

Arab American University-Jenin

Faculty of Graduate Studies

Engineering the Optical and Electrical Conduction Parameters of ZnSe Thin Films via YAu Alloy Nanosandwiching

By

Maram Fawzi Husien Taleb

Supervisor

Prof. Dr. Atef Fayez Qasrawi

This thesis was submitted in partial fulfillment of the requirements for

The Master's degree in

Physics

February/2018

© Arab American University – Jenin 2018. All rights reserved.

Engineering the Optical and Electrical Conduction Parameters of ZnSe Thin Films via YAu Alloy Nanosandwiching

By

Maram Fawzi Husien Taleb

This thesis was defended successfully on2018..... and approved by:

Committee members

Signature

1. Prof. Dr. Atef Fayez Qasrawi (Supervisor)	
2. Prof. Dr. Zaki Mohammad Saleh (Internal examiner)	
3. Asso. Prof. Khaled Faisal Ilaiwi (External examiner)	

Declaration

I am Maram Fawzi Husien Taleb declares that I have written this Master thesis and the works presented in it are my own. This thesis has been generated by me as a result of my original research and it hasn't been published before submission.

Signed:

Date:

To My Parents

Acknowledgments

First and foremost, I have to thank my Almighty Allah for giving me the health and opportunity to finish the master study. Thank my God for all courage and the determinations to do this work. I would be honor to dedicate this thesis to my lovely parents, who support me to be where I am standing today. My lovely mother thanks for all love and support step per step in my life and study. I always remember your special words "learn and grow from each setback". Really, the word thanks does not enough to express my super mom. Thank my Dad for all your love and work to give me a happy life, thank you for your trust, effort and proud. I promise you that I will stay like this in your eyes.

A special thanks and heartfelt gratitude to my research supervisor Prof. Dr. Atef Qasrawi. Thanks for your assistance and dedicated involvement in this thesis. I would like to thank you very much for your support and understanding over these past sixth years. I learned from you how to be good person in your life and work hard at yourself to achieve your dreams. Thanks for your trust, support and courage.

Besides my advisor, I would like to thank the rest of my thesis committee: The internal examiner Prof. Dr. Zaki Mohammad Saleh, from the Arab American University-Jenin and the external examiner Asso. Prof. Khaled Faisal Ilaiwi, from An-Najah National University-Nablus. Thanks for their insightful comments and encouragement, also for the questions which helped me to widen my research from various perspectives.

Also, I wish to express my sincere thanks to Dr. Moyad Abu-Saa Dean of the Faculty, for his continue encouragement.

My sincere thanks also go to Assoc. Prof. Dr. Zaki Saleh, Dr. Ahmad Omar, Dr. Adli Saleh, Dr. Mohamad abo Samra, Dr. Sulyman Rabaa, Dr. Moyad Abu-Saa and Mr. Anan Husein, lecturer, in the Department of physics. Thanks for the time that I spent with you, I learn from you a lot. I am extremely thankful to them for sharing expertise, and sincere and valuable guidance and encouragement extended to me.

My aunt Mrs. Alia Assaf, you are my hero in challenging the odds. I learned from you that, you can achieve great successes if you have faith, determination and insistence on your goals. Thanks for your love and supports. Thanks for my uncle Dr. Adwan Taleb for all love, support and encouragement to complete the master degree. My sincere thanks go to my grandmother. My sisters, Maryana, Dayana and Rama and my brothers Jihad and Husien, thanks for your kindness and extensive support, I hope to make you proud of your big sister the same way that I am proud of having you in my life.

	Title)		Page No.
List of Tables				ix
List of Figures				Х
List of Symbols				xiii
Abstract				Xvii
Chapter One	Intro	oduction	and Literature Survey	1
Chapter Two	The	oretical	Background	6
	2.1	The x-	ray Diffraction Technique	6
	2.2	Zinc S	elenide (ZnSe) Crystal Structure	7
	2.3	Crysta	Defect	9
		2.3.1	Point Defect	9
		2.3.2	Linear Defect	10
		2.3.3	Planer defect	10
	2.4	Scherr	er Equation	10
	2.5	The O	ptical Properties of Semiconductors	12
	2.6	Drude	Lorentz Model	14
	2.7	The O	otical and Electrical Conductivity	16
	2.8	AC Co	nduction	16
		2.8.1	The Small Polaron Tunneling (SPT) Model	18
		2.8.2	The Overlapping Large Polaron Tunneling (OLPT) Model	18
		2.8.3	The Quantum Mechanical Tunneling (QMT) Model	19
			2.8.3.1 The AC Conductivity for the Quantum Mechanical Tunneling (QMT) Model	20

List of contents

		2.8.4	The Correlated Barrier Hopping (CBH) Model	23
Chapter Three	Exp	erimenta	ll Details	25
	3.1	Thin F	ilms Preparation	25
	3.2	Thin F	ilms Analysis	28
		3.2.1	The Hot-Probe Technique	28
		3.2.2	The x-ray Diffraction (XRD) Measurements	29
		3.2.3	Optical Measurements	30
		3.2.4	The Current-Temperature Measurement	31
		3.2.5	The Conductance Spectroscopy Measurement	32
Chapter Four	Res	ults and	Discussion	33
	4.1	Structu	ral Analysis	33
	4.2	Optical	l Analysis	39
	4.3	Dielect	ric Analysis	54
	4.4	DC Me	easurements	68
	4.5	The Co	onductance Spectroscopy Analysis	74
Chapter Five	Con	clusions		83
References				85
List of publication				92
Conferences				92
Abstract (in Arabic)				93

List of Tables

No.	Title	Page No.
4.1	The structural parameters of ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.	36
4.2	The optical results for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.	53
4.3	The optical conduction parameters for electron-Plasmon interactions at the ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.	64
4.4	The AC conductivity fitting parameters for the quantum mechanical tunneling (QMT) and the correlated barrier hopping (CBH) conduction mechanism for Yb/ZnSe/Au, Yb/ZnSe/Y/ZnSe/Au, Yb/ZnSe/Au/ZnSe/Au and Yb/ZnSe/YAu/ZnSe/Au sandwiched films at T=300 K.	81

List of Figures

No	Caption	Page No.
2.1	Bragg's Law for x-ray diffraction.	7
2.2	The crystal structure of ZnSe: (a) zinc blend structure and (b) wurtzite structure.	8
3.1	The vacuum evaporation system.	25
3.2	The geometrical design of (a)ZnSe, (b)ZnSe/Y/ZnSe, (c)ZnSe/Au/ZnSe, (d)ZnSe/YAu/ZnSe, (e)Yb/ZnSe/ZnSe, (f)Yb/ZnSe/Y/ZnSe, (g)Yb/ZnSe/Au/ZnSe, and (h)Yb/ZnSe/YAu/ZnSe nanosandwiched films.	26
3.3	The experimental set-up of Hot-Probe technique.	29
3.4	The Rigaku MiniFlex 600 x-ray unit.	30
3.5	The Evolution 300 UV-VIS spectrophotometer unit.	30
3.6	The Current - Temperature characteristic experiment.	31
3.7	The Agilent 4291B 12F Impedance-Material Analyzer.	32
4.1	The x-ray diffraction patterns for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe films.	34
4.2	The transition (T) spectra for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films at wavelength range of 300-1100 nm.	40
4.3	The reflection coefficient (R) spectra for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films at wavelength range of 300-1100 nm.	41
4.4	The absorbance (A) spectra for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films at wavelength range of 300-1100 nm.	43
4.5	The absorbability (R_{λ}) as function of photon energy for ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.	44

- 4.6 45 The absorption coefficient (α) for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films. 4.7 $\ln(\alpha) - E$ dependence for ZnSe, ZnSe/Y/ZnSe, 47 The ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films. 4.8 $(\alpha E)^{1/p}$ versus incident photon energy for ZnSe, 49 The ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films with p values (a) p=2, (b) p=1/2, (c) p=3 and (d) p=3/2. 4.9 The $(\alpha E)^2 - E$ for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and 50 ZnSe/YAu/ZnSe sandwiched films in the high absorption region. The real part ε_r of dielectric constant for ZnSe and 4.10 55 ZnSe/Y/ZnSe sandwiched films in the incident photon frequency range of 270-1000 THz. The real part of dielectric constant ε_r for ZnSe and 4.11 57 ZnSe/Au/ZnSe sandwiched films in the incident photon frequency range of 270-1000 THz. 4.12 The real part of dielectric constant ε_r for ZnSe and 58 ZnSe/YAu/ZnSe sandwiched films in the incident photon frequency range of 270-1000 THz. 4.13 60 The imaginary part ε_{im} of dielectric constant for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films in range of 270-1000 THz. 4.14 63 The imaginary ε_{im} dielectric constant spectra for (a) ZnSe, (b) ZnSe/Y/ZnSe, (c) ZnSe/Au/ZnSe and (d) ZnSe/YAu/ZnSe sandwiched films in range of 270-1000 THz. The black colored lines are the fitting of the Drude-Lorentz equation. 4.15 The optical conductivity $\sigma(\omega)$ as a function of incident photon 67 frequency for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films. 4.16 The current (I)-voltage (V) characteristic curve at 300 K for (a) 68 ZnSe, ZnSe/Y/ZnSe and ZnSe/YAu/ZnSe at voltage rang of -100-100 V, (b) ZnSe/Au/ZnSe at voltage range of -0.5-0.5 V. 4.17 70 The variation of the conductivity with temperature for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched
- xi

films.

4.18	The logarithm of the conductivity with inverse temperature in rang of 300-460 K for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.	71
4.19	The variation of the donor energy level with temperature range of 360-460 K.	73
4.20	The conductance (G) spectra in the frequency range of (0.01 GHz -1.8 GHz) for Yb/ZnSe/Au, Yb/ZnSe/Y/ZnSe/Au, Yb/ZnSe/Au/ZnSe/Au and Yb/ZnSe/YAu/ZnSe/Au sandwiched films.	74
4.21	The $\ln(\sigma_{ac}(\omega)) - \ln(\omega)$ curves for (a) Yb/ZnSe/Au, (b) Yb/ZnSe/Y/ZnSe/Au, (c) Yb/ZnSe/Au/ZnSe/Au and (d) Yb/ZnSe/YAu/ZnSe/Au sandwiched films.	77
4.22	The variation of AC conductivity in frequency range of (0.01 GHz -1.8 GHz) for Yb/ZnSe/Au, Yb/ZnSe/Y/ZnSe/Au, Yb/ZnSe/Au/ZnSe/Au and Yb/ZnSe/YAu/ZnSe/Au sandwiched films. The brown solid lines are the fitting of the conductivity with accordance to quantum mechanical tunneling (QMT) and correlated barrier hopping (CBH) model.	80

List of Symbols

Symbol	Symbol Meaning
λ	Wavelengths
D	Interplanar distance
θ	The Bragg angle
(hkl)	Miller indices
a_{\in}	The lattice constants of the epitaxial layer
a_s	The lattice constants of the substrate layer
D	Crystallite size
K	The shape factor
β	The peak broadenings at full width half maximum peak in
	radians
3	Micro-strains
S	Stress
SF	Stacking faults
δ	Dislocation densities
Ε	Young modulus
γ	Poisson's ratio
Io	Incident light intensity
I _R	Reflected light intensity
I _A	Absorbed light intensity

Is	Scattered light intensity
Q(x)	The photon flux at depth x
α	The absorption coefficient
Eg	The band gap energy
W	The angular frequency
γ	The damping rate
τ	The electron scattering time or relaxation time
ω _e	Reduced resonant frequency
ω _{pe}	The electron bounded plasma frequency
n	The free electron density
<i>m</i> *	The effective mass of electron
$\sigma_{ac}(\omega)$	AC conductivity
S	The frequency exponent ($0 \le s \le 1$)
$n(\tau)$	Relaxation time distribution
$ au_o$	Characteristic relaxation time
v_{ph}	The phonon frequency
ξ	Random variable
W _H	The polaron activation energy
W _p	The total polaron energy
$ au_o$	The characteristic relaxation time
k _B	Boltzmann constant

T	Absolute temperature
r _P	The polaron radius
R	The intersite separation
е	The electron charge
Ep	The effective dielectric constant
$N(E_f)$	The density of state localized near the Fermi level
ł	The localization length,
ℓ^{-1}	The spatial decay parameter
R_{ω}	The hopping distance
$\alpha(au)$	The polarizability
$P(\tau)$	The distribution of the relaxation time
N _P	The number of dipole
$(\Gamma = 1/ au)$	The hopping or tunneling rate
E _F	The Fermi energy level
ε	The effective dielectric constant for the material
ε _o	The effective dielectric constant for the free space
$\sigma_{ac}(L)$	The DC value of the conductivity at low (L) frequency
$\sigma_{ac}(H)$	The DC value of the conductivity at high (H) frequency
R _λ	The absorbability
E _e	Band tail energy (or Urbach energy)
р	A constant related to the optical transition type.

E _{eff}	The effective dielectric constant
$\boldsymbol{\varepsilon}_r$	The real parts of dielectric constant
$\boldsymbol{\varepsilon}_{im}$	The imaginary parts of dielectric constant
μ	Drift mobility
N _D	Donor concentration
Ea	The thermal activation energy
E _d	Donor energy level
<i>qx</i>	The electron affinity
G	The conductance

Engineering the Optical and Electrical Conduction Parameters of ZnSe Thin Films via YAu Alloy Nanosandwiching

By

Maram Fawzi Husien Taleb

Supervisor

Prof. Dr. Atef Fayez Qasrawi

Abstract

One of the most important challenges that make the visible light communication technology hardly possible is the absence of light converters that perform without altering the properties of the incident light signal. For that reason here in this thesis, we implant an alternating approach for engineering the optical and electrical parameters of ZnSe thin films by the nanosandwiching technique. The work is promising as it indicates the ability of using the nanosandwiched ZnSe in visible light communication and as a microwave resonator. Particularly, two thin layers of yttrium and gold metals are co-evaporated onto a ZnSe thin film. The ZnSe/Y, ZnSe/Au and ZnSe/YAu films are recoated with another ZnSe film to form the nanosandwiched proposed structure. The basic properties of the sandwiched ZnSe are investigated by means of x-ray diffraction, optical spectroscopy and conductance spectroscopy in the measurement domains of 10-70°, 270-1000 THz and 0.01-1.8 GHz, respectively. The effect of the Y, Au and YAu on lattice constant, energy band gap, dielectric constant and optical and electrical the conductivities are explored. In addition, the transient optical and electrical conductivities are modeled by the existing models and theories which concern Drude-Lorentz plasmonic interaction in the terahertz range, the quantum mechanical tunneling and correlated hoping conduction of charge carriers in the frequency range 0.01-1.8 GHz to observe the variations associated with the metal sandwiching process in the optical and electrical conduction parameters like, the density of localized states near the Fermi level, scattering time constant at femtosecond levels and then electron-plasmon interactions. Particularly, an abrupt increase in the free carrier density is observed upon insertion of YAu layers. The increase in the free carrier density is associated which enhancement in the Plasmon frequency which reached \sim 4.83 GHz.

Keywords: ZnSe, nanosandwiching, alloy, YAu, x-ray diffraction, plasmon, Fermi level.

Chapter One

Introduction and Literature Survey

Thin films of zinc selenide (ZnSe) have many applications on various opto-electronic devices, hetro-junction, solar cells, thin film transistors and photochemical cells [1, 2]. It is a well known II-VI semiconductor with a direct band gap 2.7 eV, which is important for a short wavelength optoelectronic device [3]. Due to its wide range of applications in optoelectronics, the ZnSe has captured the interest of scientific society since decades. Various attempts have been carried out to improve its electrical and optical performances to make it more appropriate for technology and use doping as a preferred technique. However, each doping process has its own negatives in addition to the positive improvements [3, 4].

In this thesis, we propose the idea of nanosandwiching of a two metal alloy between two layers of ZnSe. The suggested metals are yttrium and gold. These two metals have high orbital configurations that may reach the high energy band states of ZnSe. Thus, it is expected to attenuate the conduction parameters of the ZnSe. Particularly, a ZnSe thin film layers is used as substrate to deposit a layer of Y metal 70 nm in thickness and the resulting ZnSe/Y is used to deposit 70 nm thick gold so that the ZnSe/YAu is formed, before another ZnSe film is evaporated onto the Au layer. This new approach is expected to engineer the optical and electrical conduction parameters in ZnSe.

Tan Yu and Wang Yan-Guo [4] studied the linear characteristic in the I—V relationship of ZnSe and found that it asserts elimination of the Schottky barrier and formation of ohmic contacts. Particularly, ZnSe is advantageous for terahertz applications seeking ultrafast photoconductivity with high dielectric breakdown strengths and ultrafast charge-carrier lifetimes [5].

X-ray diffraction (XRD), Transmission electron microscope (TEM) and High resolution transmission microscope (HRTEM) imaging techniques used to find the structural characterizations of ZnSe. It has a sphalerite cubic unit cell with lattice constants equals (a=5.618 Å) or a wurtzite structure has a hexagonal unit cell with lattice parameters (a=3.974 Å, c = 6.506 Å, u = 0.375). The energy band gap of ZnSe has wide range from 2.4 to 2.9 eV [6-8].

Pradip Kr Kalita et al. [1] studied the characteristics of ZnSe thin films, which revealed a polycrystal having a FCC Zincblende structure. They studied the effect of the substrate temperatures ranging from 303–623 K on the structure of ZnSe film and calculated the values of lattice constant (a), grain size (D), stress (S), micro-strain (ϵ) and dislocation density (δ), which are found to be in the range 5.6764 Å to 5.7074 Å, 17 nm to 20 nm, -1.25 ×10⁹ to -8.45 ×10⁹ dy/cm², 1.78 ×10⁻³ to 2.16 ×10⁻³, 2.31 ×10¹¹ to 3.39 ×10¹¹ line/cm², respectively.

Shaaban et al. [2, 9] studied the x-ray and optical properties of the ZnSe/flexible substrate thin films, and found that it has a cubic structure with a (111) orientation and lattice constant a = 5.667 Å. The crystallite size was found to increase with increasing film thickness, while the lattice strain was decreasing with increasing film thickness. On the other hand, optical parameters such as the refractive index (n) and the extinction coefficient (k) were calculated from the transmittance and reflectance through a wavelength between 400 nm to 2500 nm. They found that the refractive index (n) decreases with increasing film thickness.

extinction coefficient (k) decreases with increasing wavelength. The calculated direct energy gap was found to increase from 2.55 eV to 2.70 eV as the film thickness increases. That study concludes that the ZnSe/flexible substrates are good candidates for optoelectronic devices.

Min Ji Kim et al. [10] prepared ZnSe, Yb and Er-doped ZnSe by a hydrothermal method with and without hydrazine, and studied its morphology and photocatalytic activities. They found that ZnSe has a band gap ~ 2.6 eV and revealed cubic and hexagonal structure when prepared without hydrazine, while it revealed only cubic structure when the hydrazine is used. Moreover, at low Er-doping concentration a rod morphology shown, and at low Yb-doping concentration plate morphology appeared, but if it reaches a high doping concentration the morphology returns like undoped ZnSe.

ZnSe nano-crystals were synthesized using microwave irradiation method by M. Molaei et al [11]. In their work the x-ray characteristics and optical properties of ZnSe were studied. Also, the effect of Cu-doped ZnSe on the optical properties had been studied. The x-ray for ZnSe nanocrystals shows cubic zincblende ZnSe with peaks at $2\theta = 27.7^{\circ}$, 45.9° , and 54.4° , which corresponds to the (111), (220), and (311) reflection planes. The crystallite was found to be about 2.5 nm, and the bandgap was found to be about 3.15 eV. The photo-luminescence spectra of ZnSe nanocrystals have shown two peaks at 415 nm and 500 nm which relates to band edge and trap state respectively. For Cu-doped ZnSe these authors find that the increasing of Cu doping ions had an influence on the emission properties of ZnSe nanocrystal where the bandgap emission at 415 nm starts to decrease until disappeared completely at 1% ratio of Cu.

The mixture of two or more chemical elements, at least one of them is a metal are called alloys. These elements in the alloy behave in two ways, it can be uniformly distributed over the crystal lattice to form a solid solution or form different phases shown as particles in a matrix [12]. Steel and Treherne [13, 14] studied the Optical properties and electronic structure of AuMn and AgMn alloy systems with over the energy range of 0.8 eV to 4 eV. They found that increasing Mn concentration increases the classical collision frequency of the intraband absorption and the direct interband transitions had shifted to higher energies. Comparing the alloys and pure metals, they found an extra absorption band in the alloys.

The surface plasmons coupling in transition metallic alloys were studied by Abdelhak Dhibi et al. [15]. They studied Ag, Cu, Au and Al elements with different amount and found the surface plasmon resonance (SPR). They considered that a small effect on SPR appeared for alloys of two metals, and also no sufficient effect in the SRR curves appeared when a 25% of Al added to two metals alloy. They found that the SRR is highly dependent on grating parameters which discussed by rigorous coupled-wave analysis method.

Chapter two of this thesis will take attention on some theoretical subjects that are required for explanation and clarification the experimental results. The following chapter (chapter three) includes brief description about the experimental procedures that used to prepare the sample and take the measurement data. In addition, it explained some of the measurement devices that used.

In chapter four, the effect of this thin alloy which does not block the optical transmissions on the structural, optical and electrical performance are investigated in details. In addition, a theoretical modeling that fit well with the experimental data is used to verify

4

the correctness of the approach and investigate the physical phenomena laying beyond the behavior of the alloyed films. The conclusions of these results are shown in chapter five.

Chapter Two

Theoretical Background

2.1: The X-ray Diffraction Technique

The x-ray diffraction technique (XRD) is an important and useful method used to observe and characterize the crystal structure [16]. The x-rays are electromagnetic waves with a wavelength λ in range from 0.1 to 100 Å, produced when a filament in vacuum is heated until an electron is released, then accelerated by a high voltage (voltage source) until colliding with a metal anode usually Copper. This produces two types of x-ray radiation, broad continuous 'Bremsstrahlung' spectrum and narrow characteristic spectrum [17].

The atoms in a crystalline material are arranged in periodic 3-dimensional arrays to form a unit cell, which can be one of 14 groups known as bravais lattices and its dimensions are called lattice parameters. The crystalline materials structure can also describe a family of planes. Parallel planes have the same x-ray scattering effect. The lattice parameters can be determined by the reflection plane of x-ray patterns and Bragg's law [18, 19].

When two collimated monochromatic x-ray beams with a wavelength λ and incident angle θ (displayed in Fig. 2.1) interact with two parallel lattice planes separated by interplanar distance d, the constructive interference occurs if the path difference between the two beams is an integer number n of wavelengths λ . This is an important condition called Bragg's law defined by the following equation [16, 18]:

$$n\lambda = 2 d \sin(\theta) \tag{2.1}$$



Fig. 2.1: Bragg's Law for x-ray diffraction.

2.2: Zinc Selenide (ZnSe) Crystal Structure

Two crystal structures dominate in the ZnSe, the zincblende and wurtzite structures. Both structures are tetrahedrally bonded [20]. They have similar closest neighbor connections but the distances and the angles to further more neighbors quietly differ. In the unit cell, zincblende structure has four asymmetric unit (ABCABC) while the wurtzite structure has two asymmetric unit (ABAB), as shown in Fig. 2.2. The cubic zincblende (FCC) structure for ZnSe has a space group (F_4 3m). On the other hand, the wurtzite ZnSe has a hexagonal form with a space group ($P6_3$ mc) [21, 22].

For zincblende ZnSe, each Zn or Se atom is tetrahedrally surrounded by four atoms of Se or Zn, respectively. The unit cell includes four ZnSe with four Zn in (000), $(0\frac{1}{2}\frac{1}{2})$, $(\frac{1}{2}0\frac{1}{2})$, $(\frac{1}{2}\frac{1}{2}0)$ positions and four Se in $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$, $(\frac{3}{4}\frac{1}{4}\frac{1}{4})$, $(\frac{3}{4}\frac{1}{4}\frac{1}{4}\frac{1}{4})$, $(\frac{3}{4}\frac{1}{4}\frac{1}{4}\frac{1}{4})$, $(\frac{3}{4}\frac{1}{4}\frac{1}{4}\frac{1}{4})$, $(\frac{3}{4}\frac{1}{4}$



Fig. 2.2: The crystal structures for ZnSe: (a) Zinc Blend structure and (b) wurtzite structure.

The lattice parameters for a zincblende and hexagonal structures are calculated using the formulas 2.2 (a) and 2.2 (b), respectively [23]:

$$\frac{1}{d_{hkl}^2} = \left(\frac{h^2 + hk + k^2}{a^2}\right)$$
(2.2 (a))

$$\frac{1}{d_{hkl}^2} = \frac{4}{3} \left(\frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2}$$
(2.2 (b))

where, d is the interplanar distance, (hkl) are Miller indices of the reflection plane, a and c are the lattice parameters.

The physical mismatch causes dislocation at the surface and result in electronic defects; it was directly related to the maximum allowed epitaxial layer. The lattice mismatch is defined by the following equation:

$$\Delta\% = \frac{(a_{\epsilon} - a_s)}{a_{\epsilon}} \times 100\% \tag{2.3}$$

where a_{ϵ} is the lattice constants of the epitaxial layer and a_s is the lattice constants of the substrate layer [24].

2.3: Crystal Defect

Crystal defect is an imperfection in the regular geometrical arrangement of the atoms in the crystalline solid. This imperfection happens due to the deformation in the solid. Real crystal contains large number of defect ranging from variable amount of impurities to missing or misplaced atoms or ions. So the materials have different types of defects are [25, 26]:

2.3.1: Point Defect

This type of defect disturbs the crystal pattern at an isolated site. It includes intrinsic defects appear in a pure material, and extrinsic defects due to solute or impurity atoms. The intrinsic defects formed when an atom is missing creating a vacancy called schottky defect. In addition, it formed when an atom occupies an interstitial site called Frankel defect [25, 26].

The extrinsic defects are foreign atoms. It is called solutes when they are intentionally added to the material and called impurities if they are not added. The foreign atoms can be classified as interstitial or substitutional. While the interstitial usually occurs when a smaller atom (which 45% smaller than the host) fit into the octahedral or tetrahedral

holes in the metal lattice. The substitutional occurs for a different atom with about the same size that replaces one of the atoms in the host lattice [25, 26].

2.3.2: Linear Defect

It is a group of atoms in the irregular position. Linear defects called dislocations. Three types of dislocations are edg dislocation, screw dislocation and a mixed dislocation that combined the first two types [25, 26].

2.3.3: Planer Defect

This defect is a interface between homogeneous regions at the material. It includes grain boundaries, stacking fault and external surface [25, 26].

2.4: Scherrer Equation

Scherrer equation is one of many methods used to determine the crystallite size (D). It is valid for crystalline grains with size up to 200 nm [27]. Scherrer equation is important to provide a lower bound on the particle size. This can be contributed to the width of a diffraction peak in addition to instrumental effects and crystallite size [28]. In 1918, Scherrer suggested a formula that connected between the crystallite size (D) and the width of the x-ray diffraction peak. The scherrer equation is given as:

$$D = \frac{K\lambda}{\beta \cos \theta}$$
(2.4)

where, the constant *K* is the shape factor which relates to crystallite shape and normally taken 0.94, $\lambda = 0.15418$ nm is the Cu-k α x-ray wavelength, β is the peak broadenings at full width half maximum peak in radians, and θ is the Bragg angle [29, 30].

The simplest way to derive the Scherrer equation is the differentiation of Bragg's law, starting with multiplying both side of equation (2.1) by an integer m, and let n=1, then the equation becomes:

$$m\lambda = 2 m d \sin(\theta) \tag{2.5}$$

Since the interplanar distance d multiplied by integer m equals the thickness of crystal (t), then the equation (2.5) simplifies as:

$$m\lambda = 2 t \sin(\theta) \tag{2.6}$$

This equation can also be interpreted as the mth order reflection from a set of planes with an interplanar distance (t). By differentiating both sides of equation (2.6) with respect to θ and noticing that m λ is constant, this yields to:

$$0 = 2\Delta t \sin(\theta) + 2t\cos\theta \,\Delta\theta \tag{2.7}$$

$$t = \frac{\Delta t \sin(\theta)}{\cos(\theta) \ \Delta \theta}$$
(2.8)

Since the small increment in the thickness is d ($\Delta t = d$), d sin (θ) = $\lambda/2$ from equation (2.1), and $\Delta \theta$ can be positive or negative, so the absolute value must be taken. $\Delta \theta$ is the half width of the peak and ($2\Delta \theta = \beta$) is the full width at half maximum peak. Substituting these factors in equation (2.8) gives:

$$t = \frac{d \sin(\theta)}{\cos(\theta) \ \Delta\theta} = \frac{\lambda}{2\cos(\theta) \ \Delta\theta}$$
(2.9)

$$t = D = \frac{\lambda}{\cos(\theta) \ \beta} \tag{2.10}$$

If the Gaussian function is used to describe the peak, a shape factor K = 0.94 is applied. Then Scherrer equation will be given as [30-32]:

$$D = \frac{0.94\,\lambda}{\cos\left(\theta\right)\,\beta} \tag{2.11}$$

In addition, the micro-strains (ϵ), stress (S), stacking faults (SF) and dislocation densities (δ) defined by the following relations:

$$micro - strain \ (\varepsilon) = \frac{\beta}{4 \tan \theta}$$
(2.12)

Stress
$$(S) = \frac{E}{2\gamma} \left(\frac{a_{bulk} - a_{film}}{a_{bulk}} \right)$$
 (2.13)

Where, $a_{bulk} = 3.98$ Å, $c_{bulk} = 6.53$ Å are the parameter of a ZnSe hexagonal crystal, a_{film} , c_{film} are the parameter for prepared film, and $(E = 6.49 \times 10^{10} pa)$, $(\gamma = 0.28)$ are the young modulus and poisson's ratio for ZnSe, respectively [1, 33, 34]. The stacking faults (SF) can be calculated by the relation [35]:

$$(SF) = \frac{2 \pi^2 \beta}{45 \sqrt{3} \tan(\theta)}$$
 (2.14)

A dislocation is a linear crystalline defect per unit volume. The presence of dislocations has an important effect on the properties of materials. Moreover, the dislocation density (δ) is calculated from the values of micro-strains and grain sizes as following [1]:

$$\delta = \frac{15 \varepsilon}{a D} \tag{2.15}$$

Where, ε is the micro-strain, *D* is the crystalline size and a is the lattice constant for films.

2.5: The Optical Properties of Semiconductors

Semiconductor materials are very important due to many quantum optical effects. The semiconductors electronic states are restricted into energy bands instead of discrete levels. Therefore, the optical properties can be estimated through the interband transition between the valence and conduction energy bands [36].

When a beam of incident light intensity I_o interacts with a material sample of thickness d, part of the beam is reflected I_R another is transmitted I_T and the remaining is either absorbed I_A or scattered I_s . These intensities can be written as the following relation [37]:

$$I_o = I_A + I_R + I_T + I_s (2.16)$$

By substituting the coefficients for absorbance $(A = I_A/I_o)$, reflectance $(R = I_R/I_o)$, transmittance $(T = I_T/I_o)$ and scattering $(S = I_S/I_o)$, the equation (2.16) rewritten as [37]:

$$A + R + T + S = 1 \tag{2.17}$$

Assuming that the scattering part is very small, the remaining part of the light is just absorbed. In this case, the equation (2.17) re-writes as:

$$A + R + T = 1 (2.18)$$

The absorption of light is related to the creation of free carrier. The photon flux decreases in the semiconductor in accordance to the Lambert-Bouguer exponential relation [38]:

$$Q(x) = Q_0 e^{-\alpha x} = Q(1 - R)e^{-\alpha x}$$
(2.19)

Where, Q(x) is the photon flux at depth x (or thickness d) under the sample surface and α is the absorption coefficient [38]. In the absorption process, an electron in the valance band absorbs photon energy and is excited to the conduction band leaving a hole in the valance band which created an electron-hole pair [36]. The minimum value of energy required to generate an electron-hole pair called the band gap energy E_g [34]. The absorption coefficient α is employed to determine the energy gap E_g of the semiconductor using Tauc's relation:

$$\left(\alpha E\right)^{1/p} = A\left(E - E_g\right) \tag{2.20}$$

where α is the absorption coefficient, E = hv is the photon energy, A is a constant determined by transition probability and related to the material properties, Eg is the energy band gap between valance and conduction band, and p is a constant related to the optical transition type. The values of p are 3/2, 3, 1/2 or 2 for forbidding direct, forbidding indirect, allowed direct and allowed indirect optical transition, respectively. From the plot of $(\alpha E)^{1/p}$ versus photon energy, the value of the energy band gap can be estimated by the intercept with E-axis for the best linear curve of $(\alpha E)^{2/3}$, $(\alpha E)^{1/3}$, $(\alpha E)^{2}$ and $(\alpha E)^{1/2}$, which include the widest amount of data [39, 40].

2.6: Drude-Lorentz Model

The Drude free electron model was suggested in 1900 by Pual Drude to describe the transport properties of electrons in metals. Drude model is a classical treatment of the optical properties where it considers the atom's valence electrons as free electrons. This model was also accepted for semiconductors when the free carrier density due to doping sufficiently high, so the semiconductor behaves in the same way as simple metal [41,

42]. The Drude model has limitations such as; it is not valid for spatial dispersion when the dielectric constant depends on the wave vector. It also is not valid for bound holes and electrons in semiconductors [42].

On the other hand, the Lorentz model used to explain the frequency response of many materials with a strong dispersion around the resonant frequency. It is suitable for materials with bound electrons and many oscillators system [42]. The Drude model was modified by lorentz model to be Drude-Lorentz modified model for dielectric function of semiconductors. It is able to explain both bound and free electrons. The modified model connects between the coupled oscillations present in the dielectric spectra and the oscillation of the free charge carriers for positive ions (Plasmon) [42-44].

The dielectric solid atoms or molecules can be treated as numbers of oscillators. When the electric field interacts with the dielectric material, this creates the dipole oscillation. The electrons which bounded to positive nucleuses vibrate around the equilibrium position at resonant frequency accordance to Drude-Lorentz model. The metallic doping in semiconductors provides more free electrons, so this model treats with the metallic free electron vibrations [45].

The Drude-Lorentz model is used to explain the dielectric function through the dispersion relation [46]:

$$\varepsilon(\omega) = 1 - \sum_{i}^{K} \frac{\omega_{pe_{i}}^{2}}{(\omega^{2} + i\omega\gamma_{i})} + \sum_{i}^{K} \frac{\omega_{pe_{i}}^{2}}{(\omega_{e_{i}}^{2} - \omega^{2}) + i\omega\gamma_{i}}$$
(2.21)

Where, *K* is the number of peaks appeared in the dielectric spectrum and the subscript *i* refers to the relevant peak, *w* is the angular frequency, $\gamma = 1/\tau$ is the damping rate where τ is the electron scattering time, ω_e reduced resonant frequency and $\omega_{pe} =$

 $\sqrt{4\pi ne^2/m^*}$ is the electron bounded plasma frequency where *n* is the free electron density and m^* is the effective mass of electron.

2.7: The Optical and Electrical Conductivity

Optical conductivity is a material property connects between the current density and the electric field for general frequencies. It is closely related to the dielectric function and usually obtained through the optical transmission experiments, so it measured in the optical frequency ranges via the reflectivity of the sample under normal incident. On the other hand, the optical conductivity and the dielectric function indicate a response of a system of electrons to an applied electric field. However, the electrical conductivity is the reciprocal of electrical resistivity and measures the ability of the materials to conduct an electrical current. It is an electrical phenomenon where a material contains movable particles with electric charge which carry the electricity [47, 48].

2.8: AC Conduction

In general, for all amorphous semiconductors, the AC conductivity $\sigma_{ac}(\omega)$ obeys the universal Jonscher's power law. Where, the AC conductivity has a frequency and temperature dependences as expressed in the following equation [49, 50]:

$$\sigma_{ac}(\omega, T) = A(T) \,\omega^{s(T)} \tag{2.22}$$

Here, $\omega = 2\pi f$ is the angular frequency of the applied AC field, *A* and the frequency exponent *s* ($0 \le s \le 1$) are temperature-dependent parameters. The constant *A* determines the strength of polarization and *s* is the Jonscher's coefficient representing the amount of interaction between the mobile ions and the lattice around them [49].

The nearly linear frequency dependence of the AC conductivity occurs when the relaxation time distribution $n(\tau)$ is $1/\tau$. Where the relaxation time τ is:

$$\tau = \tau_o \exp(\xi) \tag{2.23}$$

and $\tau_o = v_{ph}^{-1}$ is the characteristic relaxation time which equals the inverse of the phonon frequency, and ξ is the random variable [50].

The slope for the experimental data of $\ln \sigma_{ac}(\omega) - \ln \omega$ curves yields the value of Jonscher's coefficient *s*. As the temperature increase the Jonscher's coefficient *s* value increased, and this value is only due to material properties [49]. In order to explain the behavior of the AC electrical conductivity, many models have been proposed for amorphous semiconductors. It is assumed that the dielectric loss occurs due to the carrier motion localized within pairs of sites [51]. These models are; small polaron tunneling (SPT) model, overlapping large-polaron tunneling (OLPT) model, quantum mechanical tunneling (QMT) model and correlated barrier hopping (CBH) model [49, 50].

The applicability of these models depends on the variation of Jonscher's coefficient value s with temperature. If the main value of s increase with increasing temperature, the small polaron tunneling (SPT) model is the possible mechanism. However, the s value may decrease with increasing temperature down to a minimum value at certain temperature followed by an increase in s value. In this case, the conduction is due to overlapping large-polaron tunneling (OLPT) model. While the value of s in the quantum mechanical tunneling (QMT) model is slightly increasing with increasing temperature. QMT model occurs through tunneling between two localized states near the Fermi level. On the other hand, the correlated barrier hopping (CBH) model is

usually associated with a decrease in the value of s with temperature [49, 52-55]. In (CBH) model, the charge carrier hops from site to site over the potential barrier. It assumes that conduction happens through a bipolaron process, where two polarons hop simultaneously over the potential barrier and the barrier height is correlated with the inter-site separated via coulombic interaction [49].

2.8.1: The Small Polaron Tunneling (SPT) Model

A small polaron may be created in the covalent solid when an addition charge carrier causes a large degree of local lattice distortion. The small polaron assumed that their distortion clouds don't overlap [52]. The transport of an electron having a random distribution between degenerate's sites will include activation energy:

$$W_H = \frac{1}{2} W_P$$
 (2.24)

Where, W_H is the polaron activation energy and W_p is the total polaron energy [51].

The frequency exponent s for the (SPT) model is temperature dependent and can be expressed as follows relation:

$$s = 1 - \frac{4}{\ln(1/\omega\tau_o) - W_H/k_B T}$$
(2.25)

In this equation, ω is the angular frequency, τ_o is the characteristic relaxation time, W_H is the polaron activation energy, k_B is Boltzmann constant and T is the absolute temperature [51, 52].

2.8.2: The Overlapping Large Polaron Tunneling (OLPT) Model

If the polaron tunneling model with large polaron wells of two sites overlap, the hopping energy reduced to:
$$W_H = W_{Ho}(1 - r_P/R)$$
(2.26)

Where, r_p is the polaron radius, R is the intersite separation, and $W_{Ho} = e^2/(4\varepsilon_p r_p)$ is constant for all sites (where, e is the electron charge and ε_p is the effective dielectric constant) [51].

The AC conductivity for the overlapping large polaron tunneling (OLPT) model is:

$$\sigma_{ac}(\omega) = \frac{\pi^4}{12} e^2 (k_B T)^2 \left(N(E_f) \right)^2 \frac{\omega R_{\omega}^4}{2\ell k_B T + W_{Ho} r_P / R_{\omega}^2}$$
(2.27)

Here, $N(E_f)$ is the density of state localized near the Fermi level, ℓ is the localization length, ℓ^{-1} is the spatial decay parameter, and R_{ω} is the hopping distance at frequency ω given by this quadratic equation [51]:

$$R_{\omega}^{2} + [\beta W_{Ho} + \ln(\omega\tau_{0})]R_{\omega}^{2} - \beta W_{Ho}r_{P} = 0$$
(2.28)

Where,
$$R_{\omega}^{2} = 2\alpha R_{\omega}$$
, $r_{P} = 2\ell r_{P}$ and $\beta = 1/(k_{B}T)$.

The frequency exponent s in this model is temperature and frequency dependent and can be found by the following equation [51]:

$$s = 1 - \frac{8\ell R_{\omega} + 6W_{Ho}r_P/R_{\omega}k_BT}{(2\ell R_{\omega} + W_H r_P/R_{\omega}k_BT)^2}$$
(2.29)

2.8.3: The Quantum Mechanical Tunneling (QMT) Model

The relaxation time expressed in equation (2.27) can be rewritten for the quantum mechanical tunneling (QMT) model by substituting the random variable $\xi = 2\alpha R$ (where α is the decay parameter) [51].

The AC conductivity for this model found to be [51, 52]:

$$\sigma_{ac}(\omega) = C e^2 k_B T \ell^{-1} \left(N(E_f) \right)^2 \omega R_{\omega}^4$$
(2.30)

Where C is a numerical constant may be equals $\frac{\pi^4}{24}$, $N(E_f)$ density of localized state at Fermi level which is the number of actually contributing to the ac-loss, v_{ph} is the phonon frequency, and ℓ^{-1} is the exponential decay parameter. The tunneling distance R_{ω} is given as:

$$R_{\omega} = \frac{1}{2\ell} \ln(1/\omega\tau_o) \tag{2.31}$$

On the other hand, the frequency exponent s can be evaluated for the quantum mechanical tunneling model as [51]:

$$s = 1 - \frac{4}{\ln(1/\omega\tau_o)} \tag{2.32}$$

2.8.3.1: The AC Conductivity for the Quantum Mechanical Tunneling (QMT) Model

When atomic or molecular dipole relaxation happens, the AC conductivity is given in the general formula as:

$$\sigma_{ac}(\omega) = N_P \int \alpha(\tau) \frac{\omega^2 \tau}{1 + \omega^2 \tau^2} P(\tau) d\tau$$
(2.33)

Where, N_P is the number of dipole, ω is the angular frequency, τ is the relaxation time, $\alpha(\tau)$ is the polarizability and $P(\tau)$ is the distribution of the relaxation time. Recalling that the response has a Deby form that $(1/(1 + i\omega\tau))$. The equation (2.33) takes account in the case of an isolated pair like the electric dipole. Noting that the AC conductivity $\sigma_{ac}(\omega)$ is nearly proportional to the angular frequency ω , when the distribution $P(\tau)$ is proportional to $1/\tau$. Therefore, with some constraint the equation (2.33) can also apply to the electronic hoping case [55].

The first explanation of the AC electrical conductivity $\sigma_{ac}(\omega)$ was expressed by equation (2.22). Then, in 1969 Austin and Mott [49, 55] conducted the equation (2.22) to hop of electrons near the Fermi energy E_F in a semiconductor. In the hopping case N_P is the number of carrier, and the polarizability $\alpha(\tau)$ is described as (Pollak and Geballe, 1961):

$$\alpha(\tau) = \frac{(eR)^2}{12 k_B T (\cosh(\delta E/2k_B T))^2}$$
(2.34)

Here, R is the hopping distance, k_B is the Boltzmann constant, T is the absolute temperature, and $\delta E = (E_f - E_i)$ is the average separation of the energy levels.

Starting with case of quantum tunneling electrons near the Fermi energy level E_F . The hopping or tunneling rate ($\Gamma = 1/\tau$) from a state of energy E_i to E_f ($E_f > E_i$) is given as:

$$\Gamma = v_{ph} \exp(-2R/\ell - \delta E/k_B T)$$
(2.35)

Where, v_{ph} is the phonon frequency, and $1/\ell$ is the decay parameter. Then estimate the derivative of τ with respect to R to obtain:

$$d\tau = 2\frac{v_{ph}^{-1}}{\ell} \exp\left(\frac{2R}{\ell}\right) dR = \frac{2\tau}{\ell} dR$$
(2.36)

Note that the Boltzmann constant ignores for simplification. In the case of random distribution of hopping sites N, the distribution of the relaxation time $P(\tau)$ in equation (2.33) can write as:

$$P(\tau)d\tau = P(R)dR = 4\pi NR^2 dR$$
(2.37)

By substituting the equations from (2.34) to (2.37) into equation (2.33), we obtained the AC conductivity as:

$$\sigma_{ac}(\omega) = \frac{\pi N N_P e^2 \ell \omega}{6k_B T} \int R^4 \frac{\omega^2}{1 + \omega^2 \tau^2} \frac{d\tau}{\tau}$$
(2.38)

Where both of the number of carrier for hopping near E_F and the number of unoccupied levels are given by $(N(E_F)k_BT)$. Then, substitute $NN_P = [N(E_F)k_BT]^2$ in equation (2.38). Since that $(\omega^2/(1 + \omega^2\tau^2))$ is like the δ – function sharply peaked at $(\omega\tau =$ 1), and R can be taken out of the integral. The formula of R at $(\omega\tau = 1)$, indicated by the hopping distance at a particular frequency R_{ω} can found from equation (2.35) as [55]:

$$R_{\omega} = \frac{\ell}{2} \ln(v_{ph}/\omega) \tag{2.39}$$

Then the integral in equation (2.38) can be calculated as:

$$\int \frac{\omega^2}{1+\omega^2\tau^2} \frac{d\tau}{\tau} \approx \frac{\tau}{2}$$
(2.40)

Using equations (2.37), (2.39) and (2.40) to get AC conductivity in equation (2.38) as:

$$\sigma(\omega) = C e^2 \ell^{-5} \left(N(E_f) \right)^2 k_B T \omega [\ln(v_{ph}/\omega)]^4$$
(2.41)

Where, C is a numerical constant, and ℓ^{-1} the decaying parameter [55]. This equation agreed with the equation (2.30) for the quantum mechanical tunneling (QMT) model.

2.8.4: The Correlated Barrier Hopping (CBH) Model

The correlated barrier hoping (CBH) model is a process which correlates the relaxation mechanism with the intersite separation. This model was proposed by Pike and then extended by Elliott [51, 52]. They assumed that the atoms or ions hopped over a barrier having height W separating two sites and energy difference Δ . Here, the random variable ξ in equation (2.23) is $\xi = W/k_BT$.

For two neighboring sites have a distance R, the coulomb wells overlaps. In this case, the effective barrier height lowered from W_M at infinite separation to value W:

$$W = W_M - \frac{2e^2}{\pi\varepsilon\varepsilon_o R} \tag{2.42}$$

Where, W_M is the maximum barrier height which is the binding energy of the carrier in its localized sites and can calculate from the slope of 1 - s versus temperature. Also, ε and ε_0 are the effective dielectric constant for the material and the free space, respectively [51, 52].

The AC conductivity for the correlated barrier hopping model in a narrow band limit $(\Delta_o \ll k_B T)$ is expressed as [51]:

$$\sigma(\omega) = \frac{\pi^3}{12} N^2 \varepsilon \varepsilon_o \omega R_\omega^6 \tag{2.43}$$

Where, *N* is the concentration of pair sites and the hopping distance R_{ω} are given by the relation [51]:

$$R_{\omega} = \frac{2e^2}{\pi\varepsilon\varepsilon_o[W_M + k_BT\ln(\omega\tau_o)]}$$
(2.44)

For this model the frequency exponent s found to be:

$$s = 1 - \frac{6k_BT}{W_M + k_BT\ln(\omega\tau_o)}$$
(2.45)

From the first approximation ($\Delta_0 \ll k_B T$) yields to a large value of $W_M/k_B T$, the equation (2.45) reduced to [52, 53]:

$$s = 1 - \frac{6k_BT}{W_M}$$
(2.46)

So, the frequency exponent s for the correlated barrier hopping model is a temperaturedependant predicted with decreasing the exponent value as the temperature increased.

The correlated barrier hopping (CBH) model conductivity might be a frequency independent in high and low frequency region, and takes the form [54]:

$$\sigma_{ac}(\omega) = \sigma_{ac}(H) + \left[\sigma_{ac}(L) - \frac{\sigma_{ac}(H)}{1 + (\omega\tau)^2}\right]$$
(2.47)

Where $\sigma_{ac}(L)$ and $\sigma_{ac}(H)$ are the DC value of the conductivity at low (L) and high (H) frequency in which the electrons can sense the electric field variation, and τ is the relaxation time due to hopping.

Chapter Three

Experimental Details

3.1: Thin Film Preparation

In this thesis, nanosandwiched structures of zinc selenide thin films were deposited onto ytterbium and ultrasonically cleaned glass substrates using the physical vapor deposition technique as shown in Fig. 3.1. During evaporation, the film thickness was kept at a vacuum pressure about 10^{-5} mbar. The thickness was monitored using an in situ quartz crystal thickness monitor.



Fig. 3.1: The vacuum evaporation system.

The glass substrates were cleaned in the following steps. Glass substrates were washed by distilled water then alcohol to remove dust, and then it was put in boiled peroxide water H_2O_2 for 30 min. After that, the glass substrates were immersed in alcohol, followed by ultrasonic resonator in distilled water at 70 °C for 40 min. The ytterbium substrates were masked by TEFLON strip and the rest part of metal substrates were ready to execute the first run of the evaporation.



Fig. 3.2: The geometrical design of (a) ZnSe, (b) ZnSe/Y/ZnSe, (c) ZnSe/Au/ZnSe,
(d) ZnSe/YAu/ZnSe, (e) Yb/ZnSe/ZnSe, (f) Yb/ZnSe/Y/ZnSe, (g) Yb/ZnSe/Au/ZnSe, and (h) Yb/ZnSe/YAu/ZnSe nanosandwiched films.

ZnSe powder weighing (0.3 g) is putting into a tungsten boat (Fig. 3.1, item 1), which is installed in the system. Four ytterbium and 8 glass substrates were placed in a metal holder (Fig. 3.1, item 2), located 20 cm above the evaporation source. A physical movable shatter (Fig. 3.1, item 3) located between the films samples and the evaporation source was used to control the evaporation and avoid randomization throughout the whole deposition process. The thickness of ZnSe in the grown films were about 500 nm measured by the quartz crystal monitor (Fig. 3.1, item 4).

In the second run of the evaporation system, a 70 nm of Y was deposited at the top of four ZnSe and two Yb/ZnSe substrates. The Y solid lumps were weighed (0.25 g) and placed in another tungsten boat to be deposit and form the ZnSe/Y and Yb/ZnSe/Y. The other two ZnSe and one Yb/ZnSe substrates from the first run was used to start the third run and deposit a 70 nm of gold, which was weighed (0.25 g) and put in another tungsten boat to form ZnSe/Au and Yb/ZnSe/Au. Also, in the same run the gold was reevaporated onto two of ZnSe/Y and Yb/ZnSe/Y that formed from the second run forming ZnSe/YAu and Yb/ZnSe/YAu. The final run in this evaporation process was the formation of the nanosandwiched films. The ZnSe, ZnSe/Y, ZnSe/Au, ZnSe/YAu, Yb/ZnSe, Yb/ZnSe/Y, Yb/ZnSe/Au and Yb/ZnSe/YAu substrate films were recoated by a 500 nm layer of ZnSe. The ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe, ZnSe/YAu/ZnSe, Yb/ZnSe/ZnSe, Yb/ZnSe/Y/ZnSe, Yb/ZnSe/Au/ZnSe Yb/ZnSe/YAu/ZnSe and nanosandwiched films are now formed. The geometrical designs of the samples were displayed in the Fig. 3.2.

The ytterbium metal substrates, which have small work function, were required to study the electrical characterization of prepared films. The ohmic contact was formed by deposited a gold points contact on the surface of the ytterbium substrates films by using suitable masks.

3.2: Thin Film Analysis

The effect of growing YAu metal alloy as nanosandwich in the structure of ZnSe was studied by means of structural, optical, dielectrical, conductance spectroscopy and current-temperature analysis in the following sections. In addition, a theoretical modeling that fits well with the experimental data will be used to verify the correctness of the approach and investigate the physical phenomena laying beyond the behavior of the alloyed films.

3.2.1: The Hot-Probe Technique

The conductivity types of the sandwiched films were found by using of hot-probe technique [56]. This Technique is the simplest way to distinguish between the p-type and n-type semiconductors. It is based on using a heater soldering iron with temperature reaching 400 K and a digital multi meter (DMM) to read the current signal. The cold probe connected to negative terminal (ground terminal) of the digital multi meter, and the hot soldering iron connected to the positive terminal of the DMM [58]. Fig. 3.3 displays the experimental set-up for hot probe technique. The positive reading of the multi meter indicates a n-type semiconductor. In this case, a positive external current is formed due to moving the electrons from the hot iron probe (+ve) to the cold probe (-ve). On the other hand, the p-type semiconductors indicate when read a negative current due to traveling the electrons from the cold probe (-ve) to the hot iron probe (+ve) [47]. When the technique was applied to ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe films indicating a n-type conuctivity.



Fig. 3.3: The experimental set-up of Hot-Probe technique.

3.2.2: The x-ray Diffraction (XRD) Measurements

The Rigaku MiniFlex 600 x-ray unit shown in Fig. 3.4 with K_{α} radiation of a copper anode of wavelength 1.5405 Å at voltage of 40 KV and current 15 mA were used to record the x-ray diffraction patterns in order to explore the crystalline nature of the film. The data obtained in 20 range of 10°-70° with a step of 0.1° and scan speed of rate 5.0 deg/min. The data was taken by the MiniFlex Guidance software connects with the xray unit. The x-ray data was analyzed using TREOR-92 software program.



Fig. 3.4: The Rigaku MiniFlex 600 x-ray unit.

3.2.3: Optical Measurement

The optical data of transmittance and reflectance spectra in wavelength range of 300-1100 nm were measured by using of Evolution 300 UV-VIS spectrophotometer (Thermo-scientific), which displayed in Fig. 3.5. The data was collected and manipulating with Vision-I software programmed with the system.



Fig. 3.5: The Evolution 300 UV-VIS spectrophotometer unit.

3.2.4: Current – Temperature Measurement

The current-voltage characteristics for sandwiched films were recorded with help of automated KEITHLEY 230 programmable voltage source and KEITHLEY 6485 picoammeter (Fig. 3.6), which measured the voltage and current, respectively. This system is automated by the connections with KEITHLEY low noise cables and IEE488 interface which was controlled by MATLab software. The current-temperature dependence was measured by KEITHLEY characterization systems and LakeShore 335 Temperature controller (Fig. 3.6). The current – temperature characteristic was recorded in high temperature range of 300-460 K, with a voltage source of 100, 100, 0.5 and 100 V for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe, respectively. The temperature of the sample was increased by connecting it to a power supply voltage source (0-60 V). So, the current was recorded as the temperature increased for a heating part, then it was recorded when the temperature decreased for a cooling part.



Fig. 3.6: The Current - Temperature characteristic experiment.

3.2.5: The Conductance Spectroscopy Measurement

The conductance spectra were recorded using Agilent 4291B 12F Impedance-Material Analyzer spectrometer in frequency range 1.0MHz-1.8GHz, which shown in Fig. 3.7. The samples were connected to 16453A Dielectric Material test fixture, and the data was controlled by MATLAB software.



Fig. 3.7: The Agilent 4291B 12F Impedance-Material Analyzer.

Chapter Four

Results and Discussion

4.1: Structural Analysis

The x-ray diffraction (XRD) patterns which were recorded for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films are presented in Fig. 4.1. The peak positions which were subjected to "TREOR 92" software packages reveal a hexagonal structure for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe thin films. As it is displayed in the Fig. 4.1 for ZnSe film, a maximum peak is observed at $2\theta = 28.1^{\circ}$ and a minor peak occurs at $2\theta = 25.4^{\circ}$ which could be attributed to scattering from the (002) and (100) hexagonal phase of ZnSe planes in accordance with the published data [3]. The lattice parameters for films were calculated through finding the interplanar distance from Bragg's law which is presented in equation (2.1), using the formula (2.2 (b)) and compared to the software results. The lattice parameters values presented in Table 4.1. The values being a = 4.051 Å and c = 6.354 Å for ZnSe, are consistent with literature data [6, 8].

The XRD patterns for ZnSe/Y/ZnSe sandwiched film as illustrated in Fig. 4.1 exhibited the similar peaks at $2\theta = 28.1^{\circ}$ and $2\theta = 25.4^{\circ}$ which relate to hexagonal ZnSe with (002) and (100) plans. Compared to ZnSe, the peak width increased which indicats a deformation in the structure. In addition, a new peak appeared for ZnSe/Y/ZnSe at $2\theta =$ 45.8°. This peak relates to hexagonal ZnSe at (211) direction [3] and it disappeared in the other films. The calculated lattice parameters values are a = 4.051 Å and c = 6.354 Å for ZnSe/Y/ZnSe. The appearance of the (211) reflection plane in the XRD of the ZnSe/Y/ZnSe indicate a metal induced crystallization process in ZnSe associated with the Y-presence [58].

The resulting XRD pattern for ZnSe/Au/ZnSe is also displayed in Fig. 4.1. Likewise, the peak width increased comparing with ZnSe, the peaks position shifts to $2\theta = 28^{\circ}$ and $2\theta = 25.3^{\circ}$. The calculated lattice parameters values are a = 4.066 Å and c = 6.376 Å for ZnSe/Au/ZnSe.

On the other hand, the x-ray pattern for ZnSe/YAu/ZnSe which is illustrated in Fig. 4.1 show a clear shift in the peaks position to $2\theta = 27.8^{\circ}$ and $2\theta = 25.2^{\circ}$. Narrower peak for YAu sandwiching leads to more ideal structure. For YAu metal alloy existed between two ZnSe layers, the calculated lattice parameters values are a = 4.082 Å and c = 6.421 Å.



Fig. 4.1: The x-ray diffraction patterns for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe films.

In order to understand the structural characteristic of ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films. The grain size (D), stacking fault (SF), stress (S), dislocation density (δ) and micro-strain (ϵ), which presented in the equations (2.11) to (2.15) in chapter two, were calculated. The values are illustrated in Table 4.1.

	ZnSe	ZnSe/Y/ZnSe	ZnSe/Au/ZnSe	ZnSe/YAu/ZnSe
2θ (°)	28.1	28.1	28	27.8
I (a.u.)	727	844	922	1333
d (Å)	3.177	3.177	3.188	3.210
(h kl)	(002)	(002)	(002)	(002)
a (Å)	4.051	4.051	4.066	4.082
c (Å)	6.354	6.354	6.376	6.421
D (nm)	28.54	21.41	21.41	28.53
$SF(imes 10^{-3}\%)$	265	353	354	266
$S_a(imes 10^{10})$ (dy/cm^2)	-2.07	-2.07	-2.53	-2.99
$S_c(imes 10^{10})$ (dy/cm^2)	3.12	3.12	2.73	1.93
$\delta_a(imes 10^{11}) \ (line/cm^2)$	6.78	12.1	12.1	6.81
$\delta_c(imes 10^{11})$ (<i>line/cm</i> ²)	4.33	7.69	7.69	4.33
$\epsilon(imes 10^{-3})$	5.23	6.97	7.00	5.29

Table 4.1: The structural parameters of ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.

* See Symbols Table.

The lattice mismatch between the metal and semiconductor layers is known to create large defects and force the presence of quantum confinements. The lattice plays vital role in optoelectronic properties. Returning to the tabulated data, it is clear that the presence of Y, Au and YAu highly increased the intensity indicating better crystallization process in ZnSe. The nanosandwiching of yttrium layers between two ZnSe layers has no effect on the lattice parameters and the stress (S) along the a and c axes. But yttrium reduces the grain size (D), the stacking fault (SF), dislocation density (δ) and micro-strain (ϵ) increased as shown in Table 4.1. Since the ionic radius of Y^{+3} is 102 pm [59] and that for Zn^{+2} is 74 pm [60], it is impossible for Y^{+3} to replace the vacant sites of Zn^{+2} and form Y - Se bond. The Y metal is one of the F_{m-3c} space group and exhibit an FCC structure of lattice constant 4.930 Å [61, 62], which indicate a lattice mismatch of ~21% and ~22% along the a and c axes, respectively. Large mismatched films are reported that causes a high dislocation defect in the films and this was capable of producing a highly efficient LED [63].

For the ZnSe/Au/ZnSe structure, the lattice parameter increased. The grain size (D) and the stress (S) along a and c axes reduced, while the stacking fault (SF), dislocation density (δ) and micro-strain (ε) increased as illustrated in Table 4.1. From the chemical point of view, the ionic radius of Au^+ is 137 pm [64] larger than 74 pm for Zn^{+2} [60]. In this case, substituting Au^+ in Zn^{+2} sites is impossible and interstitial Au^+ ions between Zn-Zn bonds to form Au-Zn bonds may have occurred. The Au metal belongs to F_{m-3m} space group and exhibit an FCC structure of lattice constant 4.078 Å [65, 66], which indicate a large lattice mismatch of 35% along c-axes. On the other hand, it indicates a good lattice match of 0.66% along the a-axis. This well matched along aaxes has good influence on the electrical and thermal conductivity [63]. Moreover, the nanosandwiching of the YAu alloy layer between two ZnSe layers was more preferable. It much increased the lattice parameters and decreased the stress (S) compared to other films. However, it has no effect on the grain size (D), stacking fault (SF), dislocation density (δ) and micro-strain (ϵ). For YAu alloy, the lattice mismatch between faces centered cubic-Y and face centered cubic-Au was found to be 20% along the a-axes.

The increasing of the ZnSe lattice parameters for ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films was also observed for Cobalt doped ZnSe [67] and Eu^{3+} - doped ZnSe [68]. It is reported that the increased Co doping concentration increased the lattice parameters for ZnSe due to substitution of Co ion in Zn ion site [67]. The Eu^{3+} – doped ZnSe increased the lattice parameters from a= 3.915 Å and from c= 5.973 Å to a= 3.988 Å and c= 6.125 Å. This behavior was assigned to large ionic radius of Eu^{3+} (109 pm) which causes subsequent deformation of ZnSe lattice [68]. Similarly, P. Prathap et al. report more increases in the lattice constant of AI-doped ZnSe with increase doping level [69]. In our case, the ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe may be attributed to the increase in the number of vacant sites in the ZnSe structure which causes the lattice to expand and increase the lattice parameters. On the other hand, the Y and Au ions may occupy the interstitial sites in the ZnSe host lattice. The results show that using of YAu double layer between ZnSe layers is preferable. It increased the lattice parameters and reduced the dislocation defect more than the other sandwiched films.

4.2: Optical Analysis

The optical transition (T) spectra for ZnSe (1 µm thick), ZnSe/Y/ZnSe (1.07 µm thick), ZnSe/Au/ZnSe (1.07 µm thick) and ZnSe/YAu/ZnSe (1.14 µm thick) which were measured in the incident photon wavelength range of 300-1100 nm are presented in the Fig. 4.2. The data suggest that the ZnSe film is highly transparent compared to ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films. The transmittance for ZnSe reaches a local maximum of ~82% at 530 nm and an absolute maximum value of ~92% at 956 nm. However, the transmittance for ZnSe/Y/ZnSe reaches a local maximum of \sim 76% at 510 nm which it shifted 20 nm from that of ZnSe, and an absolute maximum value of ~92% at 956 nm. On the other hand, The T% for ZnSe/Au/ZnSe exhibits a local maximum of ~65% at 528 nm, and an absolute maximum value of \sim 83% at 958 nm with a little shifted coppering to ZnSe film. When YAu alloy used as a nanosandwich in the ZnSe, it exhibits the lowest transmittance reaching a local maximum of ~61% at 516 nm, and an absolute maximum value of ~82% at 1022 nm. The position of ZnSe/YAu/ZnSe peaks shown a clear shifting compared with ZnSe.



Fig. 4.2: The transition (T) spectra for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films in the wavelength range of 300-1100 nm.

The reflectance (R) spectra for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films in the wavelength range of 300-1100 nm are illustrated in the Fig. 4.3. As shown in Fig. 4.3, the surface ZnSe/Y/ZnSe was more reflective than that of ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe. Three R% peaks appeared for all of ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe and ZnSe/YAu/ZnSe sandwiched films. The ZnSe R% peaks values reached ~16% at 330 nm, ~19% at 456 nm and a maximum R% value about ~28% at 648 nm.



Fig. 4.3: The reflection coefficient (R) spectra for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films at wavelength range of 300-1100 nm.

The reflectance spectra of ZnSe/Y/ZnSe exhibit peaks of values of ~20% at 332 nm, ~14% at 438 nm and a maximum R% value of ~33% at 638 nm. While the reflection spectra of ZnSe/Au/ZnSe exhibit peaks of values of ~16% at 336 nm, ~18% at 458 nm and the maximum R% value of ~27% at 648 nm. On the other hand, the reflection spectra of ZnSe/YAu/ZnSe exhibit peaks of values reach ~19% at 342 nm, ~14% at 464 nm and maximum R% value of ~29% at 636 nm. As we know, these peaks in the reflectance spectra appeared due to the constructive and destructive interference that occurs between the incident light to the surface and reflected light waves from the bottom of the film phenomena [43]. In addition, these peaks mostly happened near the band gap of the films [70].

The absorbance (A) spectra is found from the measurement data of T% and R% by the equation A% = (100% - T% - R%) [43]. The absorbance (A) spectra for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films were recorded in the wavelength range of 300-1100 nm and displayed in Fig. 4.4. As shown from the Fig., a sharp decay in the absorption appears $\lambda < 530$ nm. The absorbance spectra of ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe were observed to exhibit two absorption regions defined as high absorption for incident light of $\lambda < 530$ nm and low absorption region for incident light of $\lambda > 530$ nm. The A% spectra for ZnSe exhibited a lower absorbance than other sandwiched films with a minimum absorption edge value that reaches ~15% at 540 nm. For ZnSe/Y/ZnSe, the absorbance slightly increased and the minimum absorption edge of $\sim 19\%$ is reached at 528 nm. There is a shift to high absorption region compared with ZnSe film. The A% values of ZnSe/Au/ZnSe are higher than that of ZnSe and than that of the ZnSe/Y/ZnSe with a minimum absorption edge value being ~31% at 540 nm. Finally, the ZnSe/YAu/ZnSe exhibits the highest A% values with a minimum absorbance of \sim 36% at 524 nm. The absorption spectra increased when Y or Au metal were used in the ZnSe sandwiched films, but the A% was highly increased when YAu alloy was used in the ZnSe sandwiched films.



Fig. 4.4: The absorbance (A) spectra for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films at wavelength range of 300-1100 nm.

To obtain a more clear picture about the variation in the absorbance, the absorbability (R_{λ}) of the ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe nanosandwiched films were found from the ratio between the absorbance values through the relation $(R_{\lambda} = A_{ZnSe/x/ZnSe} \%/A_{ZnSe} \%)$, where (x = Y, Au, YAu) is the material used to grow the sandwiched films. The absorbability (R_{λ}) compared to ZnSe presented in Fig. 4.5 as function of incident photon energy for the sandwiched films. As appears in the Fig. 4.5, the presence of Y layer between two ZnSe layers increased the light absorbability for Y sandwiching by 1.4 times at 2.23 eV compared to ZnSe. The peak width is 0.53. The absorbability was better when an Au layer was used to form ZnSe/Au/ZnSe sandwiched film by 1.99 times at 2.32 eV. The width of the R_{λ -E} peak increased to 0.77 compared to the ZnSe/Y/ZnSe.



Fig. 4.5: The absorbability (R_{λ}) as function of photon energy for ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.

In addition, the ZnSe/Au/ZnSe light absorbability was also increased by 2.15 times at 1.24 eV. The existence of Y and Au layers together between two ZnSe layers enhanced the absorbability more than Y or Au alone. The ZnSe/YAu/ZnSe absorbability was increased by 2.36 times at 2.29 eV with peak width of 0.71 and by 2.32 times at 1.36 eV. The blue dashed lines in Fig. 4.5 shown that the peak of the absorbability increased, the width of peak increased, and it shifted to high energy region for ZnSe/YAu/ZnSe sandwiched film.

The effects of the YAu layers as a nanosandwich between two ZnSe films on the optical properties from the energy band theory point of view is also studied. The T%, R% and A% spectra were employed to determine the absorption coefficient spectra through the relation ($\alpha = (2.303A)/d$), where d is the thickness of the film [71, 72].

The absorption coefficient (α) as a function of incident photon energy for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe are displayed in Fig. 4.6. Three regions appeared are the absorption saturation region above 3.00 eV, sharp region between 2.30 – 3.00 eV and transparent region below 2.3 eV. A pronounced effect of the nanosandwiching on the absorption coefficient (α) values are observed below 2.5 eV. In the region of 2.5-1.4eV, α values for ZnSe are approximately the same as ZnSe/Y/ZnSe. Replacing Y by Au increases the values of α . The highest values of α are observed when double layer of YAu are used.



Fig. 4.6: The absorption coefficient (α) for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.

The absorption coefficient doesn't reach zero even in the transparent region. The nonzero values of α indicate the presence of the interbands or band tails. The band tails in the semiconductor are usually formed by impurities, inhomeganuities, defects and

broken bond. As the Fig. 4.6 show, while the presence of the Y doesn't strongly affect the already existing interband of ZnSe the replacement of Au alter them significantly causing higher degree of absorption, the coating of the Y with Au through the sandwiching process enhances them more.

Returning to the low absorption region, where the band tails are believed to exist, the α values in that region can be presented by the relation:

$$\alpha = \alpha_o \exp(E/E_e) \tag{4.1}$$

Where, α_0 is a constant, E is the photon energy (hv) and E_e is the band tail energy (or Urbach energy). The energy band tail usually indicates the presence of defects in the structure and the optical transition between localized and extended state in the valence and conduction band. The E_e can be estimated from the reciprocal of the slope of linearly $\ln(\alpha)$ spectra versus photon energy curve [73-75].

The logarithmic plot of the absorption coefficient verses photon energy for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films displayed in Fig. 4.7. The calculated values of the band tail energy are illustrated in Table 4.2. The calculated E_e for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe are 0.99 eV, 1.14 eV, 2.07 eV and 0.64 eV, respectively. These bands tail energy levels are related to the recombination mechanism as a result of antisite defects [76]. The increased band tail energy indicates a higher disorder of photon states in the films [74]. While the ZnSe/Y/ZnSe and ZnSe/Au/ZnSe have wider band tails than ZnSe, it is clear that the ZnSe/YAu/ZnSe has narrower band tails. This narrower band tail for the double YAu layer suggested that less defects and disorder are induced by the YAu.



Fig. 4.7: The $\ln(\alpha) - E$ dependence for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.

The (α) data reveal information about the energy gap (Eg) of ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe. The optical energy gap and the electronic transition type can be estimated from the absorption coefficient spectra by applying the well-known Tauc's relation $[(\alpha E)^{1/p} = A (E - E_g)]$, where α is the absorption coefficient, E = hv is the photon energy, A is a constant, Eg is the energy band gap, and p is a constant related to the optical transition type. The values of p are 3/2, 3, 1/2 or 2 for direct forbidden, indirect forbidden, direct allowed and indirect allowed electronic transition, respectively. From the plots of $(\alpha E)^{1/p}$ versus photon energy, the value of the energy band gap is estimated from the E-axis crossing for the best linear curves of $(\alpha E)^{2/3}$, $(\alpha E)^{1/3}$, $(\alpha E)^2$ and $(\alpha E)^{1/2}$ versus E which are shown in Fig. 4.8 [39, 40].

The linear fit which covers most of the experimental data is selected as the dominant type of electronic transition. The fitting must start from incident photon energy region below the saturation region (4.0-3.0 eV). In accordance to Fig. 4.8, the best fit which covers most of data appeared for direct allowed transition type (Fig. 4.8(b)).



Fig. 4.8: The $(\alpha E)^{1/p}$ versus incident photon energy for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films with p values (a) p=2, (b) p=1/2, (c) p=3 and (d) p=3/2.

The allowed direct Eg of ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe were estimated for high energy absorption regions as shown in Fig. 4.9. The dependence of the $(\alpha E)^2 - E$. The direct allowed energy band gap in the high absorption region (2.30-3.00 eV) for ZnSe is 2.44 eV. The direct energy band gap for the ZnSe has a highest valance band at the Γ_{15} point which split because of the spin orbit coupling into a two-fould Γ_7 and a four-fould Γ_8 state. This band gap should be considered as the transition from $\Gamma_{7\nu}$ or $\Gamma_{8\nu}$ valence band state to Γ_{6c} conduction band state [20, 77].



Fig. 4.9: The $(\alpha E)^2 - E$ for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films in the high absorption region.

The literature data for ZnSe reported an energy region of (2.55-2.70 eV) for direct allowed transition type [2, 78]. Min. Ji. Kim et al. [10] reported a band gap of 2.60 eV for the synthesized ZnSe. While, Yao et al. [79] reported an allowed energy gap value of 3.03 eV for ultrathin ZnSe nanorods. This high value was assigned to a quantum confinement effect [79].

In addition, the allowed direct Eg for ZnSe/Y/ZnSe was increased to 2.46 eV and for ZnSe/Au/ZnSe was decreased to 2.38 eV compared with that of ZnSe. Moreover, it observed that the direct allowed Eg of ZnSe/YAu/ZnSe is 2.44 eV, which is similar to that of ZnSe. G. M. Lohar et al. who reported an energy band gap value of 2.45 for Fedoped ZnSe [3], it is also less than that of pure ZnSe band gap energy of 2.63 eV. As another comparison, M. M. Ivashchenko et al. reported an energy gap of 2.81, 2.77 and 2.79 eV for Eu-doped ZnSe. These high values for Eu-doped ZnSe are due to the incorporation of Eu³⁺ ions onto the ZnSe structure or to the phonons interactions [78]. Moreover, Min. Ji. Kim et al. found that increasing of Er and Yb doping concentration in the ZnSe films decreased the absorption edge (or the band gap) [10]. It is clear that, the doping reduced the band gap of ZnSe. While the Au layer reduced the band gap energy, the Y layer increased it and the YAu layer did not change the band gap E_g value of ZnSe film.

The band gap energy values have slightly changed by nanosandwiching, so a band gap narrowing occurs. M. Harb et al. reported that the formations of incompletely delocalized electronic levels over the valence band states are responsible for the band gap narrowing of S-doped TiO₃ [80]. In addition, the lattice distortion induced by the dopant atom was also assigned as a reason for the direct band gap narrowing [81]. This effect on the energy band gap values can be attributed to the structure modifications like

decreased of the grain size, different in the electron affinity of ZnSe (3.8 eV) [20], Y (0.307 eV) [82] and Au (2.31 eV) [83], large lattice mismatch, defect, impurity level and incomplete bonds in the films structure.

In addition, the band bending mechanism plays role in shrinking and widening the band gap. The metal work function of Au and Y are 5.34 eV [71], 3.1 eV [82], respectively, and the work function of n-type ZnSe is (4. 84 eV) [20]. Since the work function of Y is less than that of n- type ZnSe, the ZnSe/Y/ZnSe shows an Ohmic nature of interfaces. In this case, the carriers flow freely in or out of the ZnSe so it exhibited less resistance at the Y contact. On the other hand, the Au has a work function larger than that of n-type ZnSe. The ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe showed a schottky type of formation. In the schottky type contact, electrons flow from the semiconductor to metal increasing the surface charge at the metal surface, and as a result they bend the conduction band down leading to the observed band gap narrowing [24]. However, as the metal is sandwiched from both sides, band bending mechanisms should be less effect.

The optical results of ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films are summarized in Table 4.2.

	ZnSe	ZnSe/Y/ZnSe	ZnSe/Au/ZnSe	ZnSe/YAu/ZnSe
Maximum T%	92% at 956 nm	92% at 956 nm	83% at 958 nm	82% at 1022 nm
Maximum R%	28% at 648 nm	33% at 638 nm	27% at 648 nm	29% at 636 nm
Minimum A% edge	15% at 540 nm	19% at 528 nm	31% at 540 nm	36% at 524 nm
Eg (eV)	2.44	2.46	2.38	2.44
E _e (eV)	0.99	1.14	2.07	0.64

Table 4.2: The optical results for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.

*See Symbols Table

4.3: Dielectric Analysis

To explain the patterns that had emerged in the reflection spectra and investigate the possible applications of this sandwiched film, the dielectric properties of ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films are investigated. The effective dielectric constant ε_{eff} was determined through the relation [44]:

$$R = \frac{\left(\sqrt{\varepsilon_{eff}} - 1\right)^2 + \left(\frac{\alpha \lambda}{4\pi}\right)^2}{\left(\sqrt{\varepsilon_{eff}} + 1\right)^2 + \left(\frac{\alpha \lambda}{4\pi}\right)^2}$$
(4.2)

In this equation, R is the reflectance at normal incidence, ε_{eff} the effective dielectric constant, α and λ are the absorption coefficient and incident photon wavelength, respectively. The real ε_r and imaginary ε_{im} parts of dielectric constant can be determined from the data of the effective dielectric constant ε_{eff} through the formulas

$$(\varepsilon_r = \varepsilon_{eff} - (\frac{\alpha \lambda}{4 \pi})^2)$$
, and $(\varepsilon_{im} = \sqrt{\varepsilon_{eff}} (\frac{\alpha \lambda}{2 \pi}))$, respectively [44, 84].

The real dielectric constant ε_r spectra for ZnSe and ZnSe/Y/ZnSe sandwiched films are illustrated in Fig. 4.10. The frequency axis was selected at THz range, to make it easier for observing the Terahertz applications. It is clear from the Fig., that the real part ε_r of the dielectric constant for ZnSe increases sharply with increasing the photon frequency reaching a maximum of ~10 at resonance frequency of 426.13 THz (1.75 eV). This peak should correspond to the interband transition in ZnSe which arises from the inhomogeneity, defect and broken bonds on the structure. In addition, it can be corresponded to the electric field due to free moving and bond charges [77]. Moreover, this resonance with energy of 1.75 eV can be assigned to the direct allowed transitions in the selenium which happens of 1.75 eV [85].


Fig. 4.10: The real part ε_r of dielectric constant for ZnSe and ZnSe/Y/ZnSe sandwiched films in the incident photon frequency range of 270-1000 THz.

The ε_r for ZnSe also exhibited two other resonating peaks with ε_r values of 8.56 and 6.12 corresponding to resonance frequency at 630.25 THz (2.59 eV) and 837.98 THz (3.45 eV), respectively. The resonant peak of energy 2.59 eV can be attributed to direct allowed electron transition for ZnSe as mentioned previously. On the other hand, the peak at 837.98 THz (3.45 eV) are probably due to the interaction between oxygen atoms and zinc atoms. The Zn-O band is reported to exhibit direct electron transitions band gap of 3.40 eV [86]. The presence of oxygen atoms in ZnSe or in the glass substrate could have resulted through the evacuation venting process.

On the other hand, the real part ε_r of dielectric spectra for ZnSe/Y/ZnSe sandwiched film that is also displayed in Fig. 4.10 revealed a clear enhancement compared to those of ZnSe. For ZnSe/Y/ZnSe, the real part ε_r exhibits a maximum value of ~12 at resonance frequency of 407.6 THz (1.68 eV). When Y layer existed between two ZnSe layers, the peaks of ε_r spectra were more insensitive and shifted toward lower frequency values. This enhancement arises from the presence of Y that was associated with strain or impurities in the films [87]. It may also attribute to the reduction in the recombination rate at the material surfaces [88].

The real part ε_r of the dielectric constant for ZnSe/Au/ZnSe is displayed in Fig. 4.11. The ε_r of ZnSe is shown to allow comparison with the Au sandwiched one. The Fig. 4.11 shows the ZnSe/Au/ZnSe film exhibits remarkable increase in ε_r with a shift to lower frequency than those observed for ZnSe. The maximum value of ε_r increased from ~10 at resonance frequency of 426.13 THz (1.75 eV) for ZnSe to ~13.82 at 414.36 THz (1.71 eV) for ZnSe/Au/ZnSe. This peak can also be assigned to interband transition of ZnSe. In addition, the other two resonance peaks of ZnSe/Au/ZnSe appeared at 600 THz (2.47 eV) and 777.20 THz (3.20 eV). The slight shift in the interband transition energy is due to the availability of more free electrons associated with the presence of Au atoms.



Fig. 4.11: The real part ε_r of dielectric constant for ZnSe and ZnSe/Au/ZnSe sandwiched films in the incident photon frequency range of 270-1000 THz.

For the ZnSe/YAu/ZnSe structure further improvement in ε_r is recognized compared to ZnSe as shown in Fig. 4.12. The maximum peak value of ε_r for ZnSe/YAu/ZnSe ~12.53 appeared at resonance frequency of 401.06 THz. It corresponds to incident photon energy of 1.65eV. Particularly, ZnSe/YAu/ZnSe sandwiched film exhibits a further shift in ε_r spectral values toward lower frequencies with an increase in the dielectric value. This improvement in dielectric constant and shift in the frequency is more preferable because it indicates more sensitivity to the light spectrum near infrared regions [44]. On the other hand, Two resonance peaks of ε_r spectra appeared at resonance frequency of 574.71 THz (2.37 eV) and 724.63 THz (2.98 eV).



Fig. 4.12: The real part ε_r of dielectric constant for ZnSe and ZnSe/YAu/ZnSe sandwiched films in the incident photon frequency range of 270-1000 THz.

While the presence of Y increased the maximum value of ε_r from ~10 to ~12, and the Au increased it from ~10 to ~14. The YAu appeared less effective, it increased the ε_r from ~10 to ~13. The decreasing value of ε_r with the presence of YAu is probably due to less contribution of charge accumulation at the interface of the films compared to ZnSe/Au/ZnSe which is more effective.

The imaginary part ε_{im} of dielectric constant spectra gives significant information about the optical conductivity, electronic motion and the electron-Plasmon interaction in ZnSe sandwiched films. The ε_{im} for the ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe nanosandwiched films are illustrated in Fig. 4.13. It is clear from the Fig. that the ε_{im} exhibits two orders of magnitude lower than those of real part. The ε_{im} spectra of ZnSe exhibited three resonating peaks at 431 THz (1.77 eV), 661 THz (2.72 eV) and 829 THz (3.41 eV).

For ZnSe/Y/ZnSe, the imaginary part shifted to lower resonance frequency. Also, the peak at 661 THz for ZnSe disappeared in ZnSe/Y/ZnSe sandwiched film. The two resonant peaks of ε_{im} for ZnSe/Y/ZnSe are formed at 410 THz (1.69 eV) and 754 THz (3.10 eV).

The imaginary part of the dielectric constant for ZnSe/Au/ZnSe also presented in Fig. 4.13 exhibits larger values than those of ZnSe and ZnSe/Y/ZnSe. In addition, Three resonances peaks appeared at 412 THz (1.70 eV), 625 THz (2.57 eV) and 777 THz (3.20 eV), which is also associated with a shift in the peak position of ZnSe film.

On the other hand, the ε_{im} for ZnSe/YAu/ZnSe exhibited similar trend of variation but with higher values. The maximum ε_{im} for ZnSe/YAu/ZnSe is 0.15 at 400 THz (1.64 eV). The second resonating peak existed at 732 THz (3.01 eV).

In addition, the ZnSe/YAu/ZnSe caused a more pronounced shifting in resonance frequency compared with ZnSe, ZnSe/Y/ZnSe and ZnSe/Au/ZnSe as shown in Fig. 4.13. The maximum resonating peak of ZnSe/YAu/ZnSe shifted toward lower frequency value.



Fig. 4.13: The imaginary part ε_{im} of dielectric constant for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films in range of 270-1000 THz.

In order to understand the reason for the resonance peaks appeared in the imaginary dielectric spectra, and explore information about the Plasmon-electron interaction, the ε_{im} was studied by Lorentz model. This model can be used to explain the frequency response the material and show strong dispersion about the resonance frequency [84]. Lorentz model connects between the imaginary part of dielectric function and the incident photon frequency for a group of linear oscillators through the relation [43, 44]:

$$\varepsilon_{im}(\omega) = \sum_{i=1}^{K} \frac{\omega_{pe_i}^{2} \omega}{\tau((\omega_{ei}^{2} - \omega^{2})^{2} + \omega_{i}^{2} \tau_{i}^{-2})}$$
(4.3)

Here, τ is being the electron scattering time, ω is the angular frequency, ω_e reduced resonant frequency and $\omega_{pe} = \sqrt{4\pi ne^2/m^*}$ is the electron bounded plasma frequency where *n* is the free electron density and m^* is the effective mass of electron. In addition, the frequency independent drift mobility, which results from the incident electromagnetic field interaction with the films samples, can be determined by the formula $\mu = e\tau/m^*$, where *e* is the electron charge. So, the equation 4.3 gives information about the values of the $\tau, \omega_e, \omega_{pe}, n, and \mu$ for the studied samples which illustrated in Table 4.3.

The electron bounded plasma frequency which is resonant oscillation of conduction electrons at the interface between two ZnSe layers and Y or Au metal, or between the two metals can be excited by incident light waves. The resonance in the dielectric spectra donated when the frequency of incident light wave equals the free surface charge carrier natural frequency ω_e . The surface free charge carriers which oscillate against the restoring force of positive nuclei cease when the energy is lost in the electronic friction that leads to a damping force of coefficient $\gamma = \tau^{-1}$ [44, 71].

In the above equation (4.3), *K* is the number possible linear oscillators. The experimental data was fitted by equation (4.3) and substituting the effective mass values $(m_{ZnSe}^* = 0.16m_o)$ [20], $(m_Y^* = 1.05m_o)$ [89], and $(m_{Au}^* = 1.10m_o)$ [89]. The effective mass of ZnSe film was evaluated from the equation $m_{ZnSe/ZnSe}^* = (2/m_{ZnSe}^*)^{-1} = 0.080m_o$. For the three layers ZnSe/Y/ZnSe, it was found as $m_{ZnSe/Y/ZnSe}^* = (2/m_{ZnSe}^* + 1/m_Y^*)^{-1} = 0.074m_o$. Thus, the effective mass of ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe were also calculated as $0.075m_o$ and $0.069m_o$, respectively.

The theoretical data of ε_{im} spectra donated by the black colored fitting curve are shown in Fig. 4.14 for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films. The black solid lines in Fig. 4.14 indict a good agreement between the experimental and theoretical data values of imaginary dielectric constant. The fitting parameters of the Plasmon-electron interaction in the ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films were revealed by tabulated data which are presented in Table 4.3.



Fig. 4.14: The imaginary ε_{im} dielectric constant spectra for (a) ZnSe, (b) ZnSe/Y/ZnSe, (c) ZnSe/Au/ZnSe and (d) ZnSe/YAu/ZnSe sandwiched films in range of 270-1000 THz. The black colored lines are the fitting of the Drude-Lorentz equation.

Table 4.3: The optical conduction parameters for electron-Plasmon interactions at the ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.

	ZnSe			ZnSe/Y/ZnSe				ZnSe/Au/ZnSe			ZnSe/YAu/ZnSe					
m^*/m_o	0.0801			0.0744				0.0746			0.0697					
$ au_i(fs)$	5.00	1.40	1.30	0.60	4.00	1.60	0.80	0.29	1.00	1.00	1.20	0.80	7.00	1.20	1.10	0.25
$n (x \ 10^{17} \ \mathrm{cm}^{-3})$	2.00	2.70	4.60	22.0	1.50	2.00	11.0	46.0	2.50	5.50	3.00	14.0	9.00	4.80	6.50	46.0
$\omega_{ei}(\mathbf{x10}^{15}Hz)$	1.30	2.72	4.13	5.28	1.30	2.60	4.70	7.00	1.00	2.65	4.00	5.00	0.60	2.55	4.60	7.00
ω_{pei} (GHz)	0.94	1.09	1.42	3.11	0.84	0.97	2.28	4.67	1.09	1.61	1.19	2.57	2.13	1.56	1.81	4.83
$\mu(cm^2/Vs)$	1097.53	307.31	285.36	5 131.70	945.29	378.12	189.06	68.53	235.69	235.69	282.83	188.55	1765.81	302.7	1 227.4	8 63.06
$\sigma_{(\Omega cm)^{-1}}$	35.1	13.3	21.0	46.4	22.7	12.1	33.3	50.4	9.43	20.7	13.6	42.2	254	23.2	28.9	46.4

*See Symbols Table.

The electron scattering time for ZnSe decreased when Y or Au layer existed between two ZnSe layers from 5 *fs* to 4 *fs* and 1 *fs*, respectively. The drift mobility 1097.53 cm^2/Vs for ZnSe decreased to 945.29 cm^2/Vs and 235.69 cm^2/Vs for ZnSe/Y/ZnSe and ZnSe/Au/ZnSe, respectively. The electron scattering time and drift mobility for ZnSe/YAu/ZnSe increased to 7 *fs* and 1765.81 cm^2/Vs , respectively, compared to those of ZnSe, ZnSe/Y/ZnSe and ZnSe/Au/ZnSe. This enhancement in the drift mobility of ZnSe was attributed to the high scattering time, and the carrier concentration variation associated with the amount of defects [88]. The two metals layers with different vacancies reduced the amount of defect which facilitated the movement of more free electrons. In scope of these observations, the improvement of μ for ZnSe/YAu/ZnSe may be due to reduced dislocation density as seen from XRD analysis. The resulting values agree with literature data of ZnSe, which shows that the drift mobility is up to 400 cm^2/Vs [20]. D. D. Nedeoglo et al. reports that for annealing ntype ZnSe enhanced the mobility form 7000 cm^2/Vs to 8000 cm^2/Vs at 77 K when adding donor imparities as Al and Ga [90].

In addition, the free electron density for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe are 2.00 x 10^{17} cm⁻³, 1.20×10^{17} cm⁻³, 2.50×10^{17} cm⁻³ and 9×10^{17} cm⁻³, respectively. The free electron density values suggest the consistency between the structural results and the dielectric analysis. Particularly, the decrease in the stress value upon YAu sandwiching is associated with more free electrons. Both result support the proposal hypotheses which indicate that the use of stacked layers improve the optical and dielectric performance of ZnSe. Moreover, the electron bounded plasma frequency ω_{pe} and the reduced resonance frequency ω_{e} increase for ZnSe/YAu/ZnSe sandwiched films and decreases for ZnSe/Y/ZnSe and ZnSe/Au/ZnSe. G. I. Rusu et al.

reported that the ZnSe has a donor concentration (N_D) of 3.67 × 10¹⁷ cm⁻³ which is consistent with the dielectric data that are shown in Table 4.3 [91].

As shown in Table 4.3, it is clear that YAu sandwiching improves the optical conduction parameters more than those of Y and Au sandwiching alone. This high value of the ZnSe/YAu/ZnSe mobility corresponds to the large scattering time values of 7*fs*, and so, less damping rate and less resistance. The high mobility of ZnSe/YAu/ZnSe makes it a batter candidate as a thin film transistor. It makes thin semiconductor more promising. In addition, it takes procedures to terahertz frequencies at femto-second electron scattering times [89, 92].

The free electron density *n*, reduced resonant frequency ω_e and the bounded Plasmon frequency ω_{pe} increased when the YAu sandwiching used. This increase corresponds to the presence of further free electrons on the metal surface [44].

The values of the electron bounded Plasmon frequency ω_{pe} for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe films are improved in the range of 0.94 – 4.83 x10⁹ Hz. The reduced resonance frequency ω_e is also increased from 1.30 x10¹⁵Hz to 7.00 x10¹⁵Hz. The interference of Plasmon frequency with the films reveals more information about the ac-signal or electromagnetic wave. For a gigahertz plasma frequency level, the microwave propagating through these films can be transmitted only if they have frequencies higher than ω_{pe} . Since the computed ω_{pe} values are in the range of 0.94 – 4.83 GHz, the ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe films can be employed as wave traps of at least four resonant frequencies which suit microwave communications [44, 71].

The dielectric functions of solids are interrelated to their optical conductivity, which is in fact the AC electrical conductivity in the presence of an alternating electric field. Therefore, the AC conductivity of metals is as important as the optical conductivity [93]. The optical conductivity $\sigma(\omega)$ can be evaluated from the relation ($\sigma(\omega) = \omega \varepsilon_{im}/4\pi$), where $\omega = 2\pi F$ is the angular frequency [94]. The optical conductivities of ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe are displayed in Fig. 4.15. It exhibits the same behavior as the imaginary dielectric spectra, and it increases with increasing incident photon frequency. In the low frequency region, ZnSe/YAu/ZnSe exhibits the highest conductivity compared to ZnSe/Au/ZnSe, ZnSe and ZnSe/Y/ZnSe.



Fig. 4.15: The optical conductivity $\sigma(\omega)$ as a function of incident photon frequency for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.

4.4: DC Measurements

The conductivity type was tested by the hot-probe technique, it revealed a n-type conduction for ZnSe sandwiched film. In addition, the technique displayed the same n-type conductivity for ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe probably due to selenide vacancies or excess zinc [95, 96]. In the ZnSe, the excess zinc which has a electron configuration $4s^23d^{10}$ [97] will give more two free electrons to the structure and causes the n-type conductivity. The Ohmic nature of the silver contacts to ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films was established by the current (I) - voltage (V) characteristic curves at room temperature which are displayed in Fig. 4.16.



Fig. 4.16: The current (I)-voltage (V) characteristic curve at 300 K for (a) ZnSe, ZnSe/Y/ZnSe and ZnSe/YAu/ZnSe at voltage rang of -100-100 V, (b) ZnSe/Au/ZnSe at voltage range of -0.5-0.5 V.

The resulting I-V curves exhibited a linear relationship for ZnSe, ZnSe/Y/ZnSe and ZnSe/YAu/ZnSe which are recorded in the voltage range of (-100-100 V). While, the ZnSe/Au/ZnSe was recorded in range of (-0.5-0.5 V) at 300 K due to instrumentation limitations the voltage range was limited.

The Ohmic nature of the contacts predominates when the work function of the metal is less than the work function of semiconductor of n-type $(q\phi_m < q\phi_{sm})$. This is expected for Ag $(q\phi_m = 4.45 \text{ eV})$ [98], which is less than ZnSe $(q\phi_{sm} = 4.84 \text{ eV})$ [20]. The linearity of the I-V plot at 300 K indicates an electrical conductivity of 1 × $10^{-4} (\Omega \text{ cm})^{-1}$. The temperature dependence of the conductivity for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe illustrated in Fig. 4.17 reveals a nonlinear relationship. The conductivity was increased with increasing the temperature from 300-460 K, further, it was illustrated that the conductivity obeys Arrhenius behavior demonstrating a semiconducting transport behavior [99].



Fig. 4.17: The variation of the conductivity with temperature for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.

In order to determine the current transport mechanism, the conductivity data in Fig. 4.17 were analyzed through plotting $\ln(\sigma)$ vs $10^3/T$ as shown in Fig. 4.18. The data was analyzed using the Arrhenius formula ($\sigma = \sigma_0 e^{(-E_a/kT)}$). In this formula, σ_0 is a parameter depending on the sample characteristics such as structure and thickness, k is Boltzmann's constant, T is absolute temperature and E_a is the thermal activation energy from the slope of $\ln(\sigma) - 10^3/T$ curve. The linear region in Fig. 4.18 indicates activation energies of 822.7, 776.2, 615.6 and 818.1 meV corresponding to ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films, respectively. The E_a values are less than $E_g/2$ for n-type semiconductor, so the activation energy is called a donor energy level E_d [91, 100]. In scope of these results, it is clear that the donor level is closer to the conduction band of the ZnSe when Y or Au are used. The

formation of the shallow donor level is due to increase the free carrier contribution which results from the energy levels overlapping between states of ZnSe and the respective metal. Particularly, as the electron configuration for Zn, Se, Y and Au are $4s^23d^{10}$ [97], $3d^{10}4s^24p^4$ [101], $4s^24p^64d^15s^2$ [102] and $4f^{14}5d^{10}6s^1$ [89], respectively, the *f*-orbitals for Au are at higher energy level compared with those of Zn, Se and Y, this causes much more bonding and the orbital's energy bands overlapping between the Au and ZnSe. So the electron will move more freely in the material.



Fig. 4.18: The logarithm of the conductivity with inverse temperature in rang of 300-460 K for ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe sandwiched films.

The large value of the activation energy assures that the observed energy gap in the spectral range of 2.2-1.1 eV during the optical analysis interbands is related to the band tails which cause the optical band transition. As the work function $(q\phi_b = q\chi + E_f)$

where $E_f = E_d/2$ and $q\chi$ are the Fermi energy and the electron affinity of the semiconductor, respectively [24]. The ZnSe, ZnSe/Y/ZnSe, ZnSe/Au/ZnSe and ZnSe/YAu/ZnSe work function are 4.21, 4.28, 4.11 and 4.21 eV, respectively. These values are less than the work function being 4.84 eV reported for ZnSe in literature [24].

The resulting value had shown a deep donor level for ZnSe which deceased when Y or Au existed between two ZnSe sandwiched films. However, it returned to increase near to ZnSe value when YAu alloy used. This value agreed with a result in other work for n-type ZnSe films in temperature range of 320-460 K. They reported that ZnSe film has activation energy of 0.67 eV [91]. Our results for E_d calculation indicate more deep level of donors compared to Hankare et al., which reported in there studied that the activation energy of ZnSe at high temperature was 0.610 eV. Also, they found that the conductivity was ranging between $1.375 \times 10^{-3} - 5.846 \times 10^{-8} (\Omega cm)^{-1}$ [103].

The analysis of the conductivity data indicates that the current transport mechanism is the thermionic emission of electrons over the potential barrier of semiconductor into the metal. In addition, the activation energy found to be greater than kT, so it was agreed with the thermionic emission assumption [24]. Moreover, Fig. 4.19 displayed the activation energy versus temperature and shown a constant variation with temperature, so the thermionic emission theory is valid.



Fig. 4.19: The variation of the donor energy level with temperature range of 360-460 K.

4.5: The Conductance Spectroscopy Analysis

The conductance spectra of the sandwiched films were recorded in the frequency range of (10 MHz - 1800 MHz) by Agilent 4291B 12F Impedance-Material Analyzer spectrometer. The ytterbium metal substrates films used to study the conductance spectra through depositing Au point in the top of the sandwiched films. The resulting conductance spectra of Yb/ZnSe/Au, Yb/ZnSe/Y/ZnSe/Au, Yb/ZnSe/Au/ZnSe/Au and Yb/ZnSe/YAu/ZnSe/Au sandwiched films were illustrated in Fig. 4.20. The Yb/ZnSe/Au interfaces displayed an increasing trend of conductance spectra below 200 MHz, it reached a maximum value of 0.03 Ω^{-1} . For Yb/ZnSe/Y/ZnSe/Au, the conductance exhibited a maximum of 0.06 Ω^{-1} at frequency of 150 MHz.



Fig. 4.20: The conductance (G) spectra in the frequency range of (0.01 GHz -1.8 GHz) for Yb/ZnSe/Au, Yb/ZnSe/Y/ZnSe/Au, Yb/ZnSe/Au/ZnSe/Au and Yb/ZnSe/YAu/ZnSe/Au sandwiched films.

The Yb/ZnSe/Au/ZnSe/Au device exhibited a maximum conductance value of 0.17 Ω^{-1} at frequency of 260 MHz. On the other hand, Yb/ZnSe/YAu/ZnSe/Au conductance spectra presented a maximum value of 0.08 Ω^{-1} at frequency of 390 MHz. Zhi Wang and others found that the un-doped n-type ZnSe has a conductance lower than 0.03 $p\Omega^{-1}$. However, they found that the Cl-doped ZnSe enhanced the conductance to 0.8 $n\Omega^{-1}$ and increased with increasing Cl doping [104]. Another study on p-type N-doped ZnSe nanobelts found that the conductance decreased with increasing the gate voltage, and the conductivity confirmed by field-effect transistor (FET) [105].

The conductance was modeled by the quantum mechanical tunneling (QMT) and correlated barrier hopping (CBH) conduction mechanisms, which be verified through the AC conductivity $\sigma_{ac}(\omega)$ spectral analysis. The frequency and temperature dependence of the AC conductivity $\sigma_{ac}(\omega)$ expressed in chapter two by equation (2.26). The frequency exponent *s* in equation (2.26) is the Jonscher's coefficient corresponds to the amount of interaction between the mobile ions and the lattice around them [49, 50].

In order to explain the behavior of the AC electrical conductivity, many models have proposed depending on the variation of Jonscher's coefficient value s with temperature. One of these models is the quantum mechanical tunneling (QMT) model is usually associated with a slightly increased in the value of s with temperature. On the other hand, the correlated barrier hopping (CBH) model is usually associated with a decrease in the value of s with temperature [49-54]. The quantum mechanical tunneling (QMT) model assumes tunneling of the charge carriers between two localized states near the Fermi level. For the correlated barrier hopping mechanism, the charge carrier hops from site to site over the potential barrier [49]. The slope for the experimental data of $\ln(\sigma_{ac}(\omega)) - \ln(\omega)$, where ω is the angular frequency, illustrated in Fig. 4.21 yields the value of Jonscher's coefficient *s* as 0.902, 0.135, 0.516 and 0.936 for Yb/ZnSe/Au, Yb/ZnSe/Y/ZnSe/Au, Yb/ZnSe/Au, Yb/ZnSe/Au, Yb/ZnSe/Au, Yb/ZnSe/Au, and Yb/ZnSe/YAu/ZnSe/Au sandwiched films, respectively. These values of *s* are tabulated in Table 4.4.



Fig. 4.21: The ln($\sigma_{ac}(\omega)$) – ln(ω) curves for (a) Yb/ZnSe/Au, (b) Yb/ZnSe/Y/ZnSe/Au, (c) Yb/ZnSe/Au/ZnSe/Au and (d) Yb/ZnSe/YAu/ZnSe/Au sandwiched films.

The temperature-dependent parameter *s* in the (CBH) model can be evaluated from the equation (2.49) in chapter 2. The maximum barrier height W_M at T = 300 k can be calculated by using equation (2.45) and substituting the experimental value of Jonscher's coefficient *s*. In addition, the hopping energy W_H in the (CBH) model is $(W_H = W_M/4)$ [54]. The values of W_M and W_H was presented in Table 4.4.

The experimental AC conductivity $\sigma_{ac}(\omega)$ which calculated from the measured conductance spectra is illustrated in Fig. 4.22. The Yb/ZnSe/Au exhibits a maximum AC conductivity $\sigma_{ac}(\omega)$ of about $4 \times 10^{-4} (\Omega cm)^{-1}$ which increased to $9 \times 10^{-4} (\Omega cm)^{-1}$ and to $12 \times 10^{-4} (\Omega cm)^{-1}$ for Yb/ZnSe/Y/ZnSe/Au and Yb/ZnSe/YAu/ZnSe/Au, respectively. On the other hand, as Fig. 4.22 shows, the Yb/ZnSe/Au/ZnSe/Au has a pronounced effect on the AC conductivity $\sigma_{ac}(\omega)$ with maximum value of $25 \times 10^{-4} (\Omega cm)^{-1}$ higher than other sandwiched films.

The fitting values of the AC conductivity $\sigma_{ac}(\omega)$ can be expressed as a two parallel conductances that dominate the conduction. To investigate the total conduction mechanism, we follow the approach which assumes that the charge carriers are scattered by two mechanisms with scattering time constant for the tunneling and hoping mechanism (τ_T and τ_H), respectively. In semiconductors, when a number of different mechanisms contribute to the carrier scattering time, the total mobility μ_{Total} is given by [106]:

$$\frac{1}{\mu_{\rm Total}} = \frac{1}{\mu_{\rm T}} + \frac{1}{\mu_{\rm H}}$$
(4.4)

Where, μ_T and μ_H are the mobility for the quantum mechanical tunneling (QMT) and correlated barrier hopping (CBH) model, respectively. Since $\sigma = ne\mu$, then:

$$\frac{1}{\sigma_{\rm ac}(\omega)} = \frac{1}{\sigma_{\rm T}(\omega)} + \frac{1}{\sigma_{\rm H}(\omega)}$$
(4.5)

Assuming the same number of free carrier in the material which are formed during the preparation process. At lower frequencies the quantum mechanical tunneling (QMT) model of $\sigma_{\rm T}(\omega)$ is more pronounced, correlated barrier hopping (CBH) model of $\sigma_{\rm H}(\omega)$ becomes significant at high frequency. The AC conductivity was found by using equations (2.30) and (2.47) in section two. A assuming that the values of phonon frequency v_{ph} and the decay parameter α in equation (2.30) are 1.5×10^{12} Hz and 10Å, respectively [54].

The fitting of experimental conductivities using equation (2.30) and (2.47), were presented the brown solid line in Fig. 4.22. The experimental AC conductivity $\sigma_{ac}(\omega)$ and the fitting curve of AC conductivity $\sigma_{ac}(\omega)$ with accordance to the (QMT) and (CBH) models are displayed in Fig. 4.22. The best fitting with the experimental conductivity found the values for the density of localized states at Fermi level $N(E_F)$, the conductivity at low frequency $\sigma_{ac}(L)$, the conductivity at high frequency $\sigma_{ac}(H)$ and the relaxation time τ for Yb/ZnSe/Au, Yb/ZnSe/Y/ZnSe/Au, Yb/ZnSe/Au/ZnSe/Au and Yb/ZnSe/YAu/ZnSe/Au sandwiched films are displayed in Table 4.4.



Fig. 4.22: The variation of AC conductivity in frequency range of (0.01 GHz -1.8 GHz) for Yb/ZnSe/Au, Yb/ZnSe/Y/ZnSe/Au, Yb/ZnSe/Au/ZnSe/Au and Yb/ZnSe/YAu/ZnSe/Au sandwiched films. The brown solid lines are the fitting of the conductivity with accordance to quantum mechanical tunneling (QMT) and correlated barrier hopping (CBH) model.

Table 4.4: The AC conductivity fitting parameters for the quantum mechanical tunneling (QMT) and the correlated barrier hopping (CBH) conduction mechanism for Yb/ZnSe/Au, Yb/ZnSe/Au, Yb/ZnSe/Au, Yb/ZnSe/Au, ZnSe/Au and Yb/ZnSe/YAu/ZnSe/Au sandwiched films at T 300 K.

	Yb/ZnSe/Au	Yb/ZnSe/Y/ZnSe/Au	Yb/ZnSe/Au/ZnSe/Au	Yb/ZnSe/YAu/ZnSe/Au
S	0.902	0.137	0.516	0.936
$W_M(\boldsymbol{eV})$	1.590	0.180	0.320	2.400
$W_H (\boldsymbol{eV})$	0.396	0.045	0.080	0.600
$N(E_f) \times 10^{19} \ (eV^{-1}cm^{-3})$	1.10	10.0	5.00	2.50
$\tau \times 10^{-9}$ (s)	5.00	1.00	1.30	1.50
$\sigma_{ac}(H) \times 10^{-3} (\Omega cm)^{-1}$	10	100	60	700
$\sigma_{ac}(L) \times 10^{-2} (\Omega cm)^{-1}$	40.0	9.20	36.0	24.0

*See Symbols Table.

Returning to the fitting parameters in Table 4.4, the Jonscher's coefficients, the maximum barrier height W_M , and the hoping energy W_H decreased for Yb/ZnSe/Y/ZnSe/Au and for Yb/ZnSe/Au/ZnSe/Au compared to Yb/ZnSe/Au. In addition, the Yb/ZnSe/YAu/ZnSe/Au device exhibits higher values of s, W_M , and W_H compared with other devices. As also shown in table 4.4, the relaxation time τ values for Yb/ZnSe/Y/ZnSe/Au, Yb/ZnSe/Au/ZnSe/Au and Yb/ZnSe/YAu/ZnSe/Au are smaller than that of Yb/ZnSe/Au. On the other hand, the density of localized states at Fermi level $N(E_F)$ for Yb/ZnSe/Y/ZnSe/Au, Yb/ZnSe/Au/ZnSe/Au and Yb/ZnSe/YAu/ZnSe/Au were greater than that of Yb/ZnSe/Au. The increase in the density of localized states near the Femi level indicate that the material become more appropriate for forcing current conduction by hopping which is very necessary for memory cell designs.

Chapter Five

Conclusions

In this thesis we have discussed the possibility of engineering the structural, optical, dielectric and electric properties of ZnSe thin films through the nanosandwiching of Y, Au and YAu metallic surfaces. The nanosandwiched layers with thickness of 70 nm each, successfully decreased the grain size by 25% upon Y or Au sandwiching and retain no change when YAu layer was used.

From the optical point of view, while the sandwiching with yttrium increased the absorbability by 1.4 times at 2.3 eV, the sandwiching with Au layer raised the absorbability to 1.9 times near 2.3 eV. The sandwiching with YAu layer enhanced the absorbability to \sim 2.4 times near 2.3 eV. On the other hand, the energy band gap did not exhibit significant shift with the nanosandwiching of Au, Y and YAu metals but a remarkable shift in the band tails was observed upon nanosandwiching. Particularly, while both of Y and Au widen the band tail from 0.99 to 1.14 and 2.07 for Y and Au nanosandwiching respectively, the YAu layer narrows the band tail width and raise it up toward the conduction band.

In addition to these observations, the real part of the dielectric spectra increased by 33% near 1.68 eV upon sandwiching with yttrium and by 67% near 1.71 eV upon Au sandwiching. The co-evaporation of Au into Y layer raised the dielectric constant by 44% near 1.65 eV. Furthermore, the modeling of the imaginary part of the dielectric spectra assuming the electron-plasmon coupling had shown that the scattering time significantly decreased via Au nanosandwiching and increased via YAu

nanosandwiching. Consistently, the free charge carriers density decreased upon Y nanosandwiching and increased upon Au and YAu sandwiching.

From electrical point of view, the alternating current conductivity exhibits much higher value for the YAu sandwiched films than those sandwiched with Y and with Au. The behavior of frequency dependent conductivity was ascribed to the domination of quantum mechanical tunneling conduction at low frequencies, and domination of correlated barrier hopping at high frequencies.

The work appears to be promising for use of the nanosandwiched ZnSe in optoelectronic technology as this way of engineering increased both of the absorbability of ZnSe and the dielectric constant without altering the energy band gaps. Meaning that, the material has formed band tails in the band gap without overlapping with the conduction or valence bands. The band tail provides a supporting step for the generated electron-hole pair transport from the valence band to the conduction band. In addition, the domination of the current conduction by tunneling moves the use of ZnSe for fabricating tunnelled barriers highly attractive.

References

[1] Pradip Kr. Kalita et al. Structural characterization of vacuum evaporated ZnSe thin films, *Bull. Mater. Sci.*, **23**, 2000, P. 313–317.

[2] E. R. Shaabanb et al. Structure Analysis and Optical Parameters of Nano-scale ZnSe/Flexible Substrate Thin Film, *Journal of Electronic Materials*, **46**, 2017, P. 527–534.

[3] G.M. Lohar et al. Studies of properties of Fe3+ doped ZnSe nanoparticles and hollow spheres for photoelectrochemical cell application, *Journal of Alloys and Compounds*, **653**, 2015, P. 22-31.

[4] Tan Yu & Wang Yan-Guo, Elimination of the Schottky Barrier at an Au-ZnSe Nanowire Nanocontact via in Situ Joule Heating, *Chinese Physics Letters*, **30**, 2013.

[5] C.M.Collier and J.F.Holzman, Ultrafast photoconductivity of crystalline, polycrystalline, and nanocomposite ZnSe material systems for terahertz applications, *Appl.Phys.Lett*, **104**, 2014, 042101.

[6] C. Bothe et al. Solid-State Chemistry on the Nanoscale: Ion Transport through Interstitial Sites or Vacancies, Wiley Online Library, 2015.

[7] Kai Ou et al. Structural, morphological and optical properties of ZnO films by thermal oxidation of ZnSe films, *Thin Solid Films*, **634**, 2017, P. 51–55

[8] Priyadharsini N. el al. Effect of temperature and pH on structural, optical and electrical properties of Ni doped ZnSe nanoparticles, *Optik*, **127**, 2016, P. 7543–7549.

[9] D. A. Gaul, W. S. Rees Jr, True Blue Inorganic Optoelectronic Devices, *Advanced Materials*, **12**, 2000, P. 935–946.

[10] M. J. Kim et al. Synthesis of Er and Yb-doped cubic and hexagonal phase ZnSe nano-assembled microspheres and their photocatalytic activities, *Ceramics International*, **40**, 2014, P. 16051–16059.

[11] M. Molaei et al. Synthesis of ZnSe nanocrystals (NCs) using a rapid microwave irradiation method and investigation of the effect of copper (Cu) doping on the optical properties, *Applied Surface Science*, **317**, 2014, P. 236–240.

[12] Wolfgang Pfeiler, *Alloy Physics: A Comprehensive Reference*, WILEY-VCH Verlag GmbH &Co.KGaA. Weinheim, 2007, P.1.

[13] M. R. Steel and D M Treherne, Optical properties and electronic structure of AuMn and AgMn alloy systems, *Journal of Physics F: Metal Physics*, **2**, 1972, P.199.

[14] S. Link, Z. L. Wang, and M. A. El-Sayed, Alloy Formation of Gold-Silver Nanoparticles and the Dependence of the Plasmon Absorption on Their Composition, *J. Phys. Chem. B*, **103**, 1999, P. 3529-3533.

[15] Abdelhak Dhibi, Mehdi Khemiri and Mohamed Oumezzine, Theoretical study of surface plasmons coupling in transition metallic alloy 2D binary grating, *Physica E*, **79**, 2016, P. 160–166.

[16] Melissa Strehle, x-ray Photoelectron Spectroscopy (XPS) Study of Single Crystal UO_2 and U_3O_8 on R-Plane Sapphire and Yttrium Stabilized Zirconium (YSZ) Substrates, University of Illinois at Urbana-Champaign, 2011, P.6-10.

[17] Kerry Simmance, *The Design and Understanding of the Mechanism of Formation of Nanoporous Catalytic Materials*, University College London, Britain, 2011, P.63-80.

[18] James D. Rachwal, x-ray diffraction applications in thin films and (100) silicon substrate stress analysis, University of South Florida, 2010, P.9-11.

[19] Albin Linder, x-ray *diffraction studies on complex metal oxides*, Lund University, 2015, P.2-8.

[20] Otfried Madelung, *Semiconductor: Data Handbook*, 3rd Ed, Springer, NewYork, 2004.

[21] Kaur N et al. A Review on Zinc Sulphide Nanoparticles: From Synthesis, Properties to Applications. *J Bioelectron Nanotechnol*, 1, 2016, P. 5

[22] D. R. Vij & N. Singh, Luminescence and Related Properties of II-VI Semiconductors, Nova Publishers, USA, 1998. P. 210.

[23] Amandeep Singh Wadhwa & Harvinder Singh Dhaliwal, A Textbook of Engineering Material and Metallurgy, University of science Press, India, 2008, P.87

[24] Sze. Simon M. & Kwok K. Ng. *Physics of semiconductor devices*. John wiley & sons, 2006, P.57.

[25] W. F. Smith & J. Hashemi, *Foundations of Materials Science and Engineering*, McGraw-Hill, Technology & Engineering, 5th Ed, 2009

[26] R. Askeland et al, *The Science & Engineering of Materials*, Cengage Learning, USA, 6th Ed, 2011.

[27] Francisco Tiago Leita^o Muniz et al, The Scherrer equation and the dynamical theory of x-ray diffraction, *Acta Cryst*, **A72**, 2016.

[28] By R. Saravanan & M. Prema Ran, *Metal and Alloy Bonding - An Experimental Analysis: Charge Density in Metals*, Springer Science & Business Media, New York, 2012, P. 26.

[29] Challa SSR Kumar, x-ray and Neutron Techniques for Nanomaterials Characterization, Springer Berlin Heidelberg, 2015.

[30] Carl Koch et al. *Structural Nanocrystalline Materials: Fundamentals and Applications*, Cambridge, New York. 2007, p.95.

[31] Ahmad Monshi et al. Modified Scherrer Equation to Estimate More Accurately Nano-Crystallite Size Using XRD, *World Journal of Nano Science and Engineering*, **2**, 2012, 154-160.

[32] P.P. Simeonova et al. *Nanotechnology - Toxicological Issues and Environmental Safety*, Springer, 2007, P.232.

[33] R. Bhargava, *Properties of Wide Bandgap II–VI*, Semiconductors Inspection, London, 1997, P.3-17.

[34] I. Ursu et al, Damage Studies in Cubic ZnSe Single Crystals Grown from Melt, *Appl. Phys. A*, **48**, 1989, P.451-456.

[35] A. Omar et al. Temperature effects on the structural and optical properties of the TIInSe_{2x}S_{2(1_x)} mixed crystals (x= 0.3), *Journal of Alloys and Compounds*, **724**, 2017, P.98-102.

[36] Mark Fox, Quantum Optics An Introduction, Oxford University Press, United States, 2006, P.60-80.

[37] Richard J. D. Tilley, *Colour and the Optical Properties of Materials*, 2nd Ed, John Wiley & Sons, UK, 2011, P.36.

[38] G. Martinez, *Optical Properties of Semiconductors*, Springer Science & Business Media,

[39] U. I. Gaya, *Heterogeneous Photocatalysis Using Inorganic Semiconductor Solids*, Springer, New York, 2014, p.17-19.

[40] Yu Liang, Ultrafast Dynamics of Metalloporphyrins, DNA and Iron-Lanthanide Clusters in the liquid phase, KIT Scientific Publishing, 2013, p.110-114.

[41] Mark Fox, *Optical Properties of Solids*, 2nd Ed, Oxford University Press, United States, 2010, P.30-150.

[42] Haeng Kon Kim et al. *IAENG Transactions on Engineering Technologies*, Springer Science & Business Media, New York, P.40-50.

[43] S. R. Alharbi & A. F. Qasrawi, Dielectric Dispersion in Ga2S3 Thin Films, *Plasmonics*, **12**, 2017, P.1045–1049.

[44] Olfat A. Omareya et al. Effect of Au nanosandwiching on the structural, optical and dielectric properties of the as grown and annealed InSe thin films, *Physica B*, **520**, 2017, P.57–64.

[45] Mark Fox, Quantum Optics An Introduction, Oxford University Press, United States, 2002, P.60-80.

[46] R. Matias et al, Fiber *Optic Sensors: Current Status and Future Possibilities*, Springer, Switzerland, 2017, P.43.

[47] Takashi Yanagisaw et al, Optical properties of unconventional superconductors, *Nova Science Publishers*, **183**, 2006, P. 1-35.

[48] Hari Singh Nalwa, *Handbook of Advanced Electronic and Photonic Materials*, Academic Press, volume 8, UK, 2001, P. 50-80.

[49] Sunita Sharma, M. M. Singh & K. D. Mandal, "Dielectric and Electrical Properties of Undoped Fe-Doped Yttrium Copper Titanate", *Ceramic Transactions*, **252**, 2015, P.95-105

[50] Bill Lee, Rainer Gadow & Vojislav Mitic, *Proceedings of the IV Advanced Ceramics and Applications Conference*, Atlantis Press, 2017, P.164-166.

[51] Aswini Ghosh, Frequency-dependent conductivity in bismuth-vanadate glassy semiconductors, *Physical Review B*, **41**, 1990.

[52] Sevi Murugavel & Manisha Upadhyay, A.C. Conduction in Amorphous Semiconductors, *Journal of the Indian Institute of Science*, **91**, 2011, P. 303-317.

[53] S. R. Elliott, A theory of ac conduction in chalcogenide glasses, *Philosophical Magazine*, **36**, 1977, P. 1291-1304.

[54] A.A.A. Darwish et al. AC electrical conductivity and dielectric studies on evaporated nanostructured InSe thin films, *Journal of Alloys and Compounds*, **586**, 2014, P.142–147.

[55] D.D. Sarma et al. Advances in Amorphous Semiconductors, Taylor & Francis, USA, 2003.

[56] Supriyo Datta, Lessons from Nanoelectronics: A New Perspective on Transport, World Scientific, USA, 2012.

[57] M. J. Sailor, *Porous Silicon in Practices: Preparation, Characterization and Applications*, WILEY-VCH, 2012.

[58] S. E. Al Garni, CHARACTERIZATION OF THE Au/ZnSe/In/ZnSe/C (ZIZ) BACK TO BACK SCHOTTKY BARRIERS, *Chalcogenide Letters*, **14**, 2017, P. 545 – 550.

[59] M.Maczka, P.Pasierb, *Synthesis and properties of barium modified yttrium borate*, Materials Research Bulletin, March 2017, P. 84-91

[60] QiuhuaYuan et al. One-pot synthesis and characterization of Zn-doped hydroxyapatite nanocomposites, *Materials Chemistry and Physics*, **199**, 2017, P. 122-130

[61] Dimitris A. Papaconstantopoulos, *Handbook of the Band Structure of Elemental* Solids: From Z = 1 To Z = 112, 2nd Ed, Springer, USA, 2015

[62] A. P. Hagen, Inorganic Reactions and Methods, John Wiley & Sons, USA, 2009.

[63] John P. Dakin & Robert G. W. Brown, *Handbook of Optoelectronics Volume 1*, CRC Press, USA, 2006.

[64] Dojalisa Sahu et al. Enhanced UV absorbance and photoluminescence properties of ultrasound assisted synthesized gold doped ZnO nanorods, *Optical Materials*, **36**, 2014, P. 1402-1407.

[65] Harald Ibach & Hans Luth, *Solid state physics: An Introduction to principles and material science*, 4th Ed, Springer-Velag Berlin Heideberg, 2009, P.155-534.

[66] G. Bums & M. Glazer, *Space group for solid state scientists*, 3rd Ed, Elsevier, China, 2013, P.337-358.

[67] P. Mallikarjuna et al, Structural, Optical and Magnetic Properties of Co-doped ZnSe Powders, *Materials Science & Engineering*, **9**, 2017 – ISSN 2412-5954.

[68] T. Rajesh Kumar et al, Optical, magnetic, and photoelectrochemical properties of electrochemically deposited Eu3+-doped ZnSe thin films, *Ionics*, **23**, 2017, P. 2497–2507.

[69] P.Prathap, Preparation and characterization of transparent conducting ZnS:Al films, *Solid State Sciences*, **11**, 2009, P. 224-232.

[70] V. Srikant and D. R. Clarke, On the optical band gap of zinc oxide, *J. Appl. Phys.* 83, 1998, P. 5446-5451.

[71] S.R. Alharbi & A.F. Qasrawi, Effect of ytterbium, gold and aluminum transparent metallic substrates on the performance of the Ga2S3 thin film devices, *Current Applied Physics*, **17**, 2017, P.835-841.

[72] S. M. El-Bashir et al. Designing of PVA/Rose Bengal long-pass optical window applications, *Results in Physics*, **7**, 2017, P. 1238-1244.

[73] Gulşen Akın Evingur, Onder Pekcan, Optical energy band gap of PAAm-GO composites, *Composite Structures*, **183**, 2018, P. 212-215

[74] M.A. Islam et al. Comparison of Structural and Optical Properties of CdS Thin Films Grown by CSVT, *CBD and Sputtering Techniques Energy Procedia*, **33**, 2013, P. 203 – 213.

[75] Y. Zhao et al, Photothermal effect on Fe3O4 nanoparticles irradiated by white-light for energy-efficient window applications, *Solar Energy Materials & Solar Cells*, **161**, 2017, P.247–254.

[76] M. Lang et al. Influence of the Cu Content in Cu₂ZnSn(S,Se)₄ solar cell absorbers on order-disorder related band gap changes, *Appl. Phys. Lett.* **109**, 2016. id.142103

[77] Najla M. Khusayfan et al, Design and performance of Yb/ZnS/C Schottky barriers, *Current Applied Physics*, **17**, 2017, P.115-119.

[78] M.M. Ivashchenko et al. Optical Properties of Pure and Eu Doped ZnSe Films Deposited by CSVS Technique, *JOURNAL OF NANO- AND ELECTRONIC PHYSICS*, **9**, 2017.

[79] T. Yao et al. Chemical synthesis, structural characterization, optical properties, and photocatalytic activity of ultrathin ZnSe nanorods, *Chemistry*, **71**, 2011, P. 8663–8670.

[80] M. Harb et al. Anionic or Cationic S-Doping in Bulk Anatase TiO_2 : Insights on Optical Absorption from First Principles Calculations, J. Phys. Chem. C, **117**, 2013, P. 8892–8902.

[81] Zhong-Hua Da et al. Effects of P, As, and Sb heavy doping on band gap narrowing of germanium as light-emitting materials, arXiv preprint arXiv:1706.04050, 2017.

[82] S. Aleiferis et al. Experimental study of H atom recombination on different surfaces in relation to H– negative ion production, *AIP Conference Proceedings*, **1869**, 2017.

[83] Charles Opoku et al, Source-Gated Transistors Based on Solution Processed Silicon Nanowires for Low Power Applications, *Advanced Electronic Materials*, **3**, 2017, 1600256.

[84] Mohamed Eldlio, Franklin Che, & Michael Cada, *Drude-Lorentz Model of Semiconductor Optical Plasmons*, IAENG Transactions on Engineering Technologies, Springer, 2014. P.41-49.

[85] Siti Nur Farhana M. Nasir et al. New Insights into Se/BiVO4 Heterostructure for Photoelectrochemical Water Splitting: A Combined Experimental and DFT Study, *J. Phys. Chem. C*, **121** (11), 2017, P.6218–6228.

[86] Walid A. Hadi et al. Steady-state and transient electron transport within the wide energy gap compound semiconductors gallium nitride and zinc oxide: an updated and critical review, *Journal of Materials Science Materials in Electronics (J Mater Sci: Mater Electron)*, **25**, 2014, P.4675–4713.

[87] M. Aven et al. Some Electrical and Optical Properties of ZnSe, *Journal of Applied Physics*, **32**, 1961, online 2004.

[88] Tamara Y. Abed et al. Investigation of the physical properties of the Yb nanosandwiched CdS films, *Journal of Alloys and Compounds*, **731**, 2018, P. 1022-1028.

[89] S.R. Alharbi & A.F. Qasrawi, Plasmon-electron dynamics at the Au/InSe and Y/InSe interfaces designed as dual gigahertz-terahertz filters, *Optik*, **136**, 2017, P.524–530.

[90] D. D. Nedeoglo et al. The effect of thermal treatment and doping on the electrical properties of zinc selenide, *Applications and materials science*, **42**, 1977, P. 675–679.

[91] G.I. Rusu et al, On the electronic transport properties of polycrystalline ZnSe films, *Applied Surface Science*, **218**, 2003, P.222–230.
[92] Po-Hsun Ho et al. High-Mobility InSe Transistors: The Role of Surface Oxides, *ACS Nano*, **11**, 2017, P. 7362–7370.

[93] Fuxiang Han, A Modern Course in the Quantum Theory of solids, Word Scientific Publishing Co. Pte. Ltd. Singapore, 2013, P.499-530.

[94] S. R. Alharbi & A. F. Qasrawi, Optical and electrical performance of Yb/InSe interface, *Materials Science in Semiconductor Processing*, **43**, 2016, P.60–64.

[95] Suresh Sagadevan & Isha Das, Chemical bath deposition (CBD) of zinc selenide (ZnSe) thin films and characterization, *Journal Australian Journal of Mechanical Engineering*, **15**, 2017, P. 222-227.

[96] Lipeng Hou et al. Bound Magnetic Polaron in Zn-rich Cobalt-Doped ZnSe Nanowires, *Nanotechnology*, 2017.

[97] Daniel Fritsch et al. Self-Consistent Hybrid Functional Calculations: Implications for Structural, Electronic, and Optical Properties of Oxide Semiconductors, *Nanoscale Research Letters*, **12**, 2017

[98] S. Karkare et al. A One-Step Model of Photoemission from Single Crystal Surfaces, *Physical Review B*, **95**, 2017.

[99] Vikas Patil et al. Effect of Annealing on Structural, Morphological, Electrical and Optical Studies of Nickel Oxide Thin Films, *Journal of Surface Engineered Materials and Advanced Technology*, **1**, 2011, P.35-41.

[100] S.R. Alharbi & A.F. Qasrawi, Structural, optical and electrical properties of YbInSe thin films, *Thin Solid Films*, **616**, 2016, P.808–814.

[101] Kaike Yang et al. Phonon-Driven Electron Scattering and Magnetothermoelectric Effect in Two-Dimensional Tin Selenide, arXiv preprint arXiv:1707.02737 (2017).

[102]Lin Hao et al. First principles study of c-axis strain effect on the magnetic structure and ferroelectricity in double perovskite Y2MnCrO6, *Journal of Alloys and Compounds*, **695**, 2017, Pages 1362-1367

[103] P. P. Hankare et al. Effect of thermal annealing on properties of zinc selenide thin films deposited by chemical bath deposition, *J Mater Sci: Mater Electron*, **20**, 2009, P.374–379

[104] Z. Wang et al. Chlorine-Doped ZnSe Nanoribbons with Tunable n-Type Conductivity as High-Gain and Flexible Blue/UV Photodetectors, *Chem. Plus. Chem*, **77**, 2012, P.470-475.

[105] Qing Su et al. Synthesis and optoelectronic properties of p-type nitrogen doped ZnSe nanobelts, *Materials Letters*, **92**, 2013, P.338-341.

[106] Dieter K. Schroder, *Semiconductor Material and Device Characterization*, John Wiley & Sons, 3rd Ed, USA, 2006, P. 450-480.

List of publications

- A.F Qasrawi, M.F Taleb, Effect of Au nanosandwiching on the optical properties of ZnSe. Under constriction.
- A.F Qasrawi, M.F Taleb, Dielectric dispersion in ZnSe nanosandwiching with YAu stacked metals. Under constriction.

Conferences

- Maram F. Taleb, S. R. Alharbi, A.F Qasrawi, Optical interactions at the ZnSenanolayers surface(poster), Fifth Palestinian Conference on Modern Trends in Mathematics and Physics, Arab American university-Jenin.
- Maram F. Taleb, Z. Saleh, A.F Qasrawi, Photo-illumination effects on the current voltage characteristics of Ga₂SeS photodiodes (Poster), Second Palestinian International Conference On Material Science and Nanotechnology, An-Najah National University- Nablus.

هندسة الخصائص الضوئية و معاملات التوصيل الكهربائي لرقائق الزنك سالنيد المزروعة بسبائك YAu

الملخص