SYNTHESIS OF GAMMA AND THETA ALUMINA PHASES COMPLEMENTED WITH FIRST PRINCIPLE CALCULATION

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A thesis submitted in fulfilment of the

requirements for the award of the degree of

Doctor of Philosophy (Physics)

Faculty of Science

Universiti Teknologi Malaysia

MARCH 2017

To the family that made me and to the family that I am to make.

ACKNOWLEDGEMENT

First and foremost I would like to express my deep gratitude and thanks to Allah, who gave me this grace to accomplish this work. I have realized how much Allah helped me during this time and all the time of my life, and I could never have done this work without Allah's willing.

I would like to thank my academic advisor, mentor, and friend during my studies at Universiti Teknologi Malaysia, Prof. Dr. Zulkafli Bin Othaman and Dr. Mohammad Alam Saeed. Their constant enthusiasm, encouragement, patience and optimism have always motivate me; their extraordinary ability to guide students in the right direction always benefited me. Whenever I had trouble with my research or personal issues, they were always there helping me. I cannot thank them enough. Allah will bless you with good health and long life.

I would like to extend my gratitude to the Ministry of Higher Education and Scientific Research (MOHESR) of Iraq for providing the scholarship during my study. Not forgetting also the Ministry of Higher Education of Malaysia and Universiti Teknologi Malaysia (UTM) for providing the necessary facilities from the preparation until this work is completed. I would also specifically like to thank members of the Center for Sustainable Nanomaterials and Physics Department, UTM for their technical supports, helps and assistance.

Words are not enough to express my feelings and sincere gratitude to my affectionate parents, brother and sisters for their unflinching love, and their presence surely made a positive impact in my life and was a constant source of moral support.

It was also all of you who originally triggered my passion for study in science. I would like to say: thank you again my mother, and may Allah bless all of you with good health and long life. I am indebted to them and my father for my successes in this regard.

From the bottom of my heart, I would like to extend my deepest thanks to my loving wife, for support, love, advice, and inspiration I have gotten from her over the years; and her believe in me that has helped to give me the strength and resolve that I needed to produce this work; and she gave me full support even during the time of the severe illness "pregnancy". She prefers to be by my side far from her family's home. I am really proud and grateful for her understanding and patience during those times. Thank you, my love, your love and prayers have been the main source of my successes in life and particularly in obtaining my PhD. May Allah bless you with good health and long life.

Also, my deep thanks go to my daughter and my son, who missed out on a lot of Daddy’s time, while I pursued my research these three past years. Thank you, my kids, for your patience, and I love you more than you will ever know.

My sincere appreciation also extends to all my dear ones who have the prayer for me at various tough times. Unfortunately, it is not possible to list all of them in this limited space. I am grateful to all my family members.

ABSTRACT

The synthesis of aluminium oxide (alumina) Al_2O_3 nanopowders has attracted much attention because of its high specific surface area and a large number of defects in its crystalline structure, which make it widely applicable in ceramic applications. In this study, co-precipitation technique was used to synthesize single-phase alumina nanopowders under various annealing temperatures. The crystalline phase, purity, morphology, chemical bonds and optical properties of the prepared powders were characterized by different spectroscopy techniques. To realize a real understanding of phenomena regarding nanoparticles growth, the material on an atomic scale must be studied. In this case, electronic and optical properties of the alumina at atomic scale have also been studied by the first principles within the framework of density functional theory (DFT). The computational approach is based on a full-potential linearized augmented plane wave method (FP-LAPW) within the generalized gradient approximation (GGA), local density approximation (LDA), and modified Becke–Johnson (mBJ) potential. The experimental results show the direct phase transitional behavior of γ-Al_2O_3 into θ-Al_2O_3 at annealing temperature of 900ºC. X-ray diffraction (XRD) and Brunauer–Emmett–Teller analysis confirm the existence of alumina nanopowders with particle diameters of < 5 nm, which also can be classified as ultrafine powder. The surface areas of prepared nanopowders were 366.67 m^2/g (200ºC) and 100 m^2/g (900ºC) for γ-Al_2O_3 and θ-Al_2O_3, respectively. The optical results indicate that γ-Al_2O_3 possesses a lower band gap (5.5 eV), compared to the θ-Al_2O_3 (5.8 eV). Theoretical results show that these compounds have a direct band gap (Γ-Γ) of 5.375 eV and 4.716 eV for γ-Al_2O_3 and θ-Al_2O_3, respectively. Several optical parameters of these materials were also investigated. The values of the real part of dielectric constant $\varepsilon_1(5)$ are found to be 3.259 and 3.694 for γ-Al_2O_3 and θ-Al_2O_3, respectively, while the refractive indices $n(5)$ are found to be 1.806 for γ-Al_2O_3 and 1.922 for θ-Al_2O_3. These GGA findings are consistent with the experimental results and are better than the other approximations. There are no salient differences between GGA and LDA results. The present results advocate the use of this material as transparent conducting layer in solar cell structure, which can be operated in a wide energy range.

ABSTRAK

Sintesis serbuknano aluminium oksida (alumina) Al_2O_3 telah menarik banyak perhatian kerana keluasan permukaan tertentu yang tinggi dan banyak kecacatan di dalam struktur kristal, menyebabkan ia digunakan dengan meluas dalam aplikasi seramik. Dalam kajian ini, teknik ko-pemendakan telah digunakan untuk mensintesis serbuknano alumina fasa tunggal di bawah pelbagai suhu sepuh lindap. Fasa kristal, ketulenan, morfologi, ikatan kimia dan sifat optik bagi serbuk yang disediakan telah dicirikan dengan pelbagai teknik spektroskopi. Bagi mendapatkan pemahaman sebenar tentang fenomena pertumbuhan nanopartikel, bahan pada skala atom perlu dikaji. Dalam hal ini, sifat elektronik dan optik alumina pada skala atom telah juga dikaji dengan prinsip pertama dalam rangka teori fungsi ketumpatan (DFT). Pendekatan komputeran adalah berdasarkan kaedah gelombang satah penuh berpotensi dilelurus dan diperkukuhkan (FP-LAPW) dalam penghampiran kecerunan umum (GGA), penghampiran kepadatan tempatan (LDA), dan keupayaan Becke-Johnson (mBJ) yang diubahsuai. Keputusan eksperimen menunjukkan transisi fasa terus γ-Al_2O_3 kepada θ-Al_2O_3 pada suhu sepuh lindap 900ºC. Pembelauan sinar-X (XRD) dan analisis Brunauer-Emmett-Teller mengesahkan kehadiran serbuknano alumina dengan diameter zarah < 5 nm, yang juga boleh dikelasifikasikan sebagai serbuk ultra-halus. Luas permukaan serbuknano yang di sediakan masing-masing adalah 366.67 m^2/g (200ºC) dan 100 m^2/g (900ºC) untuk γ-Al_2O_3 dan θ-Al_2O_3. Keputusan optik menunjukkan bahawa γ-Al_2O_3 mempunyai jurang jalur yang lebih rendah (5.5 eV), berbanding θ-Al_2O_3 (5.8 eV). Keputusan teori menunjukkan bahawa sebatian-sebatian ini mempunyai jurang jalur langsung (Γ-Γ) masing-masing adalah 5.375 eV dan 4.716 eV untuk γ-Al_2O_3 dan θ-Al_2O_3. Beberapa parameter optik bahan-bahan ini juga telah dikaji. Nilai bahagian nyata pemalar dielektrik $\varepsilon_1(5)$ masing-masing adalah 3.259 dan 3.694 untuk γ-Al_2O_3 dan θ-Al_2O_3, manakala nilai indeks biasan n (5) adalah 1.806 untuk γ-Al_2O_3 dan 1.922 untuk θ-Al_2O_3. Penemuan GGA ini adalah selaras dengan keputusan eksperimen dan adalah lebih baik daripada penghampiran lain. Tiada perbezaan yang ketara antara keputusan GGA dan LDA. Keputusan ini menyokong penggunaan bahan ini sebagai lapisan pengalir telus dalam struktur sel solar, yang boleh dikendalikan dalam julat tenaga yang luas.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

Nps	-	Nanopowders
DFT	-	Density Functional Theory
fcc	-	Face Centre Cubic
hcp	-	Hexagonal Close-Packed
XRD	-	X-ray Diffraction
FESEM	-	Field Emission Scanning Electron Microscopy
EDX	-	Energy Dispersive X-ray
XPS	-	X-ray Photoelectron Spectroscopy
BET	-	Brunauer–Emmett–Teller
FTIR	-	Fourier Transform Infrared
UV-Vis	-	Ultraviolet-Visible
FP-LAPW	-	Full Potential Linearised Augmented Plane Wave
LDA	-	Local Density Approximation
GGA	-	Generalized Gradient Approximation
mBJ	-	Modified Becke-Johnson
AACH	-	Ammonium Aluminium Carbonate Hydroxide
HF	-	Hartree Fock
CASTEP	-	Cambridge Serial Total Energy Package
VASP	-	Vienna *AB initio* Simulation Program
APW	-	Augmented Plane Wave
LAPW	-	Linearised Augmented Plane Wave
FWHM	-	Full Width at Half Maximum
HK	-	Hohenberg-Kohn
KS	-	Kohn-Sham
SCF	-	Self Consistent Field
LSDA	-	Local Spin Density Approximation
OEP	-	Optimized Effective Potential

GGA/LDA+U	-	Hubbard Corrected Energy Functional
BJ	-	Becke-Johnson
BR	-	Becke-Roussel
IR	-	Interstitial Region
MT	-	Muffin Tin
APW+lo	-	Augmented Plane Wave Plus Local Orbital
DOS	-	Density of States
No.	-	Number
BE	-	Binding Energy
2D	-	2 Dimensions

LIST OF SYMBOLS

a, b, and c	-	Lattice parameters
d_{hkl}	-	Interplanar distance
β_{hkl}	-	Full width at half maximum
S_{BET}	-	BET surface area
ρ	-	Theoretical density
AP	-	Auger parameter
KE	-	Kinetic energy
BE	-	Core-level binding energy
E_g	-	Energy band gap
F(R)	-	Kubelka-Munk function
R	-	Fractional reflectance
e and *m*	-	Electron charge and mass, respectively.
$\boldsymbol{E_F}$	-	Fermi level
$\varepsilon_1(\omega)$	-	Real part of the dielectric function
$\varepsilon_2(\omega)$	-	Imaginary part of the dielectric function
$R(\omega)$	-	Reflectivity
$n(\omega)$	-	Refractive index
$k(\omega)$	-	Extinction coefficient
$\alpha(\omega)$	-	Absorption coefficient
$\sigma(\omega)$	-	Optical conductivity

LIST OF APPENDICES

CHAPTER 1

INTRODUCTION

1.1 Background of Study

According to Drexler *et al.* (1991), the term nanotechnology means controlling the process based on molecule-by-molecule to the control of product using high precision systems. Since then, the nanotechnology term is basically used for any materials or devices, which are structured on the nanometer scale. Today, nanotechnology turned out to be a multidisciplinary science including but not limited to chemistry, biology, engineering and materials science and solid state physics.

Ceramic is another type of inorganic and non-metallic materials, which have been produced centuries ago. These materials are avaiable in bulk as well as in nanosize. The earliest ceramic compounds were made from naturally raw materials. However, it was found that natural minerals could be refined or doped to achieve required properties. Also, there is so-called composite material, which is a mixture of two or more materials that insoluble in one another, and it possesses properties eminent of any of the component materials. If the composite includes at least one material which has nanoparticles size less than 100 nm then it is named nanocomposite (Seal *et al.,* 2004; Camargo *et al.,* 2009). Kamigaito (1991) reported that the changes in material properties could be observed when nanoparticle size is less than a particular level, which is called the critical size, as follow:

I. Less than 5 nm, which makes expected changes in catalytic activities.
II. Less than 20 nm, which makes hard magnetic materials.

III. Less than 50 nm, which makes expected changes in refractive index.
IV. Less than 100 nm, which makes expected to achieve super magnetism.
V. Less than 100 nm, which makes expected changes in mechanical strengthening or restricting matrix dislocation movement.
VI. Less than 100 nm, which makes expected changes in producing toughening.
VII. Less than 100 nm, which makes expected changes in modifying hardness and plasticity.

The ceramics with grain diameter less than 100 nm known as nanocrystalline ceramics are attracting more attention in recent years, due to their unique properties and the broad diversity of utilization. Therefore, there is growing interest in the nanostructural routes to develop their synthetic pathways (Woodfield *et al.*, 2008; Kanazirev, 2010; Corr, 2013). Fang *et al.* (2016) have observed that using sol-gel method is better than the conventional solid-state reaction method for synthesizing $(K_{0.16}Na_{0.84})_{0.5}Bi_{4.5}Ti_4O_{15}$ (KNBT) nanoparticles powder, also known as nanopowders (Nps). They found an increase in Curie temperature, and a decrease in resistivity from 10^8 Ωcm to 10^7 Ωcm at 500 °C of KNBT ceramic with reducing grain size. Furthermore, measurements of the magnetization for GaMnN ceramics showed a typical paramagnetic behavior of Nps with grain size distributions in the range of 2-60 nm (Gosk *et al.*, 2016).

Synthesis of single metal oxide Nps has attracted much interest compared to other ceramic materials due to their unique electronic, thermal and mechanical properties, which make it the basis for the structural materials of mechanical parts and functional materials for many electrical parts. One such material is aluminium oxide, also called alumina with the chemical formula Al_2O_3. It has been widely used in ceramic applications depending on its high specific surface areas and large number of defects in its crystalline structure, such as microporous catalysts, ultra-hard coatings, in electroluminescent flat-screen displays (Doremus, 2008), and as nanostructured fillers for ceramic matrix composite materials (Vahtrus *et al.*, 2015). Many survey also reported alumina as a main element in ceramic matrix nanocomposites (Camargo, *et al.*, 2009; Koli *et al.*, 2014).

Currently, great challenges and opportunities in the industry of solar cells are mainly focused on incorporating nanostructure materials in their structure, which lie in making of substantial improvements in these materials to increase efficiency for the generation, conversion, transmission and use of energy. In recent years, alumina material had been instrumental in attempts overcoming these challenges. A core@shell structure like Al_2O_3@ZnO (Lung *et al.*, 2016), Ag@Al_2O_3 (Goh *et al.*, 2016) and SnO_2@Al_2O_3 (Heiba *et al.*, 2016) were used as a new strategy to improve optical absorption in solar cells. Lung, *et al.* (2016) found that by coating the Si solar cell with Al_2O_3@ZnO as the antireflection layer would create a gradient of the refractive index and this leads to a decrease in the reflectance effectively, as known that the refractive index of alumina (α-Al_2O_3) is 1.76, it is located between that of ZnO (1.931) and air (1.0). The ideal thickness of an insulating alumina shell surrounding Ag and SnO_2 nanoparticles have been investigated, where the optical absorption enhancement within the poly(3-hexylthiophene) (P3HT) film by the plasmonic electric field and the spatial separation of charge carriers from recombination centres are balanced to give the maximum polaron concentration (Goh, *et al.*, 2016). On the other hand, alumina that incorporated into the SnO_2, decreases the grain size of the mixed oxides SnO_2@xAl_2O_3 to below 10 nm compared to pure SnO_2 over 41 nm. Alumina can effectively prevent SnO_2 from further aggregations in the process of annealing by largely increasing in the specific surface area for mixed oxide samples (Heiba, *et al.*, 2016).

Properties of a material can also be studied by computational approach. Nowadays, approaches based on density functional theory (DFT) are able to calculate the physical properties such as structural, electronic and optical. These approaches are considered more and more popular in many fields as material science, condensed matter, and quantum chemistry. Even in some cases, it has replaced the experimental methods which are difficult to execute under standard conditions, or understand the behavior of physics phenomena for real materials and to make specific predictions of new materials, as well as a reducing the time and cost. Various computer packages has employed DFT such as in quantum chemistry and solid state physics software packages. They normally come along with other methods, such as WIEN2k code (Blaha *et al.*, 2001a).

1.2 Problem Statement

Nanoparticles alumina with different phases have been widely investigated and used in many applications due to their excellent mechanical and optical properties that are superior to other conventional ceramic materials. However, because of their highly disordered nature existing crystallographic models are insufficient to describe the structure of many important alumina phases (Kovarik *et al.*, 2015). Varying properties of alumina with its constituent transition phases as compared to single-phase material have been observed, where Arifa *et al.* (2016) have observed that the band gap for κ-Al_2O_3 is around 4.053 eV that is smaller than for α-Al_2O_3 8.8 eV (French, 1990). This indicates semiconductor behaviour for some alumina phases.

It has been mentioned that the powder form is a cornerstone of many materials. There is a dire need to choose suitable economical powder preparation methods, easily availability of raw materials that can be used to enhance grain size, structure and low-cost nanopowder. In-depth exploration of earlier studies reveals that these materials are usually synthesised by means conventional mechanical routes and expensive physical methods. However, inhomogeneity and non-controllable particle size of the products is always a problem. More chemical and physical methods have been used to prepare nanoparticles materials, but researchers still work on to improve their properties and reduced cost. This work will use chemical co-precipitation method to synthesize various alumina phases. Chemical co-precipitation method is one of the promising approaches to synthesize homogeneous nanoparticles. In fact, it has been recognized as one of the most simple and economical methods for preparing nanostructure materials.

A real understanding of fundamental growth-related phenomena can be achieved only by studying the material on an atomic scale. Apart from experimental computer calculations one can perform such investigations, but the time cost and accurate calculations are the main obstacles to these research. A complementary of experimental and computer simulation able to highlight the best of the two methods and produces much better solution.

1.3 Research Objectives

The following objectives are set to achieve in the proposed study.

1. To synthesize γ- and θ-Al_2O_3 -Nps materials by using chemical co-precipitation technique.
2. To determine the structure and morphology of both alumina phases.
3. To determine the optical properties of γ- and θ-Al_2O_3 -Nps experimentally, and complemented by theoretical computing of absorption coefficient, optical conductivity, refractive index, extinction coefficient, real and imaginary part of the dielectric function, and reflectivity spectra.
4. To calculate the electronic properties including the band structure, and the total and partial density of states of both γ- and θ-Al_2O_3.

1.4 Scope of Research

The goal of this work is to make new insights and to advance knowledge for phase's transitional behaviour of alumina. It consists of two parts; an experimental and theoretical work. As for the experimental study, co-precipitation method is used to synthesize alumina Nps under different annealing temperature of 200 $^{\circ}$C, 400 $^{\circ}$C, 600 $^{\circ}$C, 800 $^{\circ}$C, 900 $^{\circ}$C, 1000 $^{\circ}$C, 1100 $^{\circ}$C, 1200 $^{\circ}$C. X-ray diffraction (XRD) is used to determine the various phase of alumina. The structure parameters can be calculated from XRD results that help to create structure files for the next part of this study. Additionally, further morphology and structure analysis are performed using field emission scanning electron microscopy (FESEM), energy dispersive X-ray spectroscopy (EDX), X-ray photoelectron spectroscopy (XPS), and single point Brunauer–Emmett–Teller (BET). In particular, Fourier transform infrared spectroscopy (FTIR) and Raman spectra are employed to confirm chemical bonds of materials. In addition optical properties of alumina powders and estimation of band gap will be performed using ultraviolet-visible spectroscopy (UV-Vis).

The theoretical work involved to develop and innovate unit cell for both alumina phases depends on the parameters obtained from XRD analyses, and then assess the reality of findings by comparing with experimental results. Fundamental electronic and optical properties of γ- and θ- alumina are explored by first principles within the framework of DFT. The commercial WIEN2k package is employed for this task, which is based on full-potential linearized augmented plane wave method (FP-LAPW) within the local density approximation (LDA), generalized gradient approximation (GGA), and by modified Becke-Johnson (mBJ) potential as the exchange-correlation functions. Therefore, this calculation focus on many parameters like band structure, the total and partial density of states, absorption coefficient, optical conductivity, refractive index, extinction coefficient, real and imaginary part of the dielectric function, and reflectivity coefficient. These calculations can be used to cover the lack of data for the studied alumina phases.

1.5 Significance of Study

In an attempt to investigate nanostructured material including the development of method of its synthesis for the improvement of its performance and properties, γ-Al_2O_3 and θ-Al_2O_3 were synthesized by means of co-precipitation method under different heat treatment effect. This is to achieve the transition phase behaviour with careful processing of the specimens to produce a high purity phases. The report on the formation of phase transformation of alumina (γ→ θ) within 200 $^{\circ}$C -1200 $^{\circ}$C, which enhances the stability of these two phases can be a major breakthrough. In addition, the characterization and analysis of their properties provide fundamental information on morphology, composition and chemical bonds as fingerprints of these two phases, which can be considered references to update FTIR and Raman data bases. Present optical results prove that γ-Al_2O_3 (θ-Al_2O_3) have a band gap 5.5 eV (5.8 eV) smaller than α-Al_2O_3 band gap 8.8 eV (French, 1990), which show the material can be utilized in many optoelectronic devices.

The contribution of this work extends to include investigation of electronic and optical parameters theoretically, which in some cases cannot be achieved by

experiment. For this reason, the framework of DFT with a highly accurate FP-LAPW method as implemented in the WIEN2k code contributed in showing the discrepancies associated with the phase transformations of alumina, which is coupled with a number of modified theoretical tools like LDA, GGA, and mBJ. The theoretical findings strongly reveal the different features of these two alumina phases. The comparison has been done with α-Al_2O_3 phase because no experimental optical data are available in the literature for comparison of these phases.

Finally, new possibilities and insights are presented with the expectations that selected alumina phases herein would suitable for applications such as solar cells industry. The results of this work help in the understanding of alumina nanoparticles growth processes and transformation phases that provide groundwork for the solar cells development. The information obtained here is potentially useful to reinforce optical absorption by means of incorporation these materials in solar cells design as transparent conducting layer that could be useful to absorb all photons from UV range. Also, the present results would reveal a new trend of these alumina phases that may put it in a semiconductor list.

1.6 Thesis Outlines

A short background of alumina includes phases and structure is introduced in Chapter 1, which includes the research problem, objectives, scope, and significance of the present study. Chapter 2 gives a review of the previous research related to this work. This chapter describes the structural properties, alumina transition behaviour, applications, synthesis methods, and followed by electronic and optical properties alumina phases under DFT calculation.

Chapter 3 presents details description of research methodology about experimental and computational work. Experimental results such as: XRD, BET, FTIR, FESEM, EDX, Raman, XPS, UV-Vis are shown and discussed in Chapter 4. Also, there are many physical parameters of γ-Al_2O_3 and θ-Al_2O_3 that have been

provided from DFT code and discussed in Chapter 5. Finally, summary of the thesis, conclusions drawn along with recommendations for future research work is given in Chapter 6. At the end of this thesis the bibliography and relevant appendices are arranged.

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