



PAPER

An in-depth look at the structural, electronic, optical, and thermal properties of the cubic $\text{Be}_x\text{Mg}_y\text{Zn}_{1-x-y}\text{O}$ quaternary alloysRECEIVED
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E-mail: moussa.rabah@univ-djelfa.dz, rabah_khenata@univ-mascara.dz and shakeelkhandy11@gmail.com**Keywords:** quaternary semiconductor alloys, crystalline structure, optoelectronic characteristics, thermodynamic properties, electronic structure

Abstract

In the present research work, the structural, electrical, optical, and thermodynamic properties of the $\text{Be}_x\text{Mg}_y\text{Zn}_{1-x-y}\text{O}$ quaternary alloy were investigated. Its conventional structure, which is composed of the binary compounds ZnO, BeO, and MgO, and their ordered ternary alloys $\text{Be}_x\text{Zn}_{1-x}\text{O}$, $\text{Be}_x\text{Mg}_{1-x}\text{O}$, and $\text{Mg}_x\text{Zn}_{1-x}\text{O}$ are examined. A non-linear variation of lattice constants (a) and bulk modulus (B) as a function of the compositions (x, y) in $\text{Be}_x\text{Mg}_y\text{Zn}_{1-x-y}\text{O}$ alloys is observed due to varying atomic radii of the constituent elements leading to the structural distortion against compositional changes. Both the ternary and quaternary alloys exhibit semiconducting properties, characterized by a direct bandgap ranging from 2–4 eV. This indicates their absorption and emission of light in the visible region of the spectrum, making them promising candidates for optoelectronic applications. The results of optical characteristics display the variation of refractive index and absorption coefficient of these alloys with respect to composition and wavelength. Present results will forecast the possible applications and guidelines for synthesizing such alloys under extreme conditions.

1. Introduction

Nowadays, there has been a growing interest in ultrawide-bandgap semiconductors due to their exceptional electrical and optical properties. These materials have found applications in the field of ultraviolet (UV) detection, luminescence, laser, optoelectronics, and high-power/high-frequency range microelectronic devices [1]. ZnO, MgO, BeO and their alloys, are considered as promising wide bandgap materials with potential applications in spintronic and optoelectronic devices [2]. ZnO stabilizes in a wurtzite crystal structure and displays an insulating gap of 3.3 eV at room temperature. Additionally, it demonstrates high exciton binding energies, measuring around 60 meV [3]. This material gains significant attention due to its favorable optical and electrical characteristics, including its potential applications in transparent thin-film transistors [4].

Numerous experimental and theoretical investigations have been carried out on ternary $\text{Mg}_x\text{Zn}_{1-x}\text{O}$ alloys to adjust the bandgap range from 3.37 to 7.8 eV to suit the solar blind field. Ohtomo *et al* [5] first reported a bandgap of about 3.99 eV with phase separation occurring after the concentration of $x = 0.33$. Through continuous