OPTICAL AND ELECTRICAL CHARACTERISTICS
OF E-BEAM EVAPORATED ZnS$_x$Se$_{1-x}$ THIN FILMS

By

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A thesis submitted for the degree of Doctor of Philosophy
At the Institute of Postgraduate Studies and Research
University of Malaya
Kuala Lumpur

December, 1997
ACKNOWLEDGEMENT

To the Almighty Allah I give thanks for giving me the help and strength to complete this research. I would also like to express my sincere gratitude to both of my supervisors: Professor Dr. S. Radhakrishna and Professor Dr. Muhamad Rasat Muhamad whose guidance, advice, patience and assistance provided me the impetus to begin and complete this work.

I am indebted to Mrs Vijaya Lakshmi from I. P. S. P., University of Malaya for her great effort in obtaining SEM micrographs and EDX spectra.

My thanks are also due to the staff members in Physics Department, especially in the Solid State Laboratory, for allowing me to use the equipment and facilities during the experimental part of this work.

To my friends and colleagues in I. P. S. P. and in Material Science Laboratory, especially Mr. S. Anandan, I express my deep appreciation for constructive discussion.

I am grateful to Miss Habibah binti Shaari in the office of the Department of Physics, and Miss Zubaidah binti Yusup in the office of I. P. S. P. for their assistance. My special thanks are registered to Miss Teoh Mei Lin for her encouragement and assistance in reading the draft of this thesis.

I would like to acknowledge here that this work has been supported by Physics Department, IRPA 09-02-03-0138. My gratitude and appreciation also go to Public Service Department Malaysia for awarding me a scholarship under the Malaysian Technical Cooperation Programme (MTCP) during the course of this work.

I would like to express my profound gratitude to the Arab Student Aid International for awarding me a scholarship loan during this study.

Finally, this work would not have been possible without the encouragement of my beloved parents, Mohamed and Zarifa, four brothers and five sisters and their families who prayed for my success and gave me every kind of support I need.
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ABSTRACT

Thin films of ZnS$_x$Se$_{1-x}$ ($0 \leq x \leq 1$) were prepared by electron beam (e-beam) evaporation technique. The films were deposited onto glass substrates held at about 60 °C and were fixed horizontally 15 cm above the source material. The vacuum chamber base pressure was about $2 \times 10^{-5}$ torr during the deposition process. The atomic percentage of the film constituents obtained from an energy dispersive x-ray analyzer (EDX) has shown that zinc (Zn) contributes with almost 40% of the atomic percentage to the film composition. Sulphur (S) compositional fraction ($x$) has been estimated from the atomic percentages of sulphur and selenium (Se) in the individual film. The results indicated that films with $x$ between 0.12 and 1.0 have been obtained. Scanning electron micrographs of film morphology have shown that the films exhibit smooth surfaces with relatively large grains embedded in a matrix of finer grains. The analysis of the pronounced diffraction peaks detected by x-ray diffraction (XRD) technique indicates that the films are polycrystalline with cubic structure growing preferentially along <111> axis. The grain diameter has been estimated from the broadening of the diffraction peak and is found to be in the range of 158 - 662 Å. The cubic lattice parameter $a_0$ has been found to vary linearly with $x$ following Vegard's law. However, the difference between $a_0$ values for thin film and single crystal of ZnS$_x$Se$_{1-x}$ materials has been used to estimate the stress experienced inside the films. Most of the films exhibit tensile stress with values in the range of $0.51 - 17 \times 10^9$ dynes/cm$^2$ with exception of six samples which exhibit compressive stress in the range of $-4.6$ to $-0.05 \times 10^9$ dynes/cm$^2$. 
Abstract

A new method has been developed to estimate the thickness and the optical parameters of the films by using the experimental values of the transmission spectrum. The results of this method have been found to be in a good agreement when compared with the values obtained from the well-known envelope method. The empirical relations in the dielectric theory have been used to estimate the characteristic energies such as Penn energy gap, plasma energy, Fermi energy, the average energy of the valence electrons, the energy of the effective dispersion oscillator and the dispersion energy. The absorption edge shows three distinct regions, the high-absorption region ($\alpha > 10^4$ cm$^{-1}$), the exponential part and the weak-absorption tail. Depending on the film composition the direct optical energy gap $E_g$ has been determined to be in the range of 2.58-3.73 eV. The variation of $E_g$ with $x$ has been found to be in a reasonable agreement with the results previously reported by other workers. The effect of the uniaxial stress and the grain size on the energy gap has been studied and the shift produced in $E_g$ from these effects has been estimated.

The electrical dc-conductivity of the films has been investigated. The ohmic behaviour of the current - voltage (I - V) characteristics indicates a good electrical contact between the metal electrodes and the sample. The model proposed by Mott and Davis has been employed in order to explain the variation of conductivity with temperature in the range of 20 - 475 K. The effects of various parameters such as sulphur concentration, film thickness and grain size on the activation energy and the conductivity of ZnS$_x$Se$_{1-x}$ films have been investigated. It was found that, as in the other II - VI compounds the impurities and native defects, which might be unintentionally introduced into the films during their preparation, have a significant contribution to the dc - conductivity.
**ABSTRAK**

Filem-filem nipis ZnS\textsubscript{x}Se\textsubscript{1-x} (0 \leq x \leq 1) telah di sediakan dengan menggunakan penyejatan alur elektron. Filem-filem ini telah dimendapkan ke atas substrat kaca pada suhu 60 \degree C dan diletakkan melintang 15 cm di atas sumber bahan tersebut yang berada pada tekanan 2 \times 10^{-5} torr ketika proses pemendapan. Peratus atom kandungan filem yang diperolehi dari suatu pengalisis sebaran sinar - X (EDX) menunjukkan bahawa zink (Zn) menyumbangkan hampir 40 \% daripada atom kepada komposisi filem. Pecahan komposisi (x) sulfur (S) telah dianggarkan dari peratusan atom sulfur dan seleneum (Se) dalam filem individu dan keputusanya menunjukkan bahawa filem-filem yang diperolehi mempunyai nilai x antara 0.12 dan 1.0. Mikrografis mikroskop imbasan elektron (SEM) yang diambil pada permukaan filem menunjukkan bahawa filem-filem ini mempamirkkan permukaan yang rata dengan hablur bersaiz besar ditabur dalam matrik yang lebih halus. Analisis corak interferens dari kesan belauan sinar - X (XRD) menunjukkan bahawa filem-filem itu adalah polihablur dengan struktur kubus yang tumbuh berorientasikan arah < 111 >. Garis pusat hablur yang diukur dari pelebaran corak interferens dianggarkan diantara 15.8 - 66.2 nm. Pemalar kekisi a\textsubscript{0} didapat berubah secara linear dengan x mengikut Hukum Vegard. Seterusnya, perbezaan antara nilai untuk filem nipis dan hablur tunggal bahan ZnS\textsubscript{x}Se\textsubscript{1-x} digunakan untuk mengukur tegasan yang telah dihasilkan di dalam filem-filem itu. Kebanyakan filem itu menunjukkan bahawa ia mengalami tegasan tensil dengan nilai dalam lingkungan 0.51-17 \times 10^{19}
Abstrak
dynes/cm sementara enam sampel menunjukkan bahawa ia mengalami tegasan mampatan
dalam lingkungan – 4.6 ke – 0.05 × 10^{19} dynes/cm.

Satu kaedah baru telah dicadangkan untuk mengukur ketebalan dan pemalar optik
filem-filem dengan menggunakan nilai spektrum transmisi yang diukur. Keputusan yang
diperolehi dengan cara ini didapati sama tepat dengan yang diperolehi dari kaedah
bungkusuan. Hubungan empirik dalam teori dielektrik telah digunakan untuk mengukur
sifat sifat tenaga valen, cirian jurang tenaga Penn, tenaga plasma, tenaga Fermi, tenaga
purata elektron, tenaga sebaran penggetar berkesan dan tenaga sebaran. Spektrum pekali
serapan $\alpha$ menunjukkan tiga kawasan yang berlainan; kawasan penyerapan tinggi
($\alpha > 10^4$ cm$^{-1}$), bahagian eksponen dan ekor penyerapan lemah. Bergantung kepada
komposisi filem jurang tenaga optik terus $E_g$ didapati berada dalam lingkungan 2.58 -
3.73 eV. Perbezaan $E_g$ dengan $x$ didapati bersetuju dengan keputusan yang diperolehi
terdahulu. Kesan tekanan unipaksi dan saiz hablur kepada jurang tenaga dikaji dan
perubahan yang dihasilkan pada $E_g$ dari kesan-kesan ini telah diukur.

Sifat elektrik filem-filem diselidik melalui pengkonduksian arus terus (dc). Perlakuan ohm pada ciri arus – voltan (I-V) menunjukkan pengkonduksian baik antara
elektod logam dan permukaan sampel tersebut. Model yang dikemukakan oleh Mott dan
Davis telah digunakan untuk menerangkan perbezaan pengkonduksian dengan suhu pada
julat 20 - 475 K. Kesan-kesan struktur filem, seperti kepekatan sulfur, ketebalan filem
dan saiz hablur kepada tenaga pengaktifan dan pengkonduksian ZnS$_x$Se$_{1-x}$ filem
dikajikan. Adalah didapati bahawa seperti dalam semua sebatian II-VI, kecacatan dan
pengdopan yang mungkin diperkenalkan secara tak sengaja ke dalam filem-filem itu
semasa proses pemendapan, boleh mempengaruhi pengkonduksian arus terus.