UNIVERSITI PUTRA MALAYSIA

COMPUTATIONAL ANALYSIS OF SURFACE PLASMON RESONANCE

ROSMIZA MOKHTAR

FS 2008 38

COMPUTATIONAL ANALYSIS OF SURFACE PLASMON RESONANCE

ROSMIZA MOKHTAR

DOCTOR OF PHILOSOPHY
UNIVERSITI PUTRA MALAYSIA

2008

COMPUTATIONAL ANALYSIS OF SURFACE PLASMON RESONANCE

By

ROSMIZA MOKHTAR

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for the Degree of Doctor of Philosophy

January 2008

TABLE OF CONTENTS

DEDICATION

To my dearest husband, daughter and son,

ABD. HALIM B. BAIJAN
AMEERA FARZANA BT. ABD. HALIM
AMEER FARHAN B. ABD. HALIM

To my father and mother,

MOKHTAR B. YAHYA
RABIAH BT. YA'ACOB

To my sisters and brother,

ROSMAYA BT. MOKHTAR
MOHD. RIDZUAN B. MOKHTAR
ROSLINA BT. MOKHTAR

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirement for the degree of Doctor of Philosophy

COMPUTATIONAL ANALYSIS OF SURFACE PLASMON RESONANCE

By

ROSMIZA MOKHTAR

January 2008

Chairman : **Zainul Abidin Hassan, PhD**

Faculty : **Science**

The Surface Plasmon Resonance (SPR) technique was used as a sensitive optical sensor as well as characterizing materials. To achieve these, two computer programs were developed to carry out an accurate curve fitting of theory to reflectivity data. Two programs were developed preceding from the following requirement that SPR technique can be carried out by using two configurations. The first configuration was the prism coupling, where the program was developed based on the Fresnel's Equations. The second configuration was the grating coupling, where the program was developed based on the coordinate-transformation-based differential method of Chandezon et al. (1980) (the C Method). The fitting process was done by adjusting the relevant parameters (i.e., thickness and dielectric constants) until the lowest sum of square error was obtained. In order to know whether the results from the developed computer program represent the real situation, we have examined our program with the experimental results carried out by other researchers. We have

achieved a satisfactory agreement. Furthermore, surface plasmon resonance simulations on single and multilayer were presented to motivate an effort to understand the shape of the resonances when a surface was exposed to the environment filled with toxic gas. The film growth due to the exposition was studied by understanding the effect of increasing thickness and also the modification of effective permittivity. We also investigated the effect on surface plasmon resonance by varying the grating period and grating profile. We achieved an excellent understanding of the shape of reflectivity curve when the optical constants of layers, the grating period and grating profile, were varied, for both prism coupling and grating coupling, respectively.

In the SPR measurement, the angle of resonance is very sensitive to any surface layer over a metal thin film. The existence of extremely thin surface layer can cause a detectable shift of the SPR curve, which indicates the sensitivity of resonance angle to the changes in the environment of the metal layer. In the present work, SPR technique was used as a tool for the detection of toxic gases, i.e. hydrogen sulfide (H_2S) gas and carbon monoxide (CO) gas. The gold-coated prism was used as a sensor head. The experiments were carried out by measuring the reflected intensity as a function of incident angle. By using the developed programs, the optical permittivity of the material was obtained giving an accurate characterization of the changes brought about by the H_2S and CO gases. This is one of the important characteristics of constructing the optical gas sensor.

We have theoretically modeled a surface plasmon resonance device that is sensitive to both the refractive index and thickness of an adsorbed film. An extensive numerical simulation of the sensor is performed using the scattering matrix approach. The method is capable of monitoring environmental changes in a wide range of applications. With further effort and modification, we believe it is possible to expand the functionality of the surface plasmon resonance sensor to provide powerful tools for the determinations of optical constant of materials and also the determination of grating profiles and grating period. Some of the limitations and breakdowns may also be fixed in the future.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

ANALISIS KOMPUTER BAGI RESONAN PLASMON PERMUKAAN

Oleh

ROSMIZA MOKHTAR

Januari 2008

Pengerusi : **Zainul Abidin Hassan, PhD**

Fakulti : **Sains**

Teknik Resonan Plasmon Permukaan (SPR) telah digunakan sebagai sensor optik yang sensitif dan juga untuk mencirikan bahan-bahan. Untuk mencapai tujuan ini, dua program komputer telah dibangunkan untuk melakukan dengan tepat penyesuaian data-data ujikaji dengan data-data teori. Dua program tersebut dibangunkan berdasarkan kepada keperluan berikut, iaitu teknik SPR boleh dilakukan dengan menggunakan dua konfigurasi. Konfigurasi yang pertama adalah gandingan prisma, di mana program komputer telah dibangunkan berdasarkan persamaan Fresnel. Konfigurasi kedua adalah gandingan parutan, di mana program komputer telah dibangunkan berdasarkan kaedah pembezaan asas-transformasi-koordinat oleh Chandezon dan rakan-rakan (1980) (C Method). Proses penyesuaian data-data ujikaji dengan data-data teori dilakukan dengan cara memasukkan parameter-parameter tertentu (iaitu ketebalan saput tipis dan pemalar-pemalar dielektrik) secara kaedah cuba jaya sehingga ralat jumlah kuasa dua terkecil diperolehi. Untuk mengetahui sama ada hasil yang diperolehi dari program komputer

yang dibangunkan menyamai situasi sebenar, program komputer tersebut telah diuji dengan data-data eksperimen yang telah dilakukan oleh penyelidik-penyelidik lain. Didapati hasil dari program komputer tersebut memberikan persetujuan yang memuaskan. Tambahan lagi, simulasi resonan plasmon permukaan ke atas satu atau berbilang lapisan dilakukan bagi mendorong usaha untuk memahami bentuk resonan apabila sesuatu permukaan didedahkan kepada persekitaran yang dipenuhi dengan gas toksid. Pembetukan saput tipis akibat dari pendedahan tersebut dikaji dengan cara memahami kesan pertambahan ketebalan dan juga pengubahsuaian pemalar dielektrik. Kesan perubahan tempoh parutan dan profil parutan ke atas resonan plasmon permukaan turut dikaji. Pemahaman yang mendalam tentang bentuk lengkungan keterpantulan apabila pemalar-pemalar optik lapisan-lapisan, tempoh parutan dan profile parutan diubah telah dicapai.

Dalam pengukuran SPR, sudut resonan adalah sangat sensitif terhadap mana-mana lapisan permukaan di atas saput tipis logam. Kewujudan lapisan pemukaan yang sangat tipis boleh menyebabkan anjakan lengkungan SPR dikesan, menunjukkan kepekaan sudut resonan terhadap perubahan dalam persekitaran lapisan logam. Dalam kajian ini, teknik SPR digunakan sebagai alat untuk mengesan gas-gas toksid seperti gas hidrogen sulfida (H_2S) dan gas karbon monoksida (CO). Prisma yang disaput dengan logam emas digunakan sebagai alat pengesan. Eksperimen dijalankan dengan mengukur keamatan keterpantulan optik sebagai fungsi kepada sudut tuju. Dengan menggunakan program-program komputer yang dibangunkan, pemalar dielektrik bahan diperolehi, memberikan ketepatan dalam pencirian bahan akibat dari perubahan yang disebabkan oleh gas H_2S dan CO. Ini merupakan satu daripada ciri-ciri penting dalam membina alat pengesan gas secara optik.

Alat pengukuran resonan plasmon permukaan yang peka terhadap kedua-dua indeks biasan dan ketebalan saput tipis bahan telah berjaya dimodelkan secara teori. Simulasi angka secara meluas ke atas alat pengesan dijalankan dengan menggunakan pendekatan ‘scattering matrix’. Kaedah ini berupaya untuk memantau perubahan-perubahan persekitaran dalam julat aplikasi yang besar. Dengan usaha dan pengubahsuaian lanjut, fungsi alat pengesan resonan plasmon permukaan ini boleh dikembangkan lagi untuk menyediakan satu alat bagi menentukan pemalar optik bahan dan juga tempoh dan profil parutan. Sebahagian daripada kelemahan program yang dibangunkan boleh dibaiki pada masa hadapan.

ACKNOWLEDGEMENTS

In the name of Allah, Most Gracious, Most Merciful, Praises and thanks belong only to ALLAH S.W.T. for giving me the strength and patience and enable me to complete this work.

My immense gratitude to Dr. Zainul Abidin Hassan, chairman of my supervisory committee, for his excellent supervision, invaluable suggestions, helpful discussions, beneficial advices, valuable support, endless patience and continuous encouragement throughout this project. Similar appreciation is extended to members of my supervisory committee, Prof. Dr. W. Mahmood Mat Yunus and Associate Prof. Dr. Zainal Abidin Talib for their help in providing equipments for depositing thin layers and measurements and also for their assistance, suggestions and guidance throughout this work.

I would also like to express my thanks to ITMA (Dr. Hishamuddin Zainuddin) for providing Mathematica V5.2 software and Universiti Tenaga Nasional (ITMS) for providing the Visual Basic 6.0 Standard Edition software for the development of computer programs.

Thanks to PASCA for providing the scholarship throughout this work. To Electron Microscopic Unit, Faculty of Veterinar for letting me used the SEM equipment. To Chemistry Department, Faculty of Science, UPM for providing the chemicals resources. To Mechanical Workshop, Physics Department, Faculty of Science, UPM for their helps in experimental set up manufacture. To all my friends in UPM and UNITEN for their endless supports.

My deepest thanks to my mother, my father, my sisters and brother for their supports, care and patience without which this work would never have succeeded. To my dearest husband, daughter and son who have been always beside me, with endless love and support and have made my life enjoyable.

Finally, may Allah rewards the people who helped me directly or indirectly in finishing this work.

I certify that an Examination Committee met on 9th January 2008 to conduct the final examination of Rosmiza Mokhtar on her Doctor of Philosophy thesis entitle "Computational Analysis of Surface Plasmon Resonance" in accordance with Universiti Pertanian Malaysia (Higher Degree) Act 1980 and Universiti Pertanian Malaysia (Higher Degree) Regulations 1981. The Committee recommends that the student be awarded the degree of Doctor of Philosophy.

Members of the Examination Committee were as follows:

Zaidan Abdul Wahab, PhD
Assoc. Professor
Faculty of Science
Universiti Putra Malaysia
(Chairman)

Elias Saion, PhD
Professor
Faculty of Science
Universiti Putra Malaysia
(Internal Examiner)

Maarof Moksin, PhD
Professor
Faculty of Science
Universiti Putra Malaysia
(Internal Examiner)

Ibrahim Talib, PhD
Professor
Faculty of Science and Technology
Universiti Kebangsaan Malaysia
(External Examiner)

HASANAH MOHD. GHAZALI, PhD
Professor and Deputy Dean
School of Graduate Studies
Universiti Putra Malaysia

Date: 28 April 2008

This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philosophy.

The members of the Supervisory Committee were as follows:

Zainul Abidin Hassan, PhD
Lecturer
Faculty of Science
Universiti Putra Malaysia
(Chairman)

W. Mahmood Mat Yunus, PhD
Professor
Faculty of Science
Universiti Putra Malaysia
(Member)

Zainal Abidin Talib, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Member)

AINI IDERIS, PhD
Professor and Dean
School of Graduate Studies
Universiti Putra Malaysia

Date: 8 May 2008

DECLARATION

I declare that the thesis is my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously, and is not concurrently, submitted for any other degree at UPM or at any other institution.

ROSMIZA MOKHTAR

Date: 9 January 2008

LIST OF TABLES

LIST OF FIGURES