

The Application and Limitations of PECVD for Silicon-based Photonics

Marc Spooner

A thesis submitted for the Degree of

Doctor of Philosophy



THE AUSTRALIAN NATIONAL UNIVERSITY

November 2005

Declaration

This thesis does not incorporate any material submitted for a degree or diploma at any university and to the best of my knowledge and belief, does not contain any material previously published or written by another person except where due reference is made in the text.

Marc Spooner

Acknowledgements

First of all, I would like to thank my supervisor, Rob Elliman for his help and guidance during the course of this project. This project would not have been completed without his encouragement.

Tessica Dall has helped considerably with experimental design as well as providing feedback on my writing. Nat Smith, Andrew Wilkinson and Taehyun Kim, the fellow Ph.D. students with whom I have worked closely with have been a source of invaluable discussion. For that I thank you.

Tim Walsh, Shannon Orbons and Wilson Pok are the honour students that I have had a pleasure to work with. Tim started the work on the $\text{SiO}_2/\text{Si}_3\text{N}_4$ microcavities, while Shannon has helped with the study concerning the microcavity effects in single layers of SiO_x .

I would also like to thank David Llewellyn for his help with TEM imaging and who, along with Harri Kokkonen has helped prepare the cross sectional SEM samples. I have appreciated the help provided by Damien McGrouther of the University of New South Wales regarding the images obtained with the Focused Ion Beam.

I would also like to thank Katie Pilypas, the love of my life, for her patience and understanding these last few months as well as the time she spent providing feedback on this thesis.

Abstract

This thesis presents results on the applications and limitations of plasma enhanced chemical vapour deposition for silicon-based photonics, with an emphasis on optical microcavities for the control of light emission from silicon nanocrystals.

Silicon nanocrystals were formed by precipitation and growth within Si-rich oxide layers (SiO_x) deposited by plasma enhanced chemical vapour deposition. The films were found to exhibit strong room temperature photoluminescence, with the optimum emission depending on the composition and processing of the films. The strongest emission was achieved for films with a silicon content of ~40%, following hydrogen passivation. Hydrogen was introduced into the samples by two different methods: by annealing in forming gas (95% N_2 : 5% H_2) or by annealing with a hydrogenated silicon nitride capping layer. Both methods caused an increase in photoluminescence intensity due to the passivation of defects. In contrast, the presence of low levels of iron and gold were shown to reduce the concentration of luminescent nanocrystals due to the creation of non-radiative centres.

Optical microcavity structures containing silicon nanocrystals were also fabricated by Plasma enhanced chemical vapour deposition, using silicon dioxide, silicon nitride and silicon-rich oxide layers. The microcavities consisted of a silicon-rich oxide layer between two distributed Bragg reflectors formed of alternating silicon dioxide/nitride layers. The optical emission from these and related structures were examined and compared with that from individual layers in the structure. This revealed a complex interplay between defect and nanocrystal luminescence, hydrogen passivation and materials structure. The resulting

microcavity structures were shown to be suitable for producing a stop-band over the wavelength range of interest for nanocrystal emission, 500-1000nm, and to produce significant intensity enhancement and spectral narrowing. Quality factors of 50-200 were demonstrated.

The application of plasma deposited films was shown to be limited by stress-induced failure that resulted in cracking and delamination of the films during annealing. The SiO_x films thicker than about 600nm failed predominantly by cracking. This was shown to be caused by tensile stress in the film caused by hydrogen desorption during high temperature annealing. The resulting cracks showed preferred alignment depending on the crystallographic orientation of the silicon substrate. For films deposited on (100) silicon, two modes of crack propagation were observed, straight cracks aligned along <100> directions, and wavy cracks aligned along <110> directions. For films deposited on (110) silicon, straight cracks were observed along [1 $\bar{1}$ 0] directions, with a lesser number aligned along [001] directions. Cracks were also observed for films on (111) silicon. These showed 3-fold symmetry consistent with crack propagation along <211> directions due to plastic deformation. Details of these crack geometries and their dependencies are discussed.

Table of contents

Declaration	ii
Acknowledgements	iii
Abstract	iv
Table of contents.....	vi
Chapter 1 Introduction	1
1.1 Motivation	1
1.2 Thesis organisation	2
1.3 Literature review	3
1.3.a Bandgap of bulk silicon	3
1.3.b Porous silicon	4
1.3.c Silicon nanocrystals in SiO ₂	5
1.3.d Passivation of nanocrystals.....	6
1.3.e Microcavities and silicon nanocrystals	7
1.4 Summary.....	8
Chapter 2 Theoretical Considerations.....	9
2.1 Modelling of PL spectra	9
2.1.a The reflectivity of an interface.....	10
2.1.b The reflectivity of a stack of layers	10
2.1.c Electric field distribution	14
2.1.d Extraction efficiency of a microcavity	15
2.1.e Modelling of PL.....	17
2.2 Summary.....	18

Chapter 3 Experimental.....	19
3.1 Sample Preparation.....	19
3.1.a PECVD and RIE	19
3.1.b Annealing	20
3.2 Spectroscopy.....	21
3.2.a PL Spectroscopy	21
3.2.b PL Lifetime.....	23
3.2.c Reflectivity	24
3.2.d Index of Refraction and Thickness Measurements.....	25
3.3 Sample Imaging.....	27
3.3.a Optical Microscopy	27
3.3.b PL Imaging and PL Profiling	27
3.3.c Scanning Electron Microscopy (SEM)	29
3.3.d Focused Ion Beam	29
3.3.e Transmission Electron Microscopy	30
3.4 Ion Beam Equipment.....	31
3.4.a Ion Implantation.....	31
3.4.b Rutherford Backscattering Spectroscopy (RBS)	33
3.4.c Elastic Recoil Detection (ERD).....	34
3.5 Stress measurements.....	34
Chapter 4 Components & their Properties	38
4.1 Thickness & index.....	38
4.1.a M-line	38
4.1.b Film-tek	39
4.2 Composition	41

4.2.a RBS results	41
4.2.b ERD results.....	42
4.3 Structural properties of nanocrystals	45
4.4 Photoluminescence	46
4.4.a Effect of sample composition	46
4.4.b Effect of anneal time.....	47
4.4.c Effect of anneal temperature.....	48
4.4.d Effect of passivation	50
4.4.e Effect of impurities	55
4.5 Summary & Conclusions.....	58
Chapter 5 Microcavities.....	60
5.1 Single layers	60
5.1.a Single layers of PECVD SiO _x	60
5.1.b Ion implanted samples.....	62
5.2 Silicon Dioxide / Silicon Nitride cavities	65
5.2.a PL from cavity	65
5.2.b Angular dependence of emission.....	68
5.2.c Effect of layer thickness	70
5.2.d Effect of number of layers	71
5.3 Effect of annealing microcavities	73
5.3.b Anomalously strong PL.....	76
5.4 Passivation of microcavities	78
5.4.a Hydrogenated silicon nitride passivation.....	78
5.5 SiO ₂ /SiO _x structures	80
5.6 Summary & Conclusions.....	83

Chapter 6 Mechanical Properties	84
6.1 Nature of cracks.....	84
6.1.a SiO _x films on (100) silicon	84
6.1.b SiO _x films on (110) silicon	90
6.1.c SiO _x films on (111) silicon	91
6.2 Cause of cracks.....	92
6.2.a Stress.....	92
6.2.b The Elastic Modulus	95
6.2.c Lomer dislocations.....	96
6.3 Effect of cracks on the microcavities	97
6.4 Delamination	100
6.5 Methods to minimise defects.....	101
6.5.a Thermal treatment.....	101
6.5.b Patterning.....	101
6.5.c Layer order.....	103
6.6 Summary and Conclusions	104
Chapter 7 Conclusions	106
7.1 Future work	108
References	110