

ห้องสมุดงานวิจัย สำนักงานคณะกรรมการวิจัยแห่งชาติ



E46983



PREPARATION OF POLYCRYSTALLINE SILICON
BY ALUMINUM DIFFUSION INTO AMORPHOUS SILICON
AS MONITORED BY SPECTROSCOPIC ELLIPSOMETRY

MISS PUENISARA LIMNONTAKUL

A DISSERTATION SUBMITTED IN PARTIAL FULFILLMENT OF
THE REQUIREMENTS FOR
THE DEGREE OF DOCTOR OF PHILOSOPHY (PHYSICS)
FACULTY OF SCIENCE
KING MONGKUT'S UNIVERSITY OF TECHNOLOGY THONBURI

2010



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A Dissertation Submitted in Partial Fulfillment of the Requirements for
the Degree of Doctor of Philosophy (Physics)

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| Dissertation Title | Preparation of Polycrystalline Silicon by Aluminum Diffusion into Amorphous Silicon as Monitored by Spectroscopic Ellipsometry. |
| Dissertation Credits | 48 |
| Candidate | Miss Puenisara Limnonthakul |
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| Program | Doctor of Philosophy |
| Field of Study | Physics |
| Department | Physics |
| Faculty | Faculty of Science |
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E46983

Abstract

In this research, Al/a-Si film stacks were deposited on single crystal silicon (c-Si) wafers. Aluminum (Al) films with a thickness of 100 nm were firstly deposited by DC unbalanced magnetron sputtering on c-Si wafers. Then, the amorphous silicon (a-Si) films with a thickness of 60 nm were subsequently deposited by pulsed DC unbalanced magnetron sputtering. The deposition time for both films was 20 minutes. During the deposition of Al and a-Si films, the thicknesses of Al and a-Si films were monitored by *in situ* spectroscopic ellipsometry. The diffusion of Al into a-Si film was observed using another *in situ* spectroscopic ellipsometry by post annealing of each Al/a-Si film stack, with nitrogen flow at 1 atm for 30 minutes, from room temperature to 50, 100, 150, 200, 250 and 300°C, respectively. It was found that Al started to diffuse into a-Si film at 200°C. The various annealing times of 10, 20 and 30 minutes at 200°C were further studied using *ex situ* spectroscopic ellipsometry. The results show that a-Si become polycrystalline silicon if the samples were annealed at 200°C and above for longer time than 20 minutes and the SE simulation of Al the diffused into a-Si film was carried out successfully. Moreover, the crystal structure, composition of depth profile and microstructure of the films were characterized by Grazing Incidence X-ray Diffractometer (GIXRD), Auger Electron Spectroscopy (AES) and Transmission Electron Microscopy (TEM), respectively.

In addition, a Al/a-Si film stack with the same coating condition as stated above was also prepared and annealed rapidly at temperature 100°C under vacuum. The *in situ* data at the beginning of Al diffusion can be dynamically modeled and the diffusion coefficient of Al diffused into a-Si film was determined. The dynamic modeling results show that the diffusion of Al occurred at Al/a-Si interface as indicated by the rapid increasing of thickness of the diffused layer. From the SE modeling and non-steady state analysis, the diffusion coefficient of Al into Si was found to be $1.799 \times 10^{-15} \text{ cm}^2/\text{s}$.

Keywords : Spectroscopic Ellipsometry / amorphous silicon/ Aluminum / Diffusion Coefficient

| | |
|----------------------|--|
| หัวข้อวิทยานิพนธ์ | การเตรียมผลึกซิลิกอนแบบหลายโครงสร้าง (Polycrystalline silicon) โดยอาศัยการแพร่ของอะลูมิเนียมเข้าไปในเนื้อฟิล์มซิลิกอน ด้วยการใช้อัลลิโพไซเมตรีทำการตรวจวัด |
| หน่วยกิต | 48 |
| ผู้เขียน | นางสาวกฤษรา ถิ่นนันทกุล |
| อาจารย์ที่ปรึกษา | ศ.ดร.พิเชษฐ ถิ่นสุวรรณ |
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| หลักสูตร | ปรัชญาดุษฎีบัณฑิต |
| สาขาวิชา | ฟิสิกส์ |
| ภาควิชา | ฟิสิกส์ |
| คณะ | วิทยาศาสตร์ |
| พ.ศ. | 2553 |

E46983

บทคัดย่อ

ในงานวิจัยนี้ ได้ทำการเตรียมชั้นฟิล์มบางอะลูมิเนียมและอะมอร์ฟัสซิลิกอนบนแผ่นรองรับซิลิกอนผลึกเดี่ยวโดยชั้นแรกเป็นฟิล์มบางอะลูมิเนียมมีความหนา 100 นาโนเมตรซึ่งถูกเตรียมด้วยวิธีสปัตเตอร์แบบกระแสตรง จากนั้นได้เตรียมฟิล์มบางอะมอร์ฟัสซิลิกอนความหนา 60 นาโนเมตรบนผิวฟิล์มบางอะลูมิเนียมด้วยวิธีสปัตเตอร์แบบกระแสตรงชนิดจ่ายไฟเป็นพัลส์ โดยฟิล์มทั้งสองต่างก็ใช้เวลาในการเคลือบเท่ากับ 20 นาที และในขณะที่ทำการเคลือบ ความหนาของฟิล์มทั้งสองถูกตรวจวัดด้วยวิธีอัลลิโพไซเมตรี จากนั้นได้ทำการศึกษาการแพร่ของอะลูมิเนียมที่แพร่เข้าไปในเนื้อฟิล์มซิลิกอนภายใต้เงื่อนไขบรรยากาศในโตรเจน ด้วยอุณหภูมิการอบฟิล์มที่ อุณหภูมิห้อง 50 100 150 200 250 และ 300 องศาเซลเซียส โดยเวลาที่ใช้ในการอบแต่ละอุณหภูมิเท่ากับ 30 นาทีตามลำดับ จากผลการทดลองพบว่าที่อุณหภูมิ 200 องศาเซลเซียส อะลูมิเนียมเริ่มแพร่เข้าไปในเนื้อฟิล์มซิลิกอนได้ เพื่อศึกษาการเกิดผลึกซิลิกอนแบบหลายโครงสร้างที่อุณหภูมิ 200 องศาเซลเซียสจึงได้แปรค่าเวลาที่ใช้ในการอบฟิล์มเป็น 10 20 และ 30 นาทีตามลำดับและตรวจวัดการเปลี่ยนแปลงด้วยวิธีอัลลิโพไซเมตรี จากผลการศึกษาพบว่าอะมอร์ฟัสซิลิกอนสามารถเกิดผลึกซิลิกอนแบบหลายโครงสร้างได้ที่อุณหภูมิ 200 องศาเซลเซียสหรือมากกว่า โดยอุณหภูมิที่ใช้ออบมีค่ามากกว่า 20 นาที หลังจากนั้นได้ทำการศึกษาลักษณะโครงสร้างของฟิล์ม โปรไฟล์ความเข้มข้นของธาตุอะลูมิเนียมและซิลิกอน โครงสร้างทางจุลภาค ของฟิล์มหลังการอบด้วยเครื่องมือวัดการเลี้ยวเบนรังสีเอกซ์แบบมุมต่ำ (Grazing Incidence X-ray Diffractometer GIXRD), Auger Electron Spectroscopy (AES) และ กล้องจุลทรรศน์อิเล็กตรอนแบบส่องผ่าน (Transmission Electron Microscopy, TEM) ตามลำดับ

นอกจากนั้น ยังได้ทำการเคลือบฟิล์มบางอะลูมิเนียมและอะมอฟสซิลิกอนภายใต้เงื่อนไขเดียวกับข้างต้น เพื่อใช้ในการหาค่าสัมประสิทธิ์การแพร่ของอะลูมิเนียมที่เข้าไปในซิลิกอน โดยฟิล์มที่เตรียมได้ถูกอบที่อุณหภูมิ 100 องศาเซลเซียสภายใต้ระบบสุญญากาศ ขณะที่ทำการอบฟิล์มนั้นได้ใช้อิทธิพลของเครื่องวัดการเปลี่ยนแปลงตลอดเวลา จากผลการวัดพบว่าอะลูมิเนียมแพร่เข้าไปในเนื้อฟิล์มซิลิกอนอย่างรวดเร็ว โดยเริ่มจากบริเวณรอยต่อระหว่างชั้นฟิล์มอะลูมิเนียมและอะมอฟสซิลิกอนสุดท้ายสามารถหาค่าสัมประสิทธิ์การแพร่ของอะลูมิเนียมเข้าไปในเนื้อซิลิกอนก่อนที่อุณหภูมิ 100 องศาเซลเซียสได้เท่ากับ 1.799×10^{-15} ตารางเซนติเมตรต่อวินาที

คำสำคัญ : สเปกโตรสโคปิกอิทธิพล/ อะลูมิเนียม/ อะมอฟสซิลิกอน/ สัมประสิทธิ์การแพร่

ACKNOWLEDGEMENTS

This dissertation arose since I came to Optical Thin Film group of National Electronics and Computer Technology Center (NECTEC). By that time, I have worked with a great number of people whose contribution in assorted ways to the research and the making of the thesis deserved special mention. It is a pleasure to convey my gratitude to them all in my humble acknowledgment.

In the first place I would like to express my sincere gratitude to Prof. Dr. Pichet Limsuwan for his dedicated guidance throughout the course of this work. His expertise and friendly advice were essential to the successful completion of this Ph.D. dissertation at KMUTT.

Special thank is directed to Dr. Pongpan Chindaudom for his supervision, advice, and guidance from the very early stage of this research as well as giving me extraordinary experiences through out the work. Above all and the most needed, he provided me unflinching encouragement and support in various ways. I am indebted to him more than he knows.

Mr. Viyapol Patthanasettakul, I would like to thank him for being the first person who taught me how to work in ultra high vacuum system. I am proud to record that I had several opportunities to work with an exceptionally experienced scientist like him.

To the role model for hard workers in the lab, Dr. Mati Horprathum, I would like to thank him for all of his invaluable assistance, including lunch discussions. He has been a wonderful source for honest, helpful advice. I would also acknowledge Wasuthep Luangtip, Dr. Yongyut Inrisapong and Dr. Artorn Pokaipisit for their advice and their willingness to share their bright thoughts with me, which were very fruitful for shaping up my ideas and research. To my other co-workers in the NECTEC and KMUTT (MEMS and Optical and Laser Lab) who are too numerous to name here, I thank all for your time and input. I am lucky to have the opportunity to meet all of you.

My special thanks go to Dr. Pitak Eiamchai and Mr. Wichai Kongsri, without them; this dissertation would be unintelligible to read at all due to my “poor” English. Thank you so much for carefully revision of this manuscript, helpful advice and fruitful discussions.

I would like to thank the other committee members, Dr. Somyod Denchitcharoen, Dr. Panita Chinvetkitvanich and Dr. Noppadon Nuntawong for the fruitful discussions and through reviews of the dissertation manuscript. In addition, I thanks so much for everybody who was important to the successful realization of this dissertation, as well as expressing my apology that I could not mention personally one by one. Moreover, I would like to thank Srinakharinwirot University which gives the scholarship for me to study the Ph.D. program.

Finally, I cannot successful if I don't have my family. My parents deserve special mention for their inseparable support and prayers. My mother is the one who sincerely raised me with her caring and gently love. My sister and my brother, thanks for being supportive and trust me. Furthermore, I appreciate to my husband whose dedication love and persistent confidence in me all the time.

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NOMENCLATURE

| | |
|----------------------|---|
| AES | Auger electron spectroscopy |
| A | a wave amplitude or area across which diffusion is occurring |
| Al | Aluminum |
| a.u. | an arbitrary unit |
| a-Si | amorphous silicon |
| \vec{B} | magnetic field |
| \tilde{B} | a magnetic flux density, complex |
| BEMA | the Bruggeman effective medium approximation |
| C | concentration |
| $^{\circ}\text{C}$ | degree Celsius |
| CCD | a charged coupled device |
| CVD | chemical vapor deposition |
| c-Si | single crystal silicon |
| CVD | chemical vapor deposition |
| cm^2 | centimeter squared |
| c-Si | crystalline silicon |
| D | diffusion coefficient |
| \vec{D} | electric field displacement vector |
| \tilde{D} | a surface charge density of a capacitor, complex |
| D_p | penetration depth of light |
| DC | direct current |
| d | thickness, film |
| d_f | thickness, film |
| d_{EMA} | thickness, BEMA layer |
| d_p | a penetration depth of light |
| d_{rough} | thickness, surface roughness |
| \vec{E} | electric field |
| \tilde{E} | an electric field, complex |
| $ E_p $ | amplitude of parallel component with the plane of incident |
| $ E_s $ | amplitude of perpendicular component with the plane of incident |
| Eg | a band gap energy |
| EMA | an effective medium approximation |
| En | a photon energy |
| eV | electron volt |
| f | volume fraction |
| \vec{F}_E | electric force |
| \vec{F}_M | magnetic force |
| FESSEM | field-emission scanning electron microscopy |
| FCC | face-centered cubic |
| GenOsc TM | General Oscillator layer, trademarked by J.A. Woollam, USA |
| GIXRD | grazing incident X-ray diffraction |
| \vec{H} | magnetic field intensity |
| HWCVD | hot wire chemical vapor deposition |
| h | the Planck's constant |

| | |
|--------------------|--|
| J_d | flux of material (is the mass of the material flowing per unit time per unit area) |
| J | real current density |
| \bar{k} | propagation vector |
| k | an extinction coefficient |
| kV | kilo volt |
| M | mass of the material |
| MIC | metal induced crystallization |
| MSE | mean-square error |
| MTEC | National Metal and Materials Technology Center, Thailand |
| m_e | an electronic mass |
| mm | millimeter |
| mW | milli watt |
| $\mu\text{c-Si:H}$ | microcrystalline hydrogenated amorphous silicon |
| \tilde{N} | a refractive index, complex |
| N_2 | nitrogen gas |
| NANOTEC | National Nanotechnology Center, Thailand |
| NECTEC | National Electronics and Computer Technology Center, Thailand |
| n | a refractive index |
| nm | nanometer |
| poly-Si | Polycrystalline silicon |
| PECVD | plasma enhanced chemical vapor deposition |
| \tilde{P} | a dielectric polarization, complex |
| P | a dielectric polarization, vector |
| q | an electronic charge |
| R | reflectance |
| RAE | rotating analyzer ellipsometer |
| RCE | rotating compensator ellipsometer |
| RF | radio frequency |
| RMS | root mean square |
| r_p | reflectance for p-polarized light |
| r_s | reflectance for s-polarized light |
| \tilde{r} | the Fresnel reflection coefficients, complex |
| rpm | round per minute |
| SE | spectroscopic ellipsometry |
| SEM | scanning electron microscopy |
| Si | silicon |
| SiO_2 | silicon dioxide |
| Srough | surface roughness |
| s | second |
| sccm | standard cubic centimeters per minute |
| T | transmittance |
| TEM | transmission electron microscopy |
| TMEC | Thai Microelectronics Center, Thailand |
| T_{m_A} | melting temperature of pure A |
| T_{m_B} | melting temperature of pure B |
| T_E | eutectic temperature |
| t | time |

| | |
|---------------------------------|---|
| \tilde{r} | the Fresnel transmission coefficients, complex |
| UV | ultraviolet |
| V | volume |
| VASE | variable-angle spectroscopic ellipsometry |
| Vis | visible |
| VSA | virtual substrate approximation |
| XRD | X-ray diffraction |
| x | the x axis in the Cartesian coordinate |
| y | the y axis in the Cartesian coordinate |
| z | the z axis in the Cartesian coordinate |
| \AA | angstrom |
| Δ | a handedness; a phase difference of p- and s-component of Fresnel reflection coefficients between incident and reflected light relative to a sample |
| γ | a damping coefficient |
| Ψ | an angle of an amplitude ratio of reflected light between p- and s-component of Fresnel reflection coefficients |
| α | an absorption coefficient of a medium |
| δ | a phase difference of a traveling wave |
| ε | a relative permittivity |
| $\tilde{\varepsilon}$ | a dielectric constant, complex |
| ε_0 | permittivity of free space equal $8.8542 \times 10^{-12} (\text{C}^2/\text{N.m}^2)$ |
| ε_1 | a real part of a complex dielectric constant |
| $\langle \varepsilon_1 \rangle$ | a real part of a pseudo-dielectric constant |
| ε_2 | an imaginary part of a complex dielectric constant |
| $\langle \varepsilon_2 \rangle$ | an imaginary part of a pseudo-dielectric constant |
| φ | a traveling wave |
| λ | a wavelength |
| I | intensity of wave |
| I_0 | intensity of the light or intensity of incident light |
| μ | a dipole moment of a pair of electric charges, vector |
| μ_0 | permeability of free space equal $4\pi \times 10^{-7} (\text{N.s}^2/\text{C}^2)$ |
| $ \vec{k} $ | propagation number |
| ν | frequency of light |
| v | a speed of a traveling wave |
| θ | an angle of light and a medium |
| θ_i, θ_0 | incident angle |
| θ_r | reflection angle |
| θ_t | transmission angle |
| σ | standard deviations on the experimental data points |
| $\tilde{\rho}$ | a complex ratio for the fundamental equation of ellipsometry |
| ρ | electric charge density |
| χ^2 | chi-square represent common maximum likelihood estimator |
| ω | an angular frequency |
| ω_0 | a resonant frequency |