UNIVERSITI TEKNOLOGI MARA

SYNTHESIS, CHARACTERIZATION AND BAND GAPS OF ZnO, $Zn_{(1-x)}Cu_xO$ AND $Zn_{(1-x)}Mn_xO$ NANOMATERIALS

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AUTHOR'S DECLARATION

I declare that the work in this thesis was carried out in accordance with the regulations of Universiti Teknologi MARA. It is original and is the results of my own work, unless otherwise indicated or acknowledge as referenced work. This thesis has not been submitted to any other academic institution or non-academic institution for any degree or qualification.

I, hereby, acknowledge that I have been supplied with the Academic Rules and Regulations for Post Graduate, Universiti Teknologi MARA, regulating the conduct of my study and research.

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ABSTRACT

The structural and optical properties of ZnO can be modified by doping. The most important issue in this research is band gap. This is because band gaps of materials can be the criteria for its usage in various device applications. The motivation for this research is to obtain substitutionally doped ZnO with various band gap values. This will enhance the light absorption properties of the modified materials. Modified ZnO materials can be used in future applications such as solar cells, gas sensors, optoelectronic devices and etc with improved performance. In this work, Copper (Cu) and Manganese (Mn) will be used as dopant in ZnO nanostructures. Fundamental studies of ZnO and Cu and Mn doped ZnO were studied. Synthesis and characterization of ZnO and (TM=Cu, Mn) doped ZnO nanostructures are analysed and the relationship with their band gaps were investigated. The nanostructures were successfully synthesized via a simple sol-gel method without using any chelating agents. The fundamental properties such as thermal behaviour, crystal structure, size, morphology, electronic configuration, oxidation states, valence band, chemical environment and band gap of these materials were studied in depth. The thermal properties of these materials were studied by Simultaneous Thermogravimetric Analysis (STA) and the purpose is to find a suitable temperature for phase formation. The annealing temperature for ZnO and doped ZnO material were chosen based on the thermal profile of the materials. The phases of the materials were studied by X-Ray Diffraction (XRD). XRD revealed that the nanostructures for ZnO and doped ZnO can be obtained at low temperature of 300 °C to 500 °C. According to the FESEM results, the morphology of the materials changed from long nanorods to spherical like-shape as annealing temperature increases. The size and morphologies of the materials were also temperature dependent. The band gaps of these materials were determined using UV-Vis Spectrophotometry. It was found that band gap changes occur with respect to morphology and size. It was also found that substitutional doping with Cu and Mn in ZnO leads to the narrowing in band gap. To further understand the reasons behind the band gap change, the chemical states and chemical environments of these materials were identified through X-Ray Photoelectron Spectroscopy (XPS). It was observed in valence band (VB) studies from XPS that introduction of dopants (Cu and Mn) in ZnO host material leads to additional new energy levels in the energy gap of ZnO. Thus, the band gaps of doped ZnO were modified according to the dopant atom.

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CHAPTER ONE
INTRODUCTION

1.1 INTRODUCTION TO ZnO AND ZnO DOPED NANOSTRUCTURES

Zinc oxide (ZnO) is one of the materials that have been investigated for over decades due to its important and unique properties which are wide band gap and large exciton binding energy. ZnO is a II-VI binary compound semiconductor and crystallizes in three forms which are hexagonal, wurtzite, cubic zincblende, and the rarely observed cubic rocksalt. The most common phase of ZnO is hexagonal wurtzite structure with a space group of P63mc and this also the most stable phase. The wurtzite ZnO structure consists of alternating zinc (Zn) and oxygen (O) atoms as shown in Figure 1.1. Each Zn^{2+} ion is surrounded by a tetrahedra of O^{2-} ions, and vice-versa.

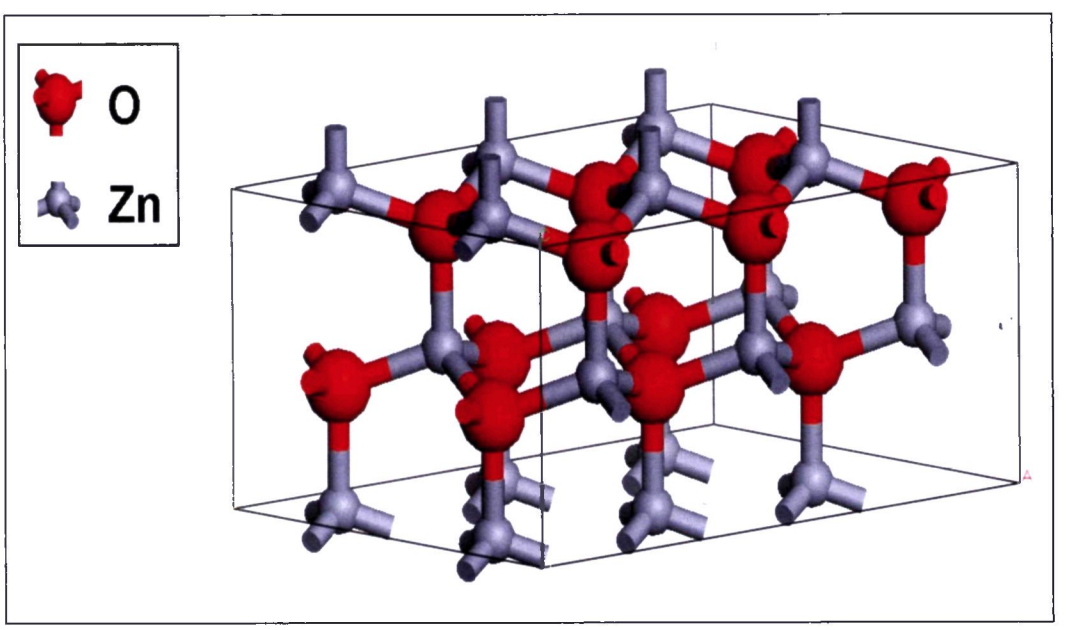

Figure1.1: Crystal structure of hexagonal wurtzite ZnO

ZnO material is already widely used in our society, and it plays a main role in many industrial manufacturing products such as paints, cosmetics, batteries, electrical equipment, rubber, pharmaceuticals, plastics, soap, textiles, etc. ZnO is a unique material that exhibits semiconducting, piezoelectric, and pyroelectric properties.