang, Ph.D
Program Coordinator

Approved by:

Jinky Bornales, Ph.D
Dean, College of Science and Mathematics

Date: August 4, 2010

IMPORTANT:

1. This form, together with a copy of the manuscript, must be submitted to the Dean's Office, College of Science and Mathematics at least one (1) week prior to the scheduled proposal hearing.
2. Each member of the panel must be provided with a copy of the manuscript.
3. The proposal hearing must be open to the public.
4. The student must attach to this form the official receipt of the proposal fee.

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CSM – GS Form 4-1 (Updated May 2009)

Date: August 11, 2010

APPROVAL OF PROPOSAL

☐ DISSERTATION
☑ THESIS

Name: Christine Marie T. Ceblano

Degree: Master of Science Specialization: Physics

Title: Design and Simulation of Silicon-based Microcavity

Comments:

See manuscript for comment.
Return/Present old manuscript to chairperson/Adviser & members
with the new manuscript

APPROVED:

Advisory Panel

Ryan B. Balili	Aug. 11, 2010
Chairperson/Adviser	Date
Florencio D. Recoleto Jr.	August 11, 2010
Member	Date
Rosario L. Reserva, M.Sc	August 11, 2010
Member	Date
Member	Date
Member	Date

Note: Submit this approval sheet and the Proposal, together with the recommendations of the examiners, to the office of the Dean of the College of Science and Mathematics.

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CSM – GS Form 4-2 (Updated May 2009)

Date: August 11, 2010

PROPOSAL HEARING

☐ DISSERTATION
☑ THESIS

Name: *Christine Marie T. Ceblano*

Title: *Design and Simulation of Silicon-based Microcavity*

Recommendations:

1. Start using a single quantum well first for your design of Si-based microcavity then after that you can employ multiple quantum wells.
2. See the thesis of Mr. Neal Lasta for the calculation of n_{eff} (the effective index of refraction). It's for VCSEL only, but maybe you will get an idea on how you could apply it for Si-based microcavity.
3. The experimental results of the reflectivity for the samples from NIP U.P Diliman are flat, perhaps the incident light is so intense, so consider using filters to minimize the intensity.

Florencio D. Recoleto Jr.
Examiner (Signature over printed name)

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CSM – GS Form 4-2 (Updated May 2009)

Date: Aug 12/10

PROPOSAL HEARING

☐ DISSERTATION
☑ THESIS

Name: *Christine Marie T. Ceblano*

Title: *Design and Simulation of Silicon-based Microcavity*

Recommendations:

- refine title and objectives of the study
- improve chapter 3 by incorporating methods to be to create a MCP model of optimum coupling.
- incorporate in the manuscript all other corrections/suggestions. Pls see questions/comments on the draft.

ROSARIO L. RESERVA

Examiner (Signature over printed name)

Table of Contents

CHAPTER 1

INTRODUCTION

With the advancement of today's technology, the realizations of crystalline microstructures with unusual and interesting optical properties are made possible. Microstructures, such as optical microcavities, can be used as controlled "laboratories" for observing large varieties of intriguing optical phenomena in semiconductor quantum optics and photonics [1].

An optical microcavity is basically an optical resonator which confines light to small volumes close to or below the dimension of the light's wavelength. It has a wide range of applications in both fundamental and applied fields of research including cavity quantum electrodynamics, optical communication, resonant cavity optoelectronics, micromechanical sensors and biosensing [2]. Fabrication of such optical microcavities can be achieved by growing multilayered structures. It can be fabricated in a way that the active medium, cavity and two mirrors consist of thin films. The light is confine to a small volume, even up to the nanometric scale of the cavity. For better confinement of light, a high refractive index contrast is needed at the interface between the layers of the structures. This result to resonant frequencies distributed at the spectrum, which is highly dependent on the cavity dimension.

There are many optical microcavities made with different semiconductor materials, but silicon-based microcavities are very interesting for optoelectronics applications such as fabrication of efficient low cost optoelectronic devices [3]. Examples of these are, vertical-cavity surface emitting lasers (VCSELS), low-threshold diodes, polariton lasers, optical switches and spin memory element [2, 4]. In particular, amorphous Silicon Nitride ($a - Si_{1-x}N_x : H$) are very suitable materials to grow optical microcavity base on multilayered structures such as Fabry-Perot microcavity. The reason is that they do not present the lattice parameter mismatch problem. Hence, you get layers with lesser effects. Also the tunable optical gap and refractive index contrast can be tuned by variation of nitrogen content in the silicon alloy [5].

Most of the researches done in microcavities are gallium - based [6, 7] made of active III-V semiconductor materials which control laser emission spectra for data transmission [1]. In this study a silicon-based microcavity is modeled. This is possible by using transfer matrix method (TM), can be useful tool in simulation and characterization of microcavities for reflectance, transmittance and absorbance. A multilayered structure can be simulated to predict optical properties before fabrication by applying the transfer matrix algorithm. To test the validity of the TM algorithm used in for ongoing studies with, amorphous silicon nitride ($a-Si_{1-x}N_x : H$) microcavity from a journal by Ballarini et al. [4] is modeled. The computed transmittance spectrum of the microcavity is then compared to their experimental result. This is to test if the transfer matrix program works for such multilayered structure. Aside from modeling an established journal, this study also simulate multilayered structures of the grown and fabricated samples from NIP, UP-Diliman for reflectivity. Reflectivity measurements of the samples will be also considered. After which is the comparison of the simulated result to the experimental result. This is also to test the TM algorithm. The program is useful for designing other silicon-based microcavities like SiGe before it goes for fabrication.

After the test of transfer matrix algorithm for various multilayered structures is the design and simulation of silicon based microcavity, specifically composed of silicon germanium ($Si_{1-x}Ge_x$) alloy, where quantum wells are embedded inside. The design parameters of the microcavity will be varied to ensure optimum overlap between exciton and photon field. Transfer matrix algorithm will be used. Acquiring the optimum resonance between exciton and photon in this microcavity may be used as parameters in future experiment for efficient and low cost optoelectronics applications. Overall, this study is an optical investigation of silicon-based microcavities and multilayered structures both in theory and experiment.

1.1 Objectives of the Study

This study investigates silicon-based microcavities for future optical applications. This also examines the reflectivity of grown and fabricated multilayered structures. Specifically, it aims the following:

1. Design a simulation algorithm using transfer matrix method.

   a. Simulate the transmittivity of a silicon-based $(a - Si_{1-x}N_x : H)$ microcavity by using transfer matrix method and compare the experimental results to the established result obtained by Ballarini et al. [4].

   b. Characterize the reflectivity of grown and fabricated multilayered structures from NIP, UP-Diliman.

   c. Simulate the reflectivity of the given multilayered structures and compare results from the experiment.

2. Design silicon-based microcavities with an optimum coupling between photon and exciton using transfer matrix method.

1.2 Significance of the Study

For the past decades, strong light-matter interactions in solid-state devices are objects of increasingly intense research [8] due to coherent and stimulated effects in such system which can lead to new optical devices [9]. The first step of this study is to create a simulation algorithm for multilayered structures or microcavities. After which is the validation of the program to various multilayered structures. If the program works, then is the design and simulation of silicon-based microcavities, particularly silicon germanium (SiGe). This is the very aim of this study. Through simulation, the silicon-based microcavity can be characterized and varied with its thickness in which there is optimum resonance between exciton and photon. The result may be used as parameters in silicon-based microcavity fabrication for future experiments. Eventually, this may lead to various and useful optical applications that are efficient and low cost. Production of such semiconductor (SiGe) material for the silicon-based microcavities will not be a problem since silicon is believed to be the optimum material for optical components fabrication due to mainly economical and practical reasons [10]. Silicons are cheaper that other group III-V and II-VI materials. It is still abundant in sources since it's the most common element in the earth's crust. Mostly, silicons are less toxic where health risks will be lesser than other semiconductor materials.

1.3 Scope and Limitation of the Study

The focus of this study is to design and simulate Silicon-based microcavities. Primary, this will consider a simulation of a microcavity made from amorphous silicon nitride $(a - Si_{1-x}N_x : H)$ [4] for transmittance using transfer matrix method (TM). Another is the simulation of multilayered structures of grown and fabricated samples from NIP, UP-Diliman for reflectance. Reflectivity measurement of the given samples will be also considered. The results from the simulation and experiment will be then compared. This is to test the TM algorithm. Then is the design and simulation of silicon-based microcavities, particularly the SiGe. This will simulate, design and characterize the microcavity using transfer matrix method. Thickness of microcavity will be varied to get the optimum resonance between exciton-polaritons. Matlab computing software will be used as the simulation tool.

On the other hand, only reflectivity experiment will be done on the grown and fabricated multilayered samples from NIP, UP-Diliman for reflectivity. This study will simply use transfer matrix method for the simulation part.

CHAPTER 2

REVIEW OF RELATED LITERATURE

2.1 Microcavities

Microcavities have wide range of applications in both fundamental and applied fields of research including cavity quantum electrodynamics, optical communication, resonant cavity optoelectronics, micromechanical sensors and biosensing [2]. Basically, a microcavity is an optical resonator which confines light to small volumes close to or below the dimension of light's wavelength. It could be a micron- or sub-micron sized optical resonator which has two different schemes to confine light (Figure 2.1). The first scheme is by using reflection of a single-interface like a metallic surface. The second scheme is by using microstructures periodically patterned on the scale of the resonant optical wavelength like Distributed Bragg Reflectors (DBRs). Microcavity has also diverse modes such as resonant optical modes, longitudinal resonant mode and transverse mode. But this traditional feature or mode can lose its precision since all modes exist at the same footing.

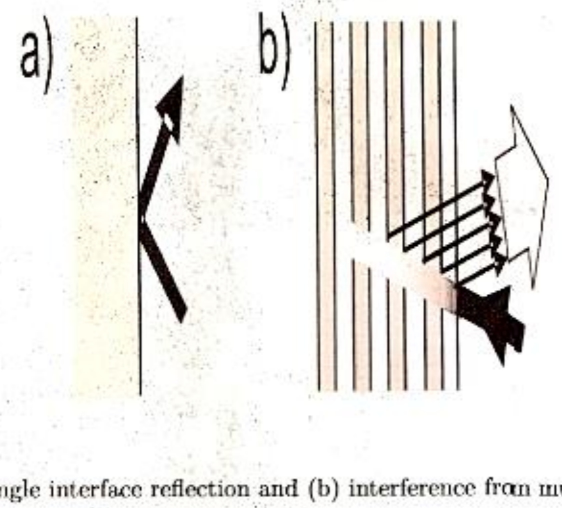

Figure 2.1: (a) single interface reflection and (b) interference from multiple interfaces [11].

Among the properties of microcavities are the quality factor (Q-factor) and finesse, intracavity field enhancement and field distribution, angular mode pattern, low threshold lasing, Purcell factor and lifetimes, strong coupling and weak coupling. This strong coupling in a microcavity will be dealt with in detail in Section 2.3.

There are different types of microcavities according to its application. The most common of all is the planar microcavity which uses two flat mirrors to confine light. These mirrors are close to proximity so only a few wavelengths of light can fit in between. Under with planar microcavity are the metal microcavities and Dielectric Bragg mirrors (DBRs). The finesse of DBRs cavity is based on the reflectivity of each mirror dependent on the number of pair repeats and the refractive index contrasts between the two materials used. So each layer is just a quarter of the desired centre wavelength of reflection. In this study we will use Silicon- based (e.g. $a - Si : N$) as DBRs.

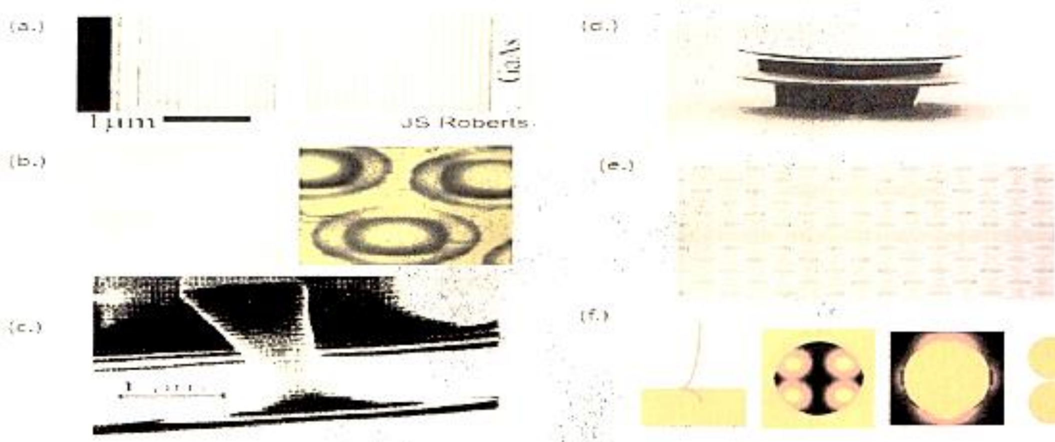

Figure 2.2: (a) Scanning electron micrograph of GaAs/AlGaAs DBR microcavity on a GaAs substrate, from Savvidis et al. (2000) (b) SEM and optical micrograph, of 5 μm diameter, 5 μm radius of curvature mirrors, from Prakash et al. (2004) (c) Pillar microcavity from an etched planar DBR semiconductor microcavity from Gerard et al. (1996) (d) microdisk (lower ring) with upper electrical contact, from Frateschi et al. (1995) (e) Plasmon localisation: on flat noble metals, metallic voids, metal spheres, and between metal spheres [11].

Other than planar are spherical mirror microcavities which control the photonic modes in the microcavity where the light has to be confined in the other two spatial directions. Another is the Pillar microcavities which are used to confine the lateral extent of the photonic modes inside planar microcavities by etching them into discrete mesas. Whispering gallery modes is an alternative approach which uses total internal reflection within a high refractive index convex body. This can exist within spheres (3D modes) or disks (2D modes), or more complicated topological structures. For photonic crystals, it employs periodic patterning in 2 or 3 dimensions to confine light to a small volume surrounding a defect of the structure. They are advantageous for many applications since it can show Q-factors exceeding 10^5 while producing extremely small mode but such cavity are hard to fabricate. Lastly is the new plasmonic cavity which is based on plasmons localized to small volumes close to metals.

Along with these are the key issues when considering microcavities. They are the optical losses or finesse, coupling to incident light, optical mode volume, fabrication complexity and tolerance, incorporation of active emitters and practicality of electrical contacting.

2.2 Fabry-Perot Microcavity

Fabry-Perot (FP) interferometer is mainly composed of two high reflecting surfaces spaced out by a spacer. It is called interferometer in the sense that the large number of rays, interfering at the two reflecting surfaces, produces an interferometer with extremely high resolution.

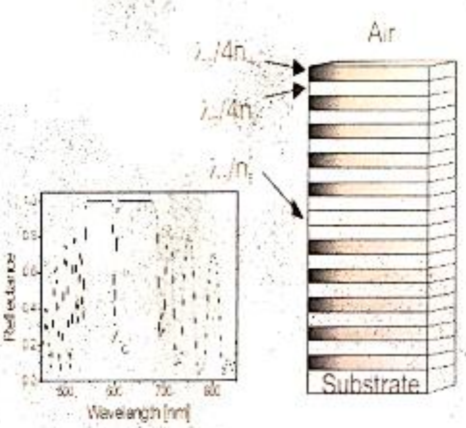

Figure 2.3: Sketch of a Fabry-Perot Microcavity [5].

The whole structure of FP filter will be a multilayered structure if two DBRs are used as reflecting surfaces and thin film as the spacer. This is commonly referred as Fabry Perot microcavity which works on low interference order. Sometimes, FP microcavity structure can also be described as a DBR structure in which the central layer has been replaced by a different refractive index layer. Figure 2.3 shows an example sketch of Fabry Perot microcavity in which two DBRs are spaced by a thin film of different refractive index with respect to those of the DBR's layers. These central layer or spacer should be of λ_c or $\lambda_c/2$ thickness for it to work on the second or first interference order. On its side is the FP reflectance spectrum centered at λ_c.

2.3 Microcavity Polaritons

A microcavity is composed of Perot-Fabry cavity sandwiched between two reflectors with quantum wells of narrower band gap embedded on it. The reflectors are quarter-wave layers of semiconductor called distributed Bragg reflectors (DBRs) with high and low indices of refraction. Conversely, quantum wells (QWs) are potential wells that confines particle like excitons to two-dimensional motion thus occupying a planar region at low temperatures [12]. When trapped in an optical cavity, photon energy is quantized in the growth direction while the in-plane photon states remain unaffected. Similarly, exciton energy states show same quantization in the growth direction and continuous states in the free in-plane motion. The strong coupling between the exciton and cavity modes gives rise to a new half light and half matter quasi-particle called polaritons. In this strong coupling regime, the photon and exciton dispersion repel each other at resonance (Figure 2.4). This eventually leads to two distinct dispersion called the polariton branches with upper and lower polariton mode [13, 14].

Considering the DBRs force of the axial wave vector kz to be quantized (see Fig 2.5), the bare cavity dispersion can be derived as,

$$E_{ph} = \hbar ck = \hbar c\sqrt{k_z^2 + k_{\parallel}^2} = \hbar c\left[\left(\frac{N\pi}{n_{eff}L_c}\right)^2 + k_{\parallel}^2\right]^{1/2} \tag{2.1}$$

where k_z is along the epitaxial growth direction, $k_{\parallel}^2$ is the wave vector parallel to the quantum well, L_c is the effective cavity length, n_{eff} is the effective intracavity index of refraction and N is the mode number or the number of half-wavelengths in the cavity.

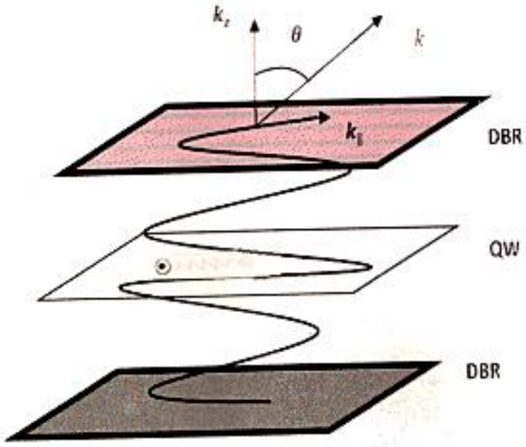

Figure 2.4: Basic structure of microcavities and illustration of the photon-exciton oscillator coupling [7].

Consequently, the exciton energy is,

$$E_{ex} = E_0 + \frac{\hbar^2 k_\parallel^2}{2(m_e + m_h)} \tag{2.2}$$

where E_0 and $m_e(m_h)$ is the ground state exciton energy and the electron in-plane mass respectively. For momentum to be conserved as required by the translational invariance of the system, the photon and exciton is given the same in-plane momentum $k_\parallel$. As a result, there is a strong coupling between exciton and photon modes with the same in-plane wave vector.

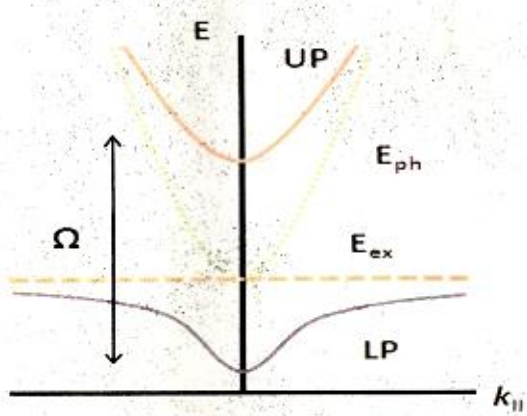

Figure 2.5: Dispersion relation of the upper and lower polariton (solid curves) [7].

The exciton and photon modes can be treated as coupled oscillators with coupling matrix element Ω. The coupling is expressed by matrix Hamiltonian with exciton states $|ex\rangle$ and photon states $|ph\rangle$ as basis. This gives us,

$$H = \begin{bmatrix} E_{ex} & \Omega/2 \\ \Omega/2 & E_{ph} \end{bmatrix} \tag{2.3}$$

where E_{ex} and E_{ph} are the energies of the exciton and cavity photon mode respectively. The eigenvectors of this Hamiltonian is expressed as a superposition of the exciton and photon states,

$$\begin{aligned} |UP\rangle &= C|ex\rangle + X|ph\rangle \\ |LP\rangle &= X|ex\rangle - C|ph\rangle \end{aligned} \tag{2.4}$$

where X and C are just the standard Hopfield coefficients which describe the fraction of the exciton and photon content of the polariton given by,

$$\begin{aligned} X^2 &= \frac{1}{2} + \frac{E_{ph} - E_{ex}}{2\sqrt{(E_{ph} - E_{ex})^2 + \Omega^2)}} \\ C^2 &= 1 - X^2 \end{aligned} \tag{2.5}$$

UP and LP are the two coupled mode eigenstates with higher and lower energy states. Eigen energies are derived by diagonalizing the Hamiltonian. We have,

$$E_{\substack{UP \\ LP}} = \frac{E_{ex} + E_{ph}}{2} \pm \left[\left(\frac{E_{ex} - E_{ph}}{2} \right)^2 + \left(\frac{\Omega}{2} \right)^2 \right]^{1/2} \tag{2.6}$$

The anticrossing or energy splitting between the exciton and photon modes at resonance is the Rabi splitting $(\Omega/2)$ pr coupling constant (Ω). Basically, it is just a function of the quantum oscillator strength f containing the electric dipole matrix elements of the atomic transition. It is also dependent on the number of atomic oscillators as well as the number of quantum wells.

2.4 Polariton Spin and Polarization

Some of the features of Microcavity polariton are its weakly interacting, light mass, lifetime variation in momentum space, bottleneck effect, magic angle, polariton spin and polarization.

Excitons have total spin of ± 1 and ± 2 . These are possible since they are formed by an electron and heavy-hole with $\pm 1/2$ and $\pm 3/2$ spin projections respectively. Exciton with ± 2 spin cannot be optically excited given that photon has spin ± 1. Spin ± 2 are optically inactive, "dark" states while spin ± 1 are optically "bright" states which can be excited by ω^+ and ω^- circularly-polarized light. Only these "bright" exciton states that are couple to light are shifted in energy by the Rabi splitting while the "dark" states remain unchanged. This eventually increases the exciton binding energy since the excited states does not couple to light.

2.5 Silicon-based microcavity

Over the last decade, optical properties of silicon nanocrystals along with its electronic properties have been a very challenging and promising field of research for technological and scientific reasons [15]. Studies have even extended over other "silicon-like" (e.g. Ge) and silicon based like SiGe nanocrystals. This is due to the poor optical properties of the bulk crystals like Si where it has a small band gap and a resulting phonon-assisted light emission.

Similarly, silicon-based multilayered structures have been intensively studied in the framework of all silicon optoelectronics [16]. A study done by Giorgis [17] shows that microcavity entirely based on hydrogenated amorphous Silicon Nitride $(a-Si_{1-x}N_x : H)$ posses appealing optical properties such as resonant enhancement of photoluminescence. Also, Fabry-Perot microcavities were used for the enhancement and inhibition of photoluminescence (PL) in a hydrogenated amorphous silicon nitride $(a-SiN_x : H)$ [18].

2.6 Transfer Matrix Formalism

Transfer Matrix (TM) method is generally used in optics and acoustics to analyze the propagation of electromagnetic or acoustic waves through stacked layers of same or different reflectivity indices. This is important for the design of anti-reflective coatings and dielectric mirrors. Thus, these materials give us a wide range of applications in instrumentation, military, medical, scientific, display, vision and space.

As stated , TM method allows the simulation of reflectivity, absorption and transmission of periodic structures [7]. Consider a system of stack dielectric materials of various thicknesses t_j and reflectivity indices n_j where a field is incident. This field will have reflected and transmitted components such as a sum of forward and backward moving waves.

$$E = E_+ e^{ikx} + E_- e^{-ikx} \tag{2.7}$$

The stack of layers can be represented as a system matrix which is the effective contribution of all the layers and interfaces (TM). Transfer matrix equation is then,

$$E' = T_M E \tag{2.8}$$

The Transfer matrix across an interface and a layer are given by

$$T_{int} = \frac{1}{2} \begin{pmatrix} n+1 & -(n-1) \\ -(n-1) & n+1 \end{pmatrix} \tag{2.9}$$

$$T_{layer} = \begin{pmatrix} e^{ik_j t_j} & 0 \\ 0 & e^{-ik_j t_j} \end{pmatrix} \tag{2.10}$$

T_M is then,

$$T_M = \begin{pmatrix} t_{11} & t_{12} \\ t_{12} & t_{22} \end{pmatrix} = T_1 T_2 T_3 \ldots T_n \tag{2.11}$$

Now, the transmitted and reflective electric fields are just

$$E_{trans} = \frac{det(T)}{t_{22}} E_{inc} \tag{2.12}$$

$$E_{ref} = -\frac{t_{21}}{t_{22}} E_{inc} \tag{2.13}$$

With reflectivity as

$$R = \frac{E_{ref}^2}{E_{trans}^2} \tag{2.14}$$

There are also studies using transfer matrix method of multilayer to investigate the transmittance at the central wavelength 720 nm of Si when using various multilayer thin film coatings [19].

2.6.1 Advantages and drawbacks of the Transfer Matrix Method

Transfer Matrix method is a very useful algorithm and has many advantages. But like any other numerical method, it has also its own drawbacks. One of its advantages is, it is fitted for reflectivity and transmission calculations multilayer structures. In this sense, this is very useful in this study where a multilayer specifically a Fabry-Perot microcavity will be simulated for these two optical properties: reflectance and transmittance. With this method, either real or complex values for the refractive index can be taken. Lossless material is represented by real refractive index while one of the two types of materials is represented by the complex refractive index. The negative imaginary part of the refractive index gives us the idea that the material is absorptive while the positive indicates a gain medium.

Another pro of TM method is its ability to handle any number of layers in a multilayer structure. With this, it is better than plane method [20] in which its key method is the matrix diagonalization. The computer time in this method required scales like N3 where N is just the number of plane waves in the expansion. This is inefficient and time consuming if large N is required for more complex structures. With TM there is no requirement that multilayer should be periodic. There is no restriction in TM regarding the order of any layer's thickness. It can define independently the thickness. So, for modeling structures with different periodic multilayer stacked together, obviously not fully periodic, TM method is the most suitable.

Now for TM's method drawbacks, first it assumes an infinite plane perpendicular to the propagation. This means that each layer in a multilayer structure extends infinitely in both of its dimensions. In order to avoid errors from this assumption, the layers to be modeled have to be wide. Next drawback is it calculates the field throughout the structure by layer by layer propagation with matrix relations. With this, it is computational speed dependent and lacks a mathematical expression that can relate the field between multiple layers. If this mathematical expression is present then it would reduce the mathematical calculation required as well as the computational time.

Lastly, TM method is only limited to continuous propagation, not for pulse propagation. Solution to model such propagation is to combine Fourier Transform with TM. But Finite Difference Time Domain Method is better for pulse propagation.

CHAPTER 3

RESEARCH METHODOLOGY

Presented in this chapter are the methods in modeling and simulating a Si-based microcavity to get the optimum resonance between the exciton and cavity mode. Furthermore, this presents the reflectivity experiment of already grown and fabricated multilayered structures from NIP, UP-Diliman.

3.1 Microcavity Structure

The general structure of the microcavity to be used in this study is a repetition of amorphous silicon nitride ($a - Si_{1-x}N_x : H$) as shown in Figure 3.1. This is consist of three sets of distributed Bragg reflectors (DBRs) namely DBR1, DBR2 and DBR3 with alternating high and low index of refraction. There are also two emitter layers spaced out by DBR2. Specifically, H for high refractive index with $n_H = 2.22$ ($x = 0.41$) and L for low refractive index with $n_L = 1.8$ ($x = 0.57$). The two spacers or cavity have refractive index of $n_c = 1.9$ ($x = 0.50$). DBR1 and DBR3 have six pairs of layers while DBR2 has 2.5 pairs. Each layer has an optical thickness of $\lambda/4n_H$ or $\lambda/4n_L$ (where $\lambda = \lambda_c$ - is the central wavelength of AL radiation spectrum). The cavity has thickness of λ_c/n_c. Only consider that the laser is at normal incidence to the top of microcavity.

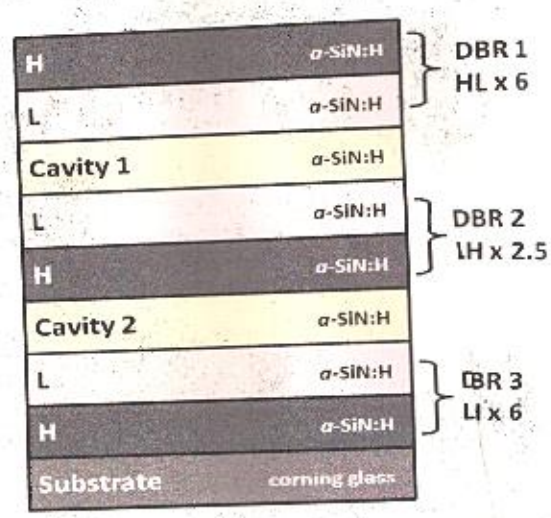

Figure 3.1: Schematic Structure of the SiGe-basd microcavity.

The structure is designed so that the resonance modes would be centered at the maximum of the cavity spacers that is why wavelength λ_c is designed to be 685nm. The numbers of pairs LH of DBR2 is also chosen to check the absorption of H layers so C2 would not be excited.

3.2 Simulation Process

The first thing to do in the simulation is the construction of the Si-based microcavity polariton using the structure in Figure 3.1 with corresponding given parameters. After which is the running of the program which will be further discussed in Section 3.3. Then finally, is the gathering of data.

These parameters are:

- Incident angle: This is the angle (θ) between the propagation of incident wave and the normal to the surface of the layer. This ranges from 0 to 90 degrees. Here, we consider that the angle is only 0 degrees which means that the incident wave is at normal incidence.

- Temperature: This considers that the microcavity is at Room temperature (300 K).

- Wavelength range: Range of the wavelength from the initial values to its final values. Also included is the step size.

- Central wavelength: This central wavelength of radiation spectrum. Transmission and reflectivity is centered at this wavelength.

- Refractive index of the ambient medium: This is the first medium before the wave arrives at the surface of the layer. Normally, ambient medium is air.

- Refractive index of the Distributed Bragg reflectors and the spacer or cavity: This is dependent in the x content of a given alloy. Here the refractive indices are dependent on the Nitrogen content of the amorphous Silicon Nitride alloy. As the Nitrogen content increases, the refractive index decreaes.

- Refractive index of the substrate: The substrate can be in the form of a material or medium.

- Thickness of Distributed Bragg reflectors: This is just a quarter of the central wavelength. Also dependent on its refractive index.

- Thickness of spacer or cavity: The thickness can be either same as the central wavelength or half of it. Also dependent on refractive index. The thickness of the spacer we use is half of the wavelength.

- Data plotted: Any combination of reflectivity or transmission.

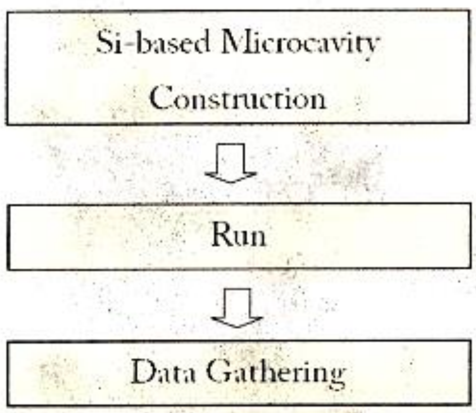

Figure 3.2: Simulation process of the SiGe-based microcavity.

3.3 Run: Algorithm

The algorithm of the program will be discussed in this section. First is the initialization of environment, the Si-based microcavity. Then is the Transfer matrix construction which will return the propagation matrix from one medium to another. Next is the list construction of the length. After which is the calling Transfer matrix functions. Reflectivity and transmittance will be then computed. Finally, the data output or the graphical data output.

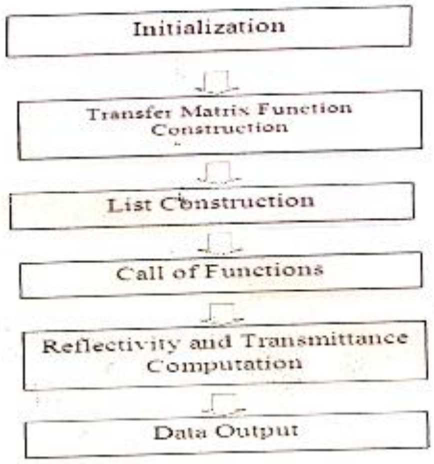

Figure 3.3: Algorithm to be used in the simulation of Silicon-based microcavity.

3.4 Reflectivity Measurement of Multilayered Structures

Figure 3.4 shows the experimental set-up for measuring reflectance of the Multilayered Structures sample at Room Temperature. The sample is attached to a plastic sample holder. Two UV fused silica Plano-convex lenses are used with different focal length, 25mm and 50mm respectively, to focus the light. An input beam is aligned parallel to the optical axis and is focused into a spot on the sample surface with 0 incident angle. The reflected beam is picked up by a 50% beam splitter and sent into HR4000 ocean optics spectrometer which records its $I(\lambda)$. A 50 W halogen lamp is used as the input light, which has relatively flat spectral distribution and supplies sufficient intensity.

3.5 Microcavity polaritons

Same process with the previous method in simulating Silicon-based microcavity will be done on this microcavity the difference is that we consider embedding quantum wells. An example of structure of the microcavity to be used is consist of three sets of four Si quantum wells embedded inside. Only consider that the laser is at normal incidence to the top of microcavity as shown in Figure 3.5. The design could be varied depending on the x component of the SiGe alloy until maximum resonance is achieve.

For the simulation part, the parameters temperature and incident angle are not

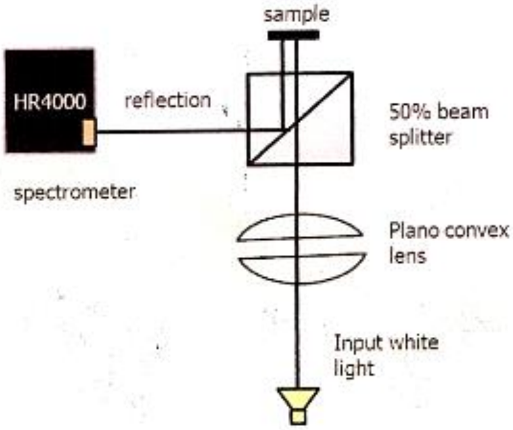

Figure 3.4: Set up for reflection measurement.

change. Note that the refractive index of the $Si_{1-x}Ge_x$ alloy is highly and directly dependent on its Germanium content. So with higher Germanium content, refractive index is high. As Germanium content decreases, the refractive index also decreases.

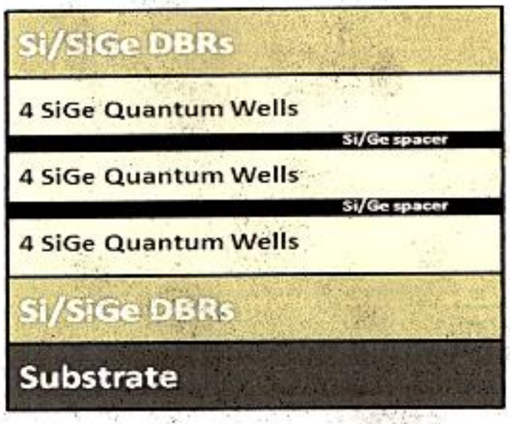

Figure 3.5: Schematic Structure of the SiGe-based microcavity..

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