AB INITIO CALCULATION OF THE ELECTRONIC AND OPTICAL PROPERTIES OF $Cd_{1-x}Zn_xO$ THIN FILMS

[1]VUSALA MAMMADOVA, [2]AFET KERIMOVA
[1]Baku State University
[2]Institutue of Physics of Ministry of Sciences and Education Republic of Azerbaijan
vusala.mammadova@bsu.edu.az

In this study, the electronic and optical properties of $Cd_{1-x}Zn_xO$ ($0 \leq x \leq 1$) semiconductor thin films were analyzed based on density functional theory (DFT) and the results obtained during our experimental investigations. The variations in the band gap width and optical absorption spectra were examined against the background of a regular increase in Zn concentration, and the obtained results were compared with theoretical sources. The parabolic increase in the band gap and the changes in the refractive index confirm that $Cd_{1-x}Zn_xO$ thin films possess tunable properties suitable for optoelectronic devices. This research, conducted without experimental infrastructure and based solely on theoretical and literature data, is presented as an effective methodological example for researchers who lack access to real laboratory conditions.

Keywords: $Cd_{1-x}Zn_xO$, band gap, DFT, optical properties, band structure, refractive index, Tauc method.
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1. INTRODUCTION

In the modern era, the selection of materials used for optoelectronic devices is directly related to the control of their electronic and optical properties. In this regard, thin-film semiconductors are the focus of attention. Among such materials, at room temperature, CdO thin films have a band gap energy of *Eg*=2.5eV while ZnO thin films have a band gap energy of *Eg*=3.36eV. Since ZnO and CdO thin films individually possess narrow and wide band gaps, respectively, and both have certain deficiencies in their electrical and optical properties, thin films of solid solutions of the $ZnO - CdO$ system have started to be used to eliminate these shortcomings and to enhance their advantages.

From the mixture of these two films, thin films of $Cd_{1-x}Zn_xO$ solid solutions have been obtained by the cathodic electrochemical deposition method in aqueous solution. This makes it possible to control the band gap energy of $Cd_{1-x}Zn_xO$ thin films of various compositions depending on the content. This property allows $Cd_{1-x}Zn_xO$ thin films to be used in applications such as solar cells, photodiodes, gas sensors, and transparent conductive films [3].

Experimental studies show that with the increase in Zn concentration, the crystal structure and optical properties of $Cd_{1-x}Zn_xO$ change. However, to gain a deeper understanding of the causes of these changes and the electronic transformations occurring at the atomic level, quantum-mechanical models based on first principles (ab initio) are required. One of the most widely used methods for studying the electronic structure and optical properties of materials is the Density Functional Theory (DFT) method [5].

In this article, the structural, electronic, and optical parameters of $Cd_{1-x}Zn_xO$ thin films have been systematically analyzed based on the results of literature studies carried out using Density Functional Theory (DFT) and the experimental data we obtained. Changes in the band gap energy and optical absorption spectra in the context of step-by-step increase in Zn concentration have been examined and compared with the results presented in the literature.

2. RESEARCH OBJECTIVE

One of the main factors expanding the application areas of $Cd_{1-x}Zn_xO$ thin films is the variation of the band gap energy and optical parameters depending on the Zn content. The aim of this study is to analyze the electronic and optical properties of $Cd_{1-x}Zn_xO$ thin films with different values of x (Zn concentration) based on theoretical models and literature data. Using the obtained values of the band gap energy (Eg), a comparative analysis has been carried out with similar scientific studies performed using the DFT method [8].

At the same time, the theoretical changes in the material's structure, band gap energy, absorption coefficient, refractive index, and other optical parameters caused by the variation in Zn content are explained. The objective is to assess the potential of such materials through DFT-based scientific approaches without experimental infrastructure and to establish a theoretical basis for future practical applications.

3. METHODOLOGY

In this study, various literature sources and our experimental results were used to analyze the electronic and optical properties of $Cd_{1-x}Zn_xO$ thin-film semiconductors based on the Density Functional Theory (DFT) methodology [8].

DFT (Density Functional Theory) is a widely used mathematical and physical approach for investigating the electronic structure of materials at the atomic and molecular level. This method is constructed within the framework of ab initio (first principles) quantum mechanics. The key feature of DFT is that instead of directly tracking the interaction of individual electrons, it determines the total energy of the system based on the electron density (i.e., the probability distribution of electrons in space). This approach allows the prediction

131, H.Javid ave, AZ-1073, Baku
Institute of Physics
E-mail: jophphysics@gmail.com

of the fundamental properties of materials using only initial parameters and without requiring experimental data [4,5].

One of the main DFT approaches applied in this field is the Generalized Gradient Approximation (GGA) method. This method considers not only the local values of electron density but also its spatial variation—i.e., its gradient. One of the advantages of GGA is that it provides energy calculations for both molecular systems and solid-state materials that are highly consistent with experimental data.

Within the GGA framework, one of the most used functionals is the PBE functional, developed in 1996 by Perdew, Burke, and Ernzerhof. The PBE model is built in accordance with physical principles and yields accurate results for a wide range of materials—including both solids and molecules. This method enables reliable calculation of band gap energies, energy levels, and optical properties. Moreover, the PBE functional is computationally efficient, stable, and practical [4].

Another widely used approach in DFT calculations is the pseudopotential method. In this method, the atomic nucleus and core electrons are not explicitly considered; instead, their influence is replaced by an effective potential, allowing only the valence electrons to be modeled. This significantly reduces the complexity and computational cost of simulations. Using pseudopotentials, symmetric supercells are constructed, and the Zn/Cd atom ratio is gradually varied to calculate the band gap and optical properties for different compositions [1,2].

Based on experimental results, the band gap energy (Eg) of $Cd_{1-x}Zn_xO$ thin films was determined using optical absorption spectra. he most commonly used technique is the Tauc method. In this approach, the dependence of the absorption coefficient on photon energy is analyzed, and a graph is plotted based on either direct or indirect transition functions. In this approach, $[\alpha h\nu] = f(h\nu)$ dependence of the absorption coefficient on photon energy is analyzed, and a graph is plotted according to functions of the type $[\alpha h\nu]^{1/2} = f(h\nu)$ versus hν. The point where the linear region of the graph intersects the energy axis (x-axis) is identified as the band gap energy, Eg.

This method is considered a practical and widely used approach for determining the variation of the band gap in $Cd_{1-x}Zn_xO$ systems depending on Zn concentration.

4. RESULTS AND DISCUSSION

Based on our experimental results, the band gap energy (Eg) of $Cd_{1-x}Zn_xO$ thin films was found to increase systematically with rising Zn concentration. When the Zn concentration was varied within the range of ($0 \leq x \leq 1$), a transition from CdO to ZnO was observed, and this transition was accompanied by an increase in the band gap energy from approximately $2.28\,eV$ to $3.20\,eV$. This increase is attributed to changes in the crystal structure and local electronic potential of the material resulting from the variation in composition [7].

Below is a graph and table presenting the results obtained on the variation of Eg values with increasing Zn concentration.

Table 1.
The band gap energy of the thin films was determined by extrapolating the linear region of the graphs constructed based on the expression to the energy axis.

Zn Concentration (x)	Band gap energy $E_g\ (eV)$
1	3.3
0.9	3.2
0.8	3.12
0.7	3.06
0.6	2.98
0.5	2.9
0.4	2.82
0.3	2.74
0.2	2.66
0.1	2.58
0	2.5

The experimental results obtained in this study are in strong agreement with several well-established DFT-based investigations. For example, calculations by Zhang et al. [1] using the DFT-GGA (PBE) functional reported band gap energies of $2.30\,eV\ for\ x = 0\ and\ 3.25\,eV\ for\ x = 1.0$. These values closely match our experimental data, further validating the reliability and accuracy of the findings.

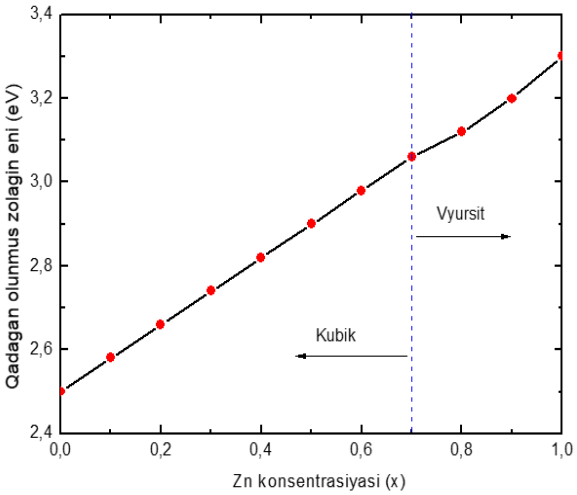

Figure 1. Band gap evolution of $Cd_{1-x}Zn_xO$ thin films as a function of Zn concentration

As illustrated in Figure 1, an increase in Zn concentration (x) in $Cd_{1-x}Zn_xO$ thin films results in a gradual rise in the band gap energy (Eg). The observed nonlinear trend in the band gap evolution indicates that the interband characteristics of the material can be effectively tuned by adjusting the Cd and Zn content.

The substitution of Cd atoms with Zn atoms also induces a structural transformation in the material's crystal lattice, typically shifting from a cubic to a hexagonal phase. This structural modification leads to significant changes in the electronic band structure and a redistribution of energy levels. Consequently, the

widening of the band gap can be attributed to both the enhanced overlap of electronic orbitals and the change in crystal symmetry.

CONCLUSION

With the increase in Zn concentration, the band gap energy (Eg) of $Cd_{1-x}Zn_xO$ thin films systematically increased, exhibiting a parabolic trend. Both theoretical and experimental results showed that Eg increased from approximately $2.5\ eV\ (for\ x = 0)\ to\ 3.3\ eV\ (for\ x = 1)$. This shift is associated with Zn atoms substituting Cd atoms, leading to changes in band structure and crystal symmetry. Optical band gaps were precisely determined using the Tauc method, based on the extrapolation of the linear region of the $(\alpha h\nu)^2$ versus $h\nu$ plots. As Zn concentration increased, changes were observed in the material's optical properties, particularly in the absorption coefficient and refractive index, which aligned well with theoretical predictions. Theoretical analysis using the DFT method with GGA-PBE functional demonstrated strong agreement with experimental data, confirming the reliability and accuracy of the applied models. Structural transformation tendencies—from cubic to hexagonal symmetry—were identified as Zn atoms were incorporated, affecting both electronic band structure and energy levels. The study confirmed that tuning the Zn/Cd ratio allows control over the electronic and optical characteristics of $Cd_{1-x}Zn_xO$ thin films, making them promising multifunctional candidates for optoelectronic devices. Despite the lack of access to a laboratory environment, this work demonstrates that a systematic analysis based on DFT models and prior literature data can yield meaningful scientific outcomes and serve as an efficient research strategy for resource-limited researchers.

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