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**13th INTERNATIONAL CONFERENCE ON MATERIALS SCIENCE AND
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Assoc.Prof.Dr. Ahmet Türker TÜZEMEN

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FOREWORD

It is a pleasure for us to offer you Abstracts Book for the 13th international conference on Materials Science and Nanotechnology for Next Generation; MSNG2026. Our goal was to create a scientific platform that introduces the newest results on internationally recognized experts to local students and colleagues and simultaneously displays relevant Turkish achievements to the world. The positive feedback of the community encouraged us to proceed and transform a single event into a conference series. Now, MSNG2026 is honored by the presence of over 150 colleagues from various cities and countries. We stayed true to the original MSNG2026 concept and accepted contributions from all fields of materials science and technology to promote multidisciplinary discussions. The focal points of the conference emerged spontaneously from the submitted abstracts: energy applications, advanced materials, electronic and optoelectronic devices. Further fields of interest include e.g. new advanced and functional materials, advanced-functional composites, biomaterials, smart materials, dielectric materials, optical materials, magnetic materials, organic semiconductors, inorganic semiconductors, electronic materials, graphene, and more. We can offer free publishing of all peer-reviewed proceedings in international journals Materials Science-Poland, Journal of Nanoelectronics and Optoelectronics, Organo Optoelectronics, Journal of Materials and Electronic Devices and provide the participants with all the commodities of a world – class conference. Therefore, we hope that getting first-hand access to so many new results, establishing new connections and enjoying the Adıyaman Turkey ambience will make you feel that your resources were spent well in MSNG2026.

Our warmest thanks go to all invited speakers, authors, and contributors of MSNG2026 for accepting our invitation, visiting Adıyaman and using MSNG2026 as a medium for communicating your research results.

We hope that you will enjoy the conference and look forward to meeting you again in one of the forthcoming MSNG2026 event.

Prof. Dr. Ali Osman AYAŞ & Prof. Dr. Fahrettin YAKUPHANOĞLU
Conference Chairs

Effect of Magnetic Field on the Electronic Confinement and Total Optical Absorption of a Aymmetric Hyperbolic Quantum Well

Habibe Sayraç^{1,2}, Fatih Ungan^{3,4,*}

¹Optical Excellence Application and Research Center, Sivas University of Science and Technology, 58000 Sivas, Turkey

²Institute of Science, Physics Department, Sivas Cumhuriyet University, 58140 Sivas, Turkey

³Faculty of Science, Physics Department, Sivas Cumhuriyet University, 58140 Sivas, Turkey

⁴Sivas Cumhuriyet University Nanophotonics Application and Research Center, CUNAM, 58140 Sivas, Turkey

Abstract

In this study, the influence of an externally applied perpendicular magnetic field on the electronic confinement potential, quantized subband energy levels, and nonlinear total optical absorption coefficient (TOAC) of an asymmetric hyperbolic GaAs/AlGaAs quantum well is theoretically investigated. Within the effective mass approximation, the one-dimensional time-independent Schrödinger equation is solved using an exact numerical diagonalization technique with an infinite potential well basis set. The optical response is calculated using the compact density matrix formalism and the electric dipole approximation, including both linear and third-order nonlinear contributions. The numerical results show that the applied magnetic field introduces an additional parabolic magnetic confinement, leading to stronger electron localization within the hyperbolic potential region. As a result, the energy separation between the ground and first excited states increases with increasing magnetic field strength. At the same time, the transition dipole matrix element is enhanced. These changes lead to a pronounced blueshift and a significant enhancement of the resonant TOAC spectrum. The results demonstrate that the magnetic field provides an effective external control parameter for tuning intersubband optical transitions in engineered hyperbolic quantum wells, highlighting their potential applications in terahertz (THz) modulators, photodetectors, and ultrafast optical switches.

Keywords: Hyperbolic quantum well, Magnetic field, Total optical absorption coefficient (TOAC), Effective mass approximation.

Corresponding Authors: funghan@cumhuriyet.edu.tr

1. Introduction

Low-dimensional semiconductor heterostructures, including quantum wells (QWs), quantum wires, and quantum dots, have attracted considerable theoretical and experimental interest over the past several decades due to their unique physical properties and important applications in modern optoelectronic technologies [1–6]. Among these structures, QWs have received particular attention because of their well-established epitaxial growth methods, such as Molecular Beam Epitaxy (MBE) and Metal-Organic Chemical Vapor Deposition (MOCVD), as well as their highly controllable quantum confinement characteristics [7–10]. The confinement of charge carriers within QWs results in discrete subband energy levels, providing an effective platform for tailoring intersubband optical transitions over the mid-infrared (MIR) and terahertz (THz) spectral regions [11–14].

Intersubband optical transitions in semiconductor QWs play a fundamental role in the operation of various advanced photonic and optoelectronic devices, including quantum cascade lasers (QCLs), quantum well infrared photodetectors (QWIPs), and high-speed optical modulators. Although linear optical absorption is essential for understanding the underlying electronic structure and transition characteristics, nonlinear optical (NLO) phenomena, particularly third-order nonlinear absorption and refractive-index changes, have gained increasing

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technological importance. Under strong optical excitation, these nonlinear effects can lead to phenomena such as absorption saturation, optical bleaching, and ultrafast optical switching, making QW structures attractive for high-speed and intensity-dependent photonic applications [15–20].

The confinement potential of QWs is commonly described using simple geometrical profiles, such as rectangular, parabolic, and triangular potentials [21–25]. However, real semiconductor heterostructures often exhibit smooth rather than abrupt interfaces due to interdiffusion and compositional variations during epitaxial growth. Generalized hyperbolic potentials therefore provide a more flexible framework for describing smoothly varying confinement profiles while introducing additional degrees of freedom through their geometrical parameters [26–28]. These characteristics make hyperbolic QWs promising candidates for investigating and controlling carrier confinement and optical transitions in semiconductor heterostructures.

In addition to the structural design of the confinement potential, external fields provide effective and non-destructive means of controlling the electronic and optical properties of QWs. Electric, magnetic, and intense non-resonant laser fields can modify the subband energy spectrum, carrier localization, and intersubband transition characteristics [29–35]. In particular, whereas an external electric field can break the spatial symmetry of a QW and induce quantum-confined Stark shifts, an applied static magnetic field introduces an additional parabolic confinement component through the vector potential [36–39]. This magnetic confinement compresses the electronic wavefunctions, modifies their spatial overlap, and generally increases the intersubband transition energy, leading to a characteristic blueshift in the optical response [40–42].

Despite extensive studies of the optical properties of conventional square and parabolic QWs in the presence of magnetic fields, the combined effects of magnetic confinement and generalized hyperbolic potential profiles have received comparatively limited attention. This motivates the present theoretical study, which investigates the influence of an externally applied static magnetic field on the electronic confinement and nonlinear optical properties of an asymmetric hyperbolic GaAs/AlGaAs QW. In particular, the effects of magnetic field strength on the confinement potential, quantized subband energy levels, intersubband dipole matrix elements, and total optical absorption coefficient (TOAC) are systematically examined for representative magnetic-field strengths. The results provide insight into the field-controlled electronic and optical behavior of hyperbolic quantum wells and demonstrate their potential as tunable structures for MIR and THz optoelectronic applications.

2. Theoretical Model and Computational Method

We consider a single conduction-band GaAs/AlGaAs QW heterostructure grown along the z -axis. Within the effective mass approximation, assuming an isotropic and parabolic conduction band, the one-dimensional time-independent Schrödinger equation governing the electron dynamics in the presence of an external magnetic field is given by [41,42]:

$$\left[\frac{1}{2m^*} \left(\vec{p} + \frac{e}{c} \vec{A} \right)^2 + V(z) \right] \Psi(x, y, z) = E \Psi(x, y, z) \quad (1)$$

where m^* is the electron effective mass, e is the elementary charge, c is the speed of light in vacuum, and p is the electron momentum operator. For a magnetic field B applied, the Landau gauge $A = (0, -Bz, 0)$ is adopted. Since the in-plane coordinates (x, y) are separable via plane-wave representations, the effective one-dimensional Hamiltonian acting on the envelope wavefunction along the z -direction becomes:

$$-\frac{\hbar^2}{2m^*} \frac{d^2 \Psi(z)}{dz^2} + \left[\frac{e^2 B^2}{2m^* c^2} z^2 + V(z) \right] \Psi(z) = E \Psi(z) \quad (2)$$

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The bare generalized hyperbolic confinement potential $V(q, z)$ is formulated as follows:

$$V(q, z) = \frac{V_0 e^{\alpha z}}{1 + q e^{\alpha z}} - \frac{8V_0 e^{\alpha z}}{(1 + q e^{\alpha z})^2} \quad (3)$$

where V_0 characterizes the well depth, q is the geometric shape parameter controlling the asymmetry and curvature, and α denotes the screening parameter. In the present investigation, we focus strictly on the asymmetric QW configuration. To accurately solve Eq. (2), an exact numerical diagonalization technique is employed [16]. The electron envelope wavefunction $\psi(z)$ is expanded in terms of the complete orthogonal basis set of an infinite quantum well of width L_∞ :

$$\Psi(z) = \sum_{n=1}^{n_p} c_n \varphi_n(z) \quad \varphi_n(z) = \sqrt{\frac{2}{L_\infty}} \cos\left(\frac{n\pi z - L_\infty \delta_n}{L_\infty}\right) \quad (4)$$

Numerical convergence was strictly verified; an expansion basis size of $n_p = 200$ states within a spatial domain of $L_\infty = 100$ nm ensures excellent eigenenergy precision with negligible truncation error.

Once the eigenvalues E_n and envelope wave-functions $\psi_n(z)$ are determined, the nonlinear optical response is computed using the compact density matrix formalism within the electric dipole approximation. The total optical absorption coefficient (TOAC), $\beta(\omega, I)$, comprises the sum of the linear absorption coefficient $\beta^{(1)}(\omega)$ and the third-order nonlinear absorption coefficient $\beta^{(3)}(\omega, I)$ [25]:

$$\beta^{(1)}(\omega) = \theta \left[\frac{|M_{21}|^2 \sigma_v \hbar Y_{21}}{(\Delta E - \hbar\omega)^2 + (\hbar Y_{21})^2} \right] \quad (5)$$

$$\beta^{(3)}(\omega, I) = -2\theta \left(\left(\frac{I}{\epsilon_0 n_r c} \right) \frac{|M_{21}|^4 \sigma_v \hbar Y_{21}}{[(\Delta E - \hbar\omega)^2 + (\hbar Y_{21})^2]^2} \right) \left[1 - \frac{|M_{22} - M_{11}|^2}{|2M_{21}|^2} \times \frac{(\Delta E - \hbar\omega)^2 - (\hbar Y_{21})^2 + 2(\Delta E)(\Delta E - \hbar\omega)}{(\Delta E)^2 + (\hbar Y_{21})^2} \right] \quad (6)$$

$$\beta(\omega, I) = \beta^{(1)}(\omega) + \beta^{(3)}(\omega, I) \quad (7)$$

Here, $E_{21} = E_2 - E_1$ represents the intersubband transition energy between the ground state (ψ_1) and the first excited state (ψ_2), $M_{ij} = \langle \psi_i | e z | \psi_j \rangle$ is the electric dipole moment matrix element, σ_v is the carrier electron density, I is the incident optical intensity, $n_r = \sqrt{\epsilon_r}$ is the refractive index, and $Y_{21} = 1 / T_{21}$ is the phenomenological relaxation rate.

3. Results and Discussion

To elucidate the magneto-optical characteristics of the asymmetric hyperbolic QW, we systematically evaluate the electronic structure and optical absorption behavior under three representative magnetic field strengths: $B = 0$ T, $B = 10$ T, and $B = 20$ T.

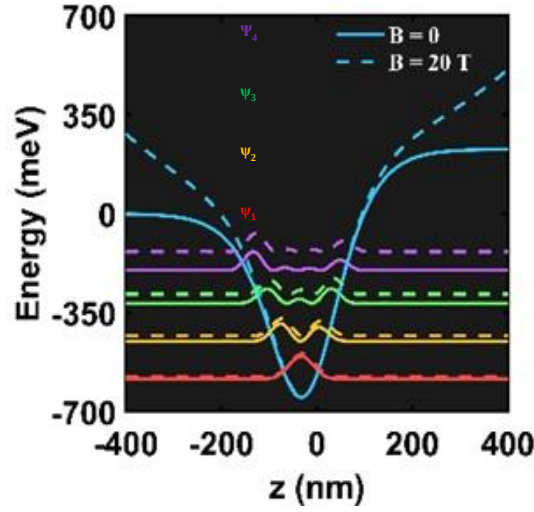


Figure 1 Potential profile and energy levels of the electron in the QW under the influence of applied magnetic field

Figure 1 displays the effective confinement potential profiles along with the spatial distributions of the lowest confined electronic subband wave functions ($\psi_1, \psi_2, \psi_3, \psi_4$) in the absence and presence of the magnetic field. In the zero-field case ($B = 0$ T), the electron experiences solely the asymmetric hyperbolic potential well. When the external magnetic field is engaged ($B = 20$ T), the additional term $\frac{e^2 B^2}{2m^* c^2} z^2$ parabolically bends the potential profile upwards away from the well center. This supplementary confinement dramatically narrows the effective well width and elevates the bound subband energy levels toward higher energies.

Furthermore, the magnetic field induces strong spatial localization of the envelope wave functions within the central core region of the hyperbolic well. Because the wave functions are compressed closer to the origin, their mutual spatial overlap increases. This directly modifies both the transition dipole matrix element M_{21} and the transition energy E_{21} , which serve as the fundamental inputs governing the optical absorption characteristics.

Table 1. Transition energy E_{21} and dipole moment matrix element M_{21} correspond to the transition between the ground state and the first excited state under different applied magnetic field strengths

	B (T)		
	0	10	20
E_{21} (meV)	133.381	136.392	148.003
$M_{21}^2 (\text{\AA}^2)$	2.791	3.061	3.998

Quantitative data detailing the electronic structure changes are compiled in Table 1. At $B = 0$ T, the intersubband energy spacing is $E_{21} = 133.381$ meV. As the magnetic field increases to $B = 10$ T, E_{21} shifts to 136.392 meV, and under $B = 20$ T, it expands significantly to 148.003 meV. This represents a substantial net energy shift of $\Delta E_{21} =$

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14.622 meV. Concurrently, the dipole matrix element squared increases monotonically from $M_{21}^2 = 2.791 \text{ \AA}^2$ to $3.061 \text{ \AA}^2$ and reaches $3.998 \text{ \AA}^2$. This remarkable enhancement in oscillator strength is a direct consequence of the enhanced magnetic spatial compression, which tightens the overlap between the odd-parity first excited state and even-parity ground state.

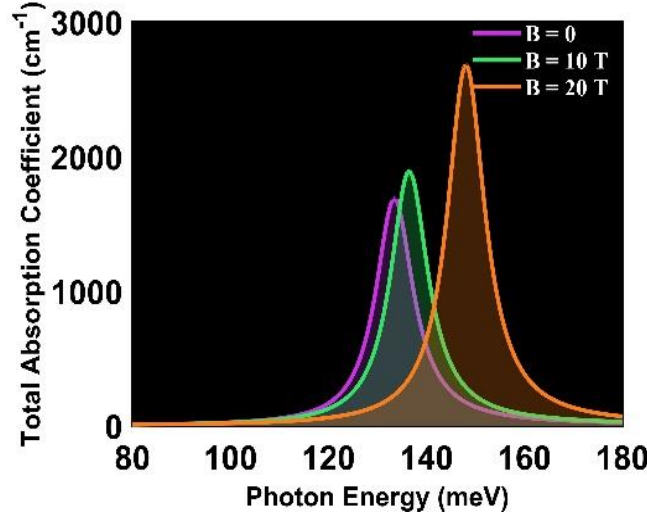


Figure 2 TOAC variation for different photon energies applied magnetic field

The spectral profile of the total optical absorption coefficient (TOAC) as a function of incident photon energy ($\hbar\omega$) is depicted in Figure 2. Under zero magnetic field ($B = 0 \text{ T}$), the TOAC spectrum exhibits a resonant peak centered precisely at $\hbar\omega = 133.38 \text{ meV}$ with an amplitude of approximately 1700 cm^{-1} . When the magnetic field is raised to $B = 10 \text{ T}$, the resonance peak experiences a noticeable blueshift, shifting to $\hbar\omega = 136.39 \text{ meV}$ with an increased absorption peak reaching $\sim 1900 \text{ cm}^{-1}$. At $B = 20 \text{ T}$, the resonant absorption peak shifts further into the higher-energy domain, peaking at $\hbar\omega = 148.00 \text{ meV}$ with a peak amplitude exceeding 2700 cm^{-1} .

This prominent blueshift and concomitant intensity surge can be comprehensively understood through Eqs. (5)-(7) and Table 1. The resonance condition for optical absorption occurs when the incident photon energy matches the intersubband energy separation. Since magnetic quantization forces the subband separation upward, the resonance peak naturally translates toward higher photon energies. Simultaneously, the linear absorption term scales directly with the dipole matrix element squared. Because M_{21}^2 increases by over 43% between 0 T and 20 T , the oscillator strength is greatly amplified, driving the marked increase in the absorption coefficient peak.

4. Conclusions

In conclusion, we have presented a comprehensive theoretical investigation of the effect of an external magnetic field on the electronic confinement and nonlinear optical absorption in an asymmetric hyperbolic GaAs/AlGaAs quantum well. By numerically diagonalizing the effective-mass Hamiltonian, we have demonstrated that the applied magnetic field significantly modifies the quantum confinement environment through the emergence of an additional parabolic potential component. The results reveal enhanced carrier localization, with the magnetic field compressing the envelope wave functions and concentrating the electron density within the central hyperbolic region, thereby increasing the spatial overlap between quantum states. Furthermore, the intersubband transition

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energy between the ground and first excited states increases monotonically from 133.381 meV at 0 T to 148.003 meV at 20 T, indicating strong spectral tunability. The transition matrix element squared, M_{21}^2 , also increases from 2.791 Å² to 3.998 Å², leading to a substantial enhancement in the optical transition probability. Consequently, the total optical absorption coefficient exhibits a pronounced blueshift of approximately 14.6 meV, accompanied by a significant increase in its amplitude from around 1700 cm⁻¹ to above 2700 cm⁻¹. These findings clearly demonstrate that generalized hyperbolic quantum wells under magnetic fields provide enhanced flexibility and spectral tunability compared with conventional rigid square quantum wells. Such field-controlled optical properties highlight the potential of these structures for the development of high-performance terahertz/infrared photonic devices, optical modulators, photodetectors, and ultrafast nonlinear optical switches.

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Electrical Characterization of an AAO-Based GEM Detector

Y. Kandeger^{1,*}, Y. Kalkan¹, A. Kosemen², S. Ozturk², R. Lok¹

¹Nuclear Radiation Detectors and Research Center, Bolu Abant İzzet Baysal University, Bolu 14030, Türkiye

²Nanotechnology and Biotechnology Research Institute, Istanbul University – Cerrahpasa, Istanbul 34500, Türkiye

Abstract

Gas Electron Multiplier (GEM) detectors require well-controlled amplification structures to achieve stable electrical behavior and high spatial granularity, motivating the investigation of alternative nanoporous materials for GEM-like detector structures. In this study, the electrical characteristics of a Nano-GEM detector based on a metallized anodic aluminum oxide (AAO) membrane with a thickness of $50 \pm 2 \mu\text{m}$ and a pore diameter of $200 \pm 24 \text{ nm}$ were experimentally investigated. Current–voltage (I–V) measurements of the metallized AAO foil showed a gradual increase in current from 0.17 nA at 1 V to 7.80 nA at 500 V without an abrupt current increase over this voltage range. After detector assembly, the electrical response was further investigated under ambient air and Ar–CO₂ (70:30) conditions. Under Ar–CO₂ (70:30), the measured avalanche current remained below 0.30 nA over the investigated ΔV_{GEM} range, with a maximum measured value of approximately 0.290 nA at 920 V. The distinct electrical responses observed under ambient air and Ar–CO₂ indicate that further optimization of the detector configuration is required for operation under the gas mixture. These results provide an experimental basis for the further development and evaluation of nanoporous AAO structures in GEM-like gaseous detector applications.

Keywords: Gas Electron Multiplier (GEM), Anodic Aluminum Oxide (AAO), nanoporous membrane, electrical characterization, gaseous detector

Corresponding authors: yelda.kandeger@cern.ch

1. Introduction

Gas Electron Multiplier (GEM) detectors are widely used in high-energy physics and radiation detection because of their high rate capability, good spatial resolution, and fast response. A conventional GEM consists of a thin insulating foil coated with conductive layers on both sides and perforated with a large number of microscopic holes. When a potential difference is applied across the foil, a strong electric field is formed inside the holes, where electrons produced by ionizing radiation can undergo avalanche multiplication [1,2].

The performance of a GEM is closely related to the properties of its amplification foil. In particular, the dimensions and geometry of the holes can influence the electric-field distribution and consequently affect electron multiplication and gain [3,4]. Variations introduced during foil fabrication may therefore contribute to spatial variations in detector response [4]. In addition, charge accumulation on dielectric surfaces can modify the detector response during operation [5]. These effects have motivated studies of different foil materials, geometries, and fabrication techniques for GEM-type detectors [6].

Anodic aluminum oxide (AAO) provides an alternative platform for producing highly ordered nanoporous structures. AAO membranes contain self-organized arrays of vertical nanochannels whose pore diameter, depth, and interpore distance can be controlled during fabrication [7]. They also exhibit a relatively uniform pore distribution and good chemical stability [7]. These properties make AAO an interesting candidate for the development of GEM-like structures with dimensions considerably smaller than those of conventional GEM holes.

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Recent work has demonstrated the fabrication of a nanostructured GEM foil based on such nanotube structures and its integration into a gaseous detector prototype [8]. However, the experimental electrical behavior of these structures under detector operating conditions still requires further investigation.

In this work, a metallized nanoporous AAO membrane was incorporated into a GEM-like detector structure, and its electrical behavior was investigated experimentally. Current–voltage (I–V) measurements were performed to characterize the electrical response of the metallized AAO foil and the assembled detector. The detector was subsequently investigated under ambient air and Ar–CO₂ (70:30) conditions to examine its electrical behavior under different operating environments. The aim of this study is to provide a preliminary electrical characterization of the AAO-based Nano-GEM structure and to evaluate its feasibility for further development as a nanoscale gaseous detector.

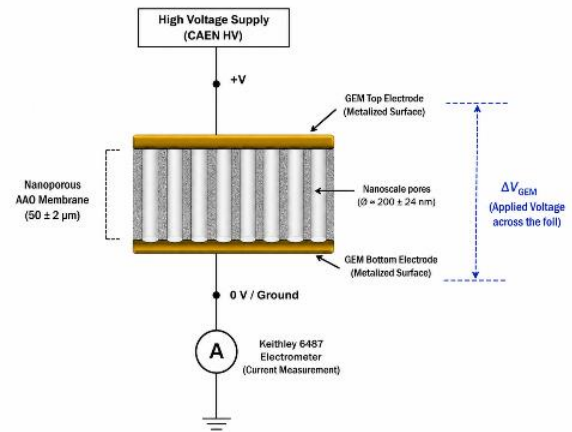
2. Experimental details

Commercial anodic aluminum oxide (AAO) membranes with a nominal thickness of $50 \pm 2 \mu\text{m}$ and a pore diameter of $200 \pm 24 \text{ nm}$ were used to fabricate the Nano-GEM structures. The AAO membranes were coated with aluminum on both surfaces to form conductive electrodes while preserving the open nanoporous structure. The metallized surfaces correspond to the GEM-top and GEM-bottom electrodes of the Nano-GEM foil.

The electrical characteristics of the metallized AAO foil were initially investigated by current–voltage (I–V) measurements. A potential difference was applied between the two metallized surfaces, and the resulting current was measured using a Keithley 6487 electrometer. These measurements were performed to evaluate the electrical behavior and voltage-dependent response of the fabricated Nano-GEM foil.



(a)



(b)

Figure 1 Experimental configuration used for the electrical characterization of the AAO-based Nano-GEM: (a) photograph of the detector setup and (b) simplified schematic representation of the electrical connection used for the I–V measurements of the metallized AAO foil.

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Following the initial foil characterization, the Nano-GEM foil was incorporated into a dedicated detector chamber. An aluminized Mylar foil was used as the cathode and detector entrance window, while a copper electrode served as the anode. The Nano-GEM foil was positioned between the cathode and anode. The assembled detector was subsequently characterized under ambient air and Ar–CO₂ (70:30) conditions. Current–voltage measurements were performed under both environments to investigate the electrical behavior of the detector under different operating conditions.

Under Ar–CO₂ (70:30) conditions, the potential difference across the Nano-GEM foil (ΔV_{GEM}) was defined as the difference between the GEM-top and GEM-bottom electrode potentials. The corresponding current was measured using a Keithley 6487 electrometer and recorded as the avalanche current.

3. Results and discussion

The current–voltage characteristics of the metallized AAO Nano-GEM foil are shown in Figure 2. The measured current increased gradually from 0.17 nA at 1 V to 1.26 nA at 100 V, 2.40 nA at 200 V, 3.90 nA at 300 V, and 7.80 nA at 500 V. No abrupt increase in current was observed over the investigated voltage range. This gradual voltage-dependent response demonstrates stable electrical behavior of the metallized AAO foil and shows that a potential difference of up to 500 V could be applied across the nanoporous AAO structure without an abrupt current increase under the investigated conditions.

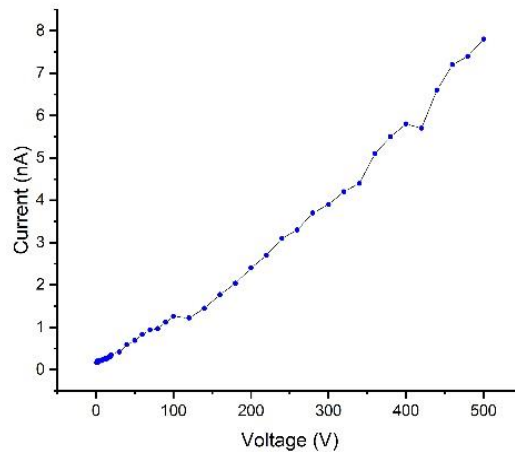


Figure 2 Current–voltage characteristics of the metallized AAO-based Nano-GEM foil

Following the initial characterization of the foil, the Nano-GEM was installed in the detector chamber and its electrical response was investigated under ambient air and Ar–CO₂ (70:30) conditions, as shown in Figure 3. Under ambient air conditions, the measured current remained in the nanoampere range up to approximately 825 V, reaching 11.1 nA at this voltage. A pronounced increase was then observed, with the current rising to approximately 1100 nA at 850 V and reaching 1900 nA at 1000 V. This sharp increase indicates a substantial change in the electrical conduction behavior of the assembled detector at higher applied voltages. In contrast, under Ar–CO₂ (70:30), the avalanche current remained below 0.30 nA throughout the investigated ΔV_{GEM} range. The current increased from approximately 0.005 nA at $\Delta V_{\text{GEM}} = 300$ V to 0.120 nA at 720 V and reached a maximum measured value of approximately 0.290 nA at 920 V. Although an overall increase with ΔV_{GEM} was observed, the measurements exhibited noticeable fluctuations at higher voltages. Based on these observations, the detector geometry was subsequently modified by increasing the drift gap to improve charge collection and electric-

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field uniformity. Overall, these measurements revealed distinctly different electrical behavior under ambient air and Ar-CO₂ conditions and guided the subsequent optimization of the detector configuration.

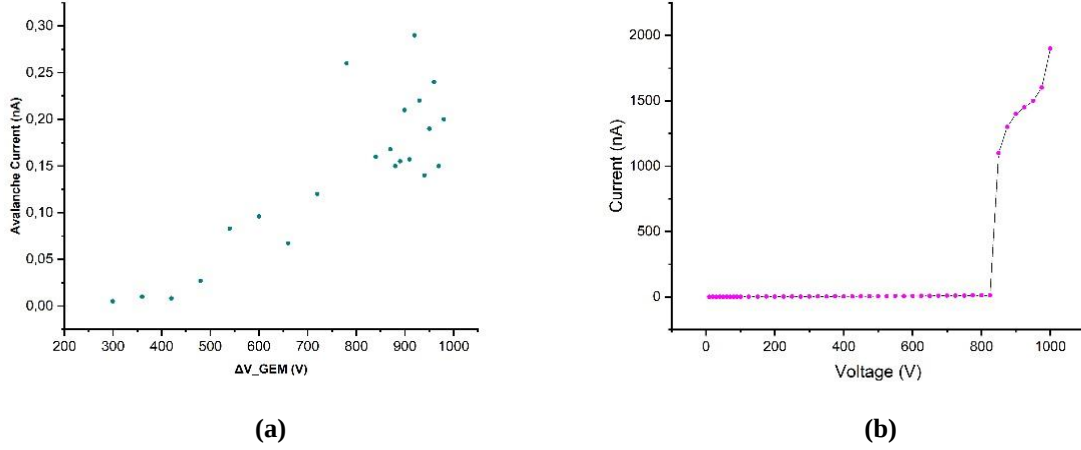


Figure 3 Electrical characteristics of the assembled Nano-GEM detector: **(a)** current as a function of applied voltage under ambient air conditions and **(b)** avalanche current as a function of ΔV_{GEM} under Ar-CO₂ (70:30) conditions.

Conclusions

The electrical behavior of an AAO-based Nano-GEM structure was investigated through current-voltage measurements. The aluminum-coated AAO foil exhibited a gradual increase in current from 0.17 nA at 1 V to 7.80 nA at 500 V without an abrupt current increase over this voltage range. After detector assembly, measurements under ambient air showed a pronounced increase in current from 11.1 nA at 825 V to approximately 1100 nA at 850 V, reaching 1900 nA at 1000 V. Under Ar-CO₂ (70:30), the avalanche current remained below 0.30 nA over the investigated ΔV_{GEM} range, with a maximum measured value of approximately 0.290 nA at 920 V. The distinctly different electrical responses observed under ambient air and Ar-CO₂ indicate that further optimization of the detector geometry and operating parameters is required. Overall, these results provide an experimental characterization of the voltage-dependent electrical behavior of the AAO-based Nano-GEM and establish a basis for its further development as a GEM-like gaseous detector structure.

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Thickness-Dependent Optoelectronic and Interfacial Response of ETL-Free and CdS-Based AgBiS₂ Solar Cells

^{1*}A. KARACA & ^{2*}D. Esra YILDIZ

¹*Department of Physics, Faculty of Sciences, Yozgat Bozok University, Yozgat 66000, Turkey,*

²*Department of Physics, Faculty of Engineering and Natural Sciences, Hitit University, Corum 19030, Türkiye.*

Abstract

The role of the electron transport layer in AgBiS₂ thin-film solar cells was investigated by comparative SCAPS-1D simulations of two device architectures, an ETL-free configuration (FTO/AgBiS₂/Au, D0) and a CdS-containing counterpart (FTO/CdS/AgBiS₂/Au, D1). A comprehensive optoelectronic analysis was carried out, including current–voltage, capacitance–voltage, external quantum efficiency, spectral responsivity, frequency-dependent conductance and impedance measurements under AM1.5G illumination. The AgBiS₂ absorber thickness was systematically varied from 100 to 1000 nm in both configurations, and the CdS buffer thickness in D1 was independently swept from 50 to 250 nm. To further separate optical and interfacial contributions, the two devices were additionally examined under three distinct illumination conditions, namely standard 1-Sun (AM1.5G), a broad white spectrum (300–1300 nm) and a narrow visible spectrum (400–800 nm). The insertion of the CdS buffer left the open-circuit voltage essentially unchanged at 0.917 V and produced a modest gain in fill factor from 82.31% to 83.64%, whereas the short-circuit current density decreased from 30.89 to 27.48 mA/cm². Impedance and conductance analyses consistently showed a larger and more complex electrical response for the CdS-containing device under all illumination conditions studied, which is consistent with a coupled contribution of short-wavelength optical attenuation and modified interfacial transport at the CdS/AgBiS₂ boundary. These findings identify CdS as an interfacial modifier rather than a universally beneficial electron transport layer for AgBiS₂ solar cells and support the ETL-free FTO/AgBiS₂/Au architecture as a viable route for low-cost and Cd-free thin-film photovoltaic applications.

Keywords: AgBiS₂ thin-film solar cell, SCAPS-1D simulation, ETL-free architecture, impedance analysis.

Corresponding authors: abdullah.karaca@bozok.edu.tr, desrayildiz@hitit.edu.tr

1. Introduction

Silver bismuth sulfide (AgBiS₂) has garnered growing interest in photovoltaic research due to its favorable optoelectronic properties, including a high absorption coefficient exceeding 10⁵ cm⁻¹ and a tunable bandgap around 1.3 eV, which is near-optimal for single-junction solar cells [1-4]. Unlike conventional absorbers such as CdTe or CIGS, AgBiS₂ offers the advantages of elemental abundance, low toxicity, and solution processability, making it an attractive candidate for scalable and environmentally benign thin-film photovoltaics [5]. In device architectures, the electron transport layer (ETL) plays a decisive role in carrier extraction and interfacial recombination dynamics. Cadmium sulfide (CdS) has long served as the benchmark ETL for chalcogenide absorbers, primarily because of its suitable conduction band alignment and mature deposition technology [6]. Nevertheless, CdS introduces parasitic light absorption at shorter wavelengths and raises sustainability concerns, prompting a search for alternatives [7-9]. Although CdS is routinely employed in solar cell simulations, the fundamental assumption that an ETL for AgBiS₂ is always necessary has not been critically tested. Prior numerical studies, such as those by Olopade and Swaray [7] and Sayeem et al. [10] and have predominantly examined buffer layers and back surface fields while treating the ETL as an indispensable component. While Sayeem et al. systematically explored multiple ETL candidates, they omitted an ETL-free reference configuration.

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Consequently, a comprehensive and direct comparative analysis between ETL-containing and ETL-free AgBiS₂ architectures remains conspicuously absent in the literature.

In this work, we employ SCAPS-1D simulations [9] to evaluate two distinct structures: a control device without any ETL (FTO/AgBiS₂/Au, D0) and a conventional CdS-based ETL device (FTO/CdS/AgBiS₂/Au, D1). A comprehensive numerical optoelectronic characterization is performed for both configurations. This characterization includes current density–voltage (J–V), capacitance–voltage (C–V), external quantum efficiency (EQE), spectral responsivity (SR), impedance (Nyquist) and frequency-dependent conductance G(f) analyses under AM1.5G illumination. The thickness of the AgBiS₂ absorber is varied between 100 and 1000 nm in both architectures. The CdS buffer thickness in D1 is independently swept from 50 to 250 nm. This dual parametric investigation enables a decoupled evaluation of absorber and buffer related contributions. To further separate parasitic optical losses from interfacial effects, the two devices are additionally compared under three distinct illumination conditions. These conditions correspond to standard 1-Sun (AM1.5G) illumination, broad white spectrum (300–1300 nm) and narrow visible spectrum (400–800 nm). Impedance spectroscopy consistently reveals larger Nyquist arcs for D1 across all illumination regimes. This trend also holds within the narrow 400–800 nm window in which CdS parasitic absorption is minimal. Such behavior indicates that interfacial recombination at the CdS/AgBiS₂ heterojunction contributes to the loss mechanism independently of optical filtering. Two coupled effects are therefore proposed to govern this outcome. The first mechanism is parasitic optical absorption in the 300–500 nm range that attenuates the photon flux reaching the AgBiS₂ absorber. The second mechanism is enhanced non-radiative recombination originating from defects and interfacial chemistry at the CdS/AgBiS₂ boundary. The following sections present the quantitative results of these analyses and evaluate the contribution of the CdS layer to the overall device performance.

2. Numerical details

The device simulations were carried out with the one-dimensional solar cell simulation software SCAPS-1D (version 3.3.11), developed at the University of Gent [11]. SCAPS-1D solves the Poisson equation together with the electron and hole continuity equations under steady-state conditions and provides the standard optoelectronic outputs required for full device characterization, including J–V, C–V, C–f, quantum efficiency and impedance spectra [12, 13]. Two device architectures were considered in this study. The first configuration (D0) consists of a control cell without any electron transport layer and follows the sequence FTO/AgBiS₂/Au. The second configuration (D1) incorporates a conventional CdS buffer layer and adopts the sequence FTO/CdS/AgBiS₂/Au. The schematic representation of both structures together with their equilibrium energy band diagrams is presented in Fig. 1. The Au back contact was defined with a metal work function of 5.1 eV, which is the accepted value for gold electrodes in the SCAPS environment.

The material parameters used for the AgBiS₂ absorber and the CdS buffer layer are summarized in Table 1. These values were compiled from previously reported experimental and theoretical studies and correspond to physically consistent input sets for SCAPS-1D [14–16]. All simulations were performed at a working temperature of 300 K under standard AM1.5G illumination with an incident optical power of 1000 W/m². A series resistance of 1.0 Ω·cm² was included in the equivalent circuit and the shunt resistance was set to a sufficiently high value (10³⁰ Ω·cm²) to isolate intrinsic device behavior. The J–V and C–V characteristics were computed over the voltage range from –3 to +3 V using 2000 points with a 0.02 V step. Capacitance–frequency (C–f) and impedance spectra were obtained between 10⁰ and 10⁶ Hz. Quantum efficiency and spectral responsivity were evaluated over the 100–1400 nm wavelength range. The thickness of the AgBiS₂ absorber was systematically varied from 100 to 1000 nm in both D0 and D1, and the CdS buffer thickness in D1 was independently swept from 50 to 250 nm. To decouple parasitic optical absorption from interfacial recombination effects, additional simulations were performed under

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three distinct illumination conditions, namely standard AM1.5G (1 Sun), broad white spectrum (300–1300 nm) and narrow visible spectrum (400–800 nm).

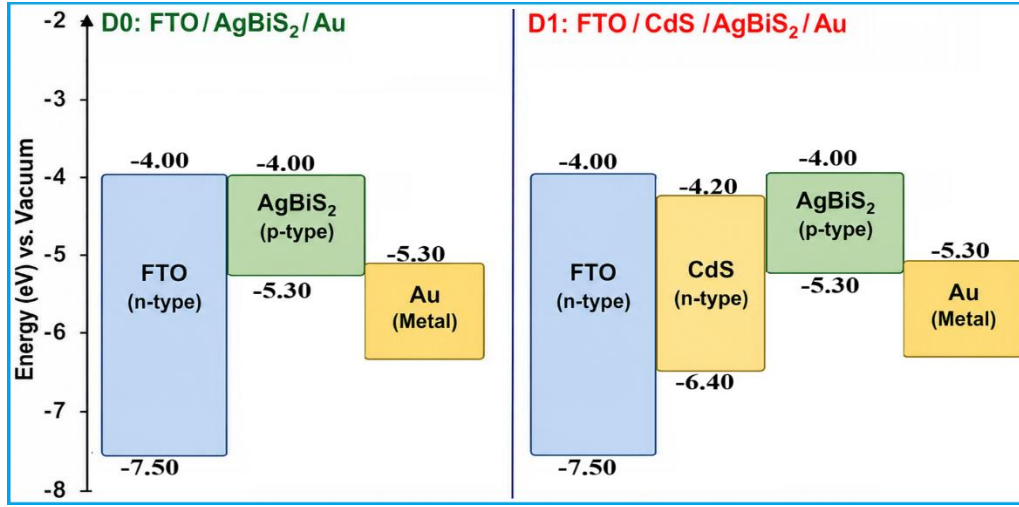


Figure 1 Schematic equilibrium energy band diagram of AgBiS_2 solar cells referenced to the vacuum level: **(a)** control device without ETL ($\text{FTO}/\text{AgBiS}_2/\text{Au}$, D0) and **(b)** device with CdS buffer layer ($\text{FTO}/\text{CdS}/\text{AgBiS}_2/\text{Au}$, D1).

Table 1 Key physical and electronic parameters of FTO, AgBiS_2 , and CdS layers used in device simulations.

Layer Parameters	FTO	AgBiS_2	CdS
d (nm)	300	100 – 1000	50 – 250
E_g (eV)	3.5	1.10	2.40
χ (eV)	4.00	4.00	4.20
ϵ_r	9.0	10	10
N_c (cm^{-3})	2.2×10^{18}	2.0×10^{18}	2.2×10^{18}
N_v (cm^{-3})	1.8×10^{19}	1.5×10^{19}	1.8×10^{19}
μ_n (cm^2/Vs)	20	50	50
μ_p (cm^2/Vs)	10	20	20
N_D/N_A (cm^{-3})	2×10^{19}	5×10^{17}	5×10^{17}
N_t (cm^{-3})	10^{15}	10^{15}	10^{15}

3. Results and discussion:

The influence of the AgBiS_2 absorber thickness on the optoelectronic response of the ETL-free device D0 is illustrated in Fig. 2. The J–V curves in Fig. 2a show a progressive increase of J_{SC} with thickness that rises steeply between 100 and 500 nm and then approaches saturation for thicknesses larger than 700 nm. This trend reflects the enhanced photon absorption in thicker absorbers and is consistent with the assumed electron diffusion length

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of $L_n = 2.3 \mu\text{m}$ in the SCAPS model, which remains well above the maximum absorber thickness examined here [17]. Nevertheless, the benefit of further increasing the absorber thickness becomes increasingly marginal at larger values and does not correspond to an unlimited improvement in device response. The capacitance–voltage response in Fig. 2b remains almost invariant with thickness over the accumulation region. The relatively similar C–V profiles suggest that the overall electrostatic response is not strongly altered by the absorber thickness within the investigated range. The external quantum efficiency spectra in Fig. 2c progressively enhance in amplitude as the thickness increases, with the improvement being particularly pronounced at longer wavelengths where the absorption coefficient of AgBiS₂ is intrinsically weaker. The spectral responsivity $R(\lambda)$ shown in Fig. 2d follows the same qualitative trend and can be related to the quantum efficiency through the standard relation $R(\lambda) = (q\lambda/hc) \times \text{EQE}(\lambda)$, which links the two datasets on physically consistent grounds. The responsivity reaches its maximum near 850 nm for the 1000 nm absorber.

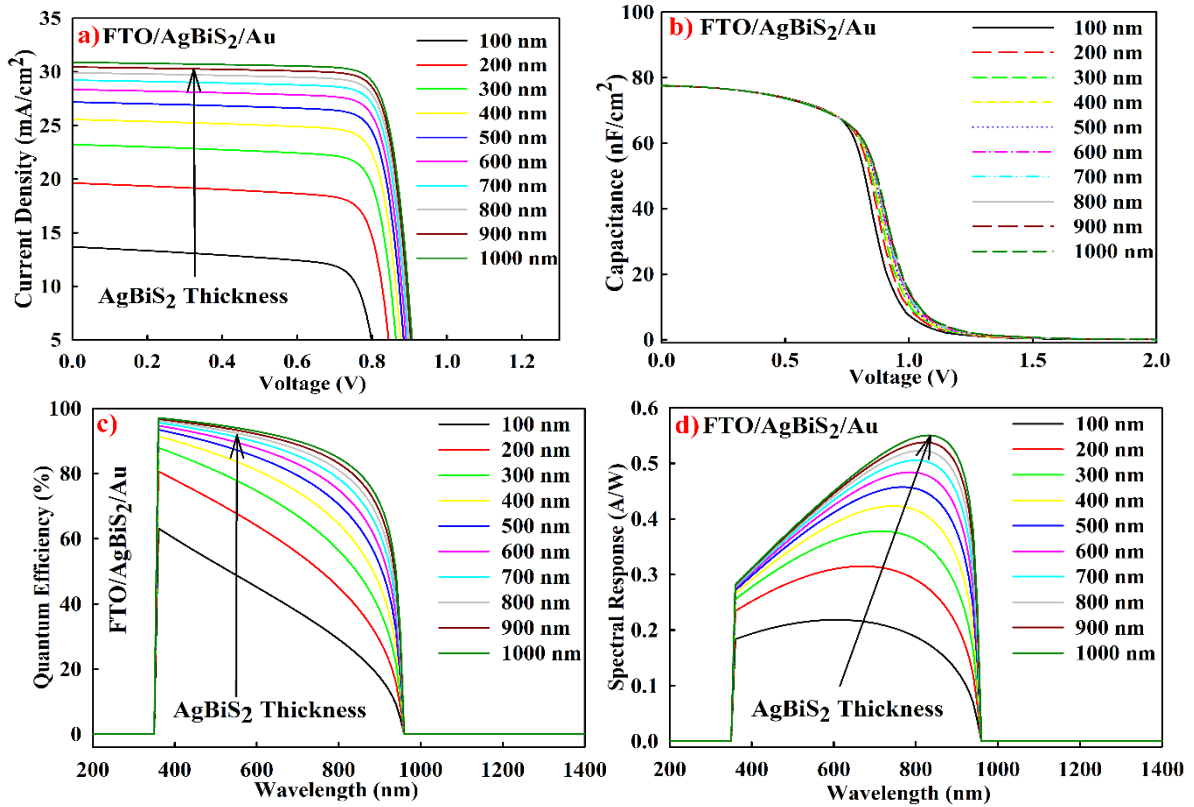


Figure 2 (a) J–V, (b) C–V, (c) EQE and (d) spectral responsivity of D0 for AgBiS₂ thicknesses from 100 to 1000 nm.

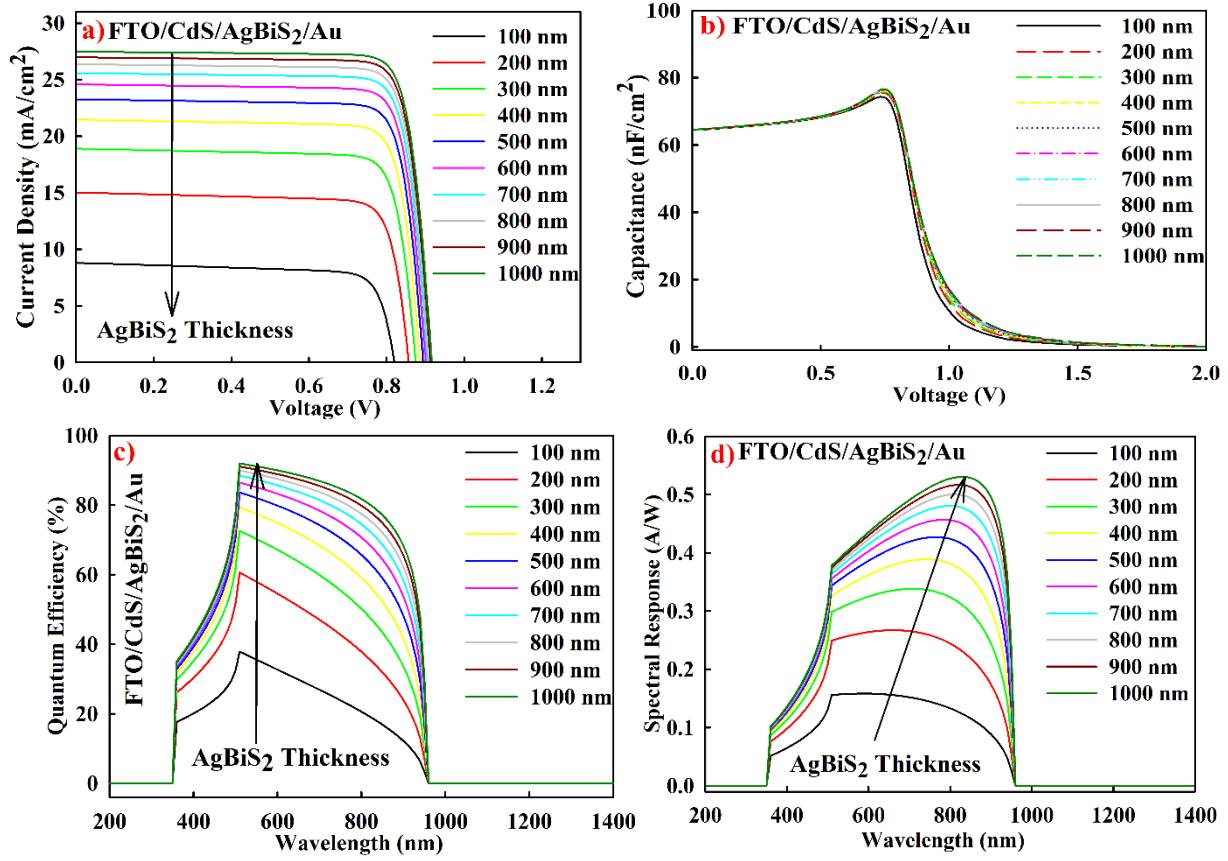
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Figure 3 (a) J–V, (b) C–V, (c) EQE and (d) spectral responsivity of D1 for AgBiS₂ thicknesses from 100 to 1000 nm.

The equivalent analysis for the CdS-containing device D1 is shown in Fig. 3. The overall trends closely follow those of D0 with three notable differences. First, the J_{SC} values in Fig. 3a are systematically lower for every AgBiS₂ thickness compared with the corresponding D0 curves. Second, the EQE spectra in Fig. 3c are strongly suppressed below 500 nm, which is consistent with additional short-wavelength absorption introduced by the CdS layer. Third, the short-wavelength cutoff of the spectral response in Fig. 3d shifts toward longer wavelengths, from approximately 350 nm in D0 to approximately 520 nm in D1. These observations indicate that the introduction of the CdS buffer modifies both the short-wavelength optical response and the effective carrier collection of the device, even though the qualitative dependence on absorber thickness is preserved [18]. A definitive separation of the underlying contributions between optical absorption in the CdS layer and modified front-interface transport would require additional wavelength-resolved optical loss analysis and is therefore treated here as a coupled effect.

The dependence of D1 performance on the CdS buffer thickness in the range of 50 to 250 nm is presented in Fig. 4. The J–V curves in Fig. 4a display a clear monotonic decrease of J_{SC} as the CdS thickness increases. Since the AgBiS₂ thickness is kept constant in this scan, this reduction cannot be attributed to bulk absorber effects and is instead governed by the CdS layer itself. The C–V response in Fig. 4b shows the emergence of a distinct thickness-dependent behavior for CdS layers thicker than 100 nm, indicating that increasing CdS thickness modifies the overall capacitance response of the multilayer structure. The EQE curves in Fig. 4c and the spectral responsivity in Fig. 4d both exhibit a progressive suppression of the short-wavelength response as the CdS thickness grows. The cutoff of the useful spectral range shifts from approximately 380 nm for a 50 nm CdS layer to about 520 nm for a 250 nm CdS layer, which is consistent with increasing optical attenuation in the CdS layer. Considered together, these results indicate a narrow thickness range over which the CdS layer can be introduced without substantial deterioration of the photocurrent response [19]. Excessively thick CdS layers become

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detrimental to the photocurrent through a combination of front-side optical losses and modified carrier extraction characteristics, and thin CdS layers are therefore preferable within the investigated range [20].

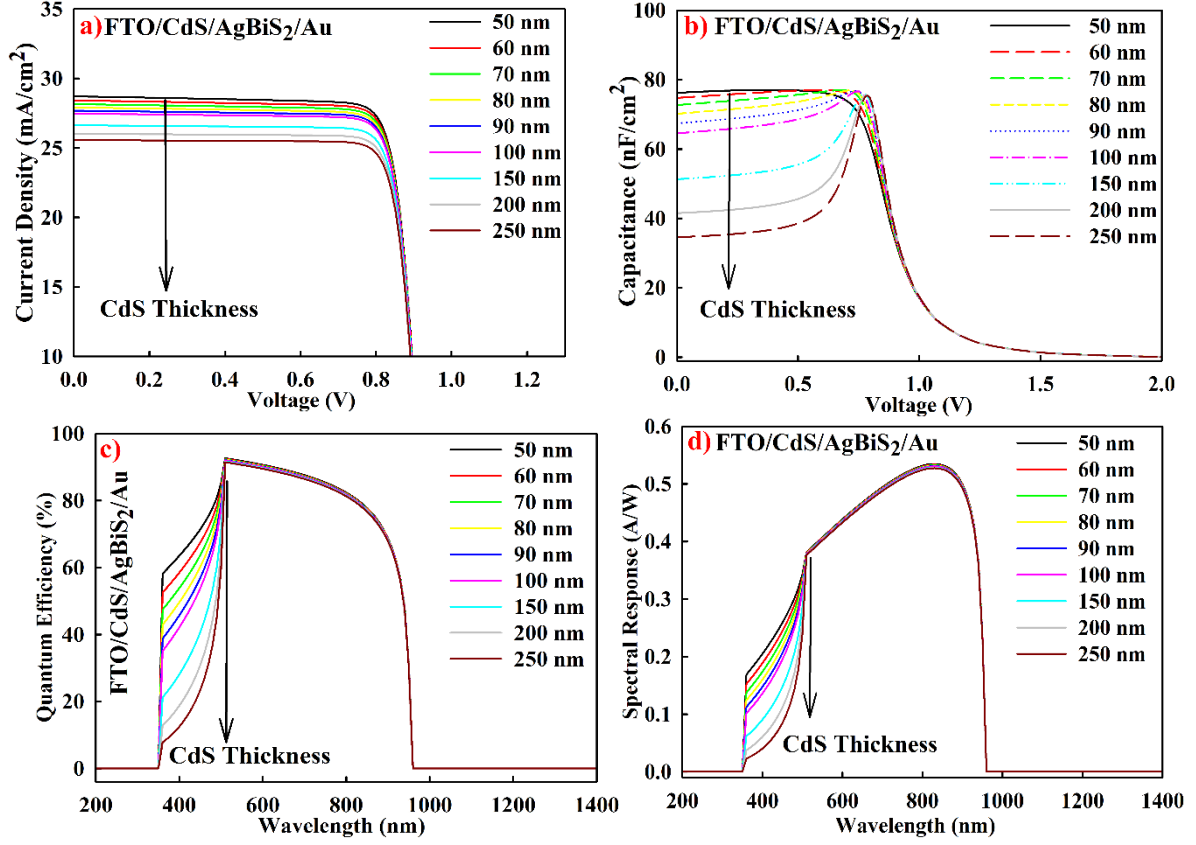


Figure 4 (a) J–V, (b) C–V, (c) EQE and (d) spectral responsivity of D1 for CdS thicknesses from 50 to 250 nm.

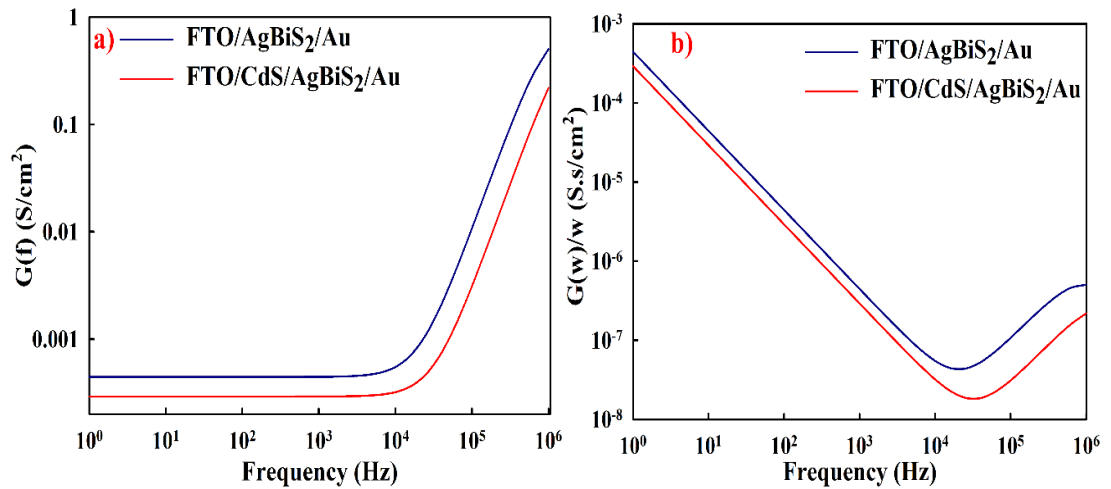


Figure 5 (a) G(f) and (b) G(ω)/ω spectra of D0 and D1.

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To probe the frequency-dependent electrical response of the two configurations, the conductance $G(f)$ and the normalized $G(\omega)/\omega$ spectra of D0 and D1 are presented in Fig. 5a and 5b. Both devices exhibit a low-frequency plateau followed by a pronounced increase above 10^4 Hz, which is consistent with frequency-dependent dielectric and interfacial contributions. The $G(\omega)/\omega$ curves display a well-defined minimum in the 10^4 – 10^5 Hz range, reminiscent of the minimum used in the Nicollian–Brews framework for interface analysis [21]. The persistence of a comparatively higher $G(\omega)/\omega$ signal in D0 across the intermediate frequency range indicates that the ETL-free configuration is not free from interfacial contributions, but that its front interface response differs qualitatively from that of D1. In contrast, the frequency response of D1 shows a broader distribution above 10^5 Hz, which is consistent with an interfacial region whose electrical response is modified by the CdS layer. A quantitative extraction of interface state densities from these curves would require the full Nicollian–Brews methodology and dedicated equivalent-circuit fitting, which are outside the scope of the present numerical analysis.

The Nyquist plots obtained under AM1.5G illumination as a function of AgBiS_2 thickness are shown in Fig. 6a and 6b for D0 and D1. Both configurations exhibit single semicircular arcs whose diameters evolve systematically with absorber thickness. This evolution reflects a thickness-dependent modification of the effective transport and interfacial impedance of the device rather than an unambiguous change in a single physical parameter. An explicit assignment of the arc diameter to a specific series, charge-transfer or recombination resistance would require dedicated equivalent-circuit fitting and is not attempted here. For a given AgBiS_2 thickness, the Nyquist arc of D1 is consistently larger than that of D0, indicating that the CdS-containing device presents a higher total impedance under the simulated conditions. The corresponding CdS thickness scan in Fig. 6c reveals a strong monotonic increase of the arc diameter as the CdS layer grows from 50 to 250 nm, in agreement with the observed decrease of J_{SC} over the same range.

The illumination-dependent Nyquist analysis presented in Fig. 7 was performed to examine whether the observed impedance difference between the two configurations persists under different spectral excitation conditions. Under standard 1-Sun illumination (Fig. 7a) the arc of D1 is clearly larger than that of D0. When a broad white spectrum in the 300–1300 nm range is applied (Fig. 7b), the difference between the two devices becomes even more pronounced, which is consistent with an additional short-wavelength contribution associated with the CdS layer. The most informative comparison appears in Fig. 7c, where a narrow visible spectrum in the 400–800 nm range is used. In this configuration the relative contribution of short-wavelength CdS absorption is reduced compared with the 300–1300 nm excitation. Despite this reduction the Nyquist arc of D1 remains significantly larger than that of D0. This observation suggests that optical filtering alone is insufficient to account for the larger impedance response of D1 and is consistent with an additional contribution from the CdS/ AgBiS_2 interface, which persists regardless of the incident spectral distribution [22].

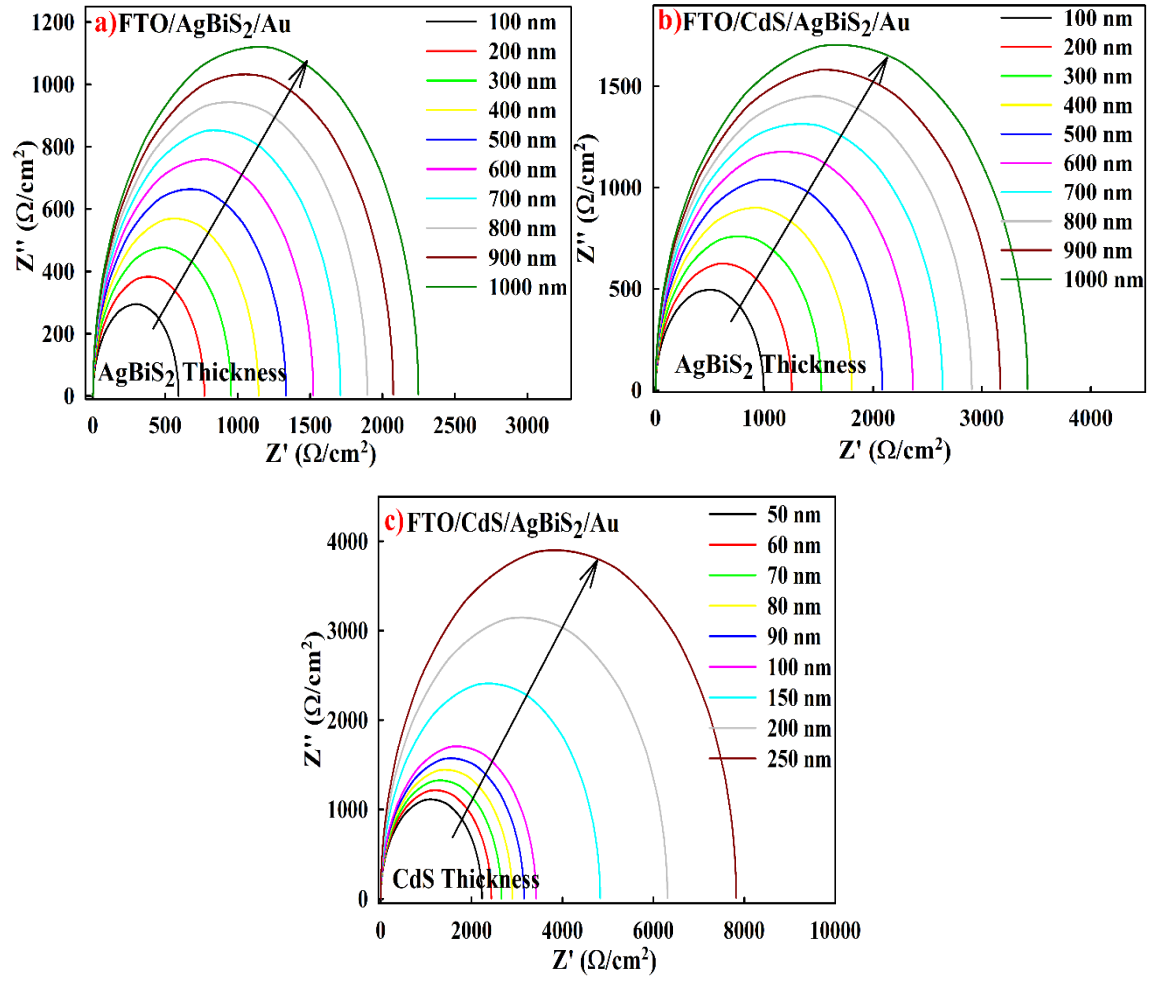
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Figure 6 Nyquist plots of D0 (a) and D1 (b) for varying AgBiS₂ thickness, and of D1 (c) for varying CdS thickness.

Table 2 Photovoltaic parameters of D0 and D1 under AM1.5G illumination.

Structure	$V_{oc}(V)$	$J_{sc}(mA/cm^2)$	$FF(\%)$	$\eta(\%)$
FTO/ABS/Au	0.917	30.885	82.31	23.32
FTO/CdS/ABS/Au	0.917	27.478	83.64	21.06
Relative Change	≈ 0	-11.0%	+1.6%	-9.7%

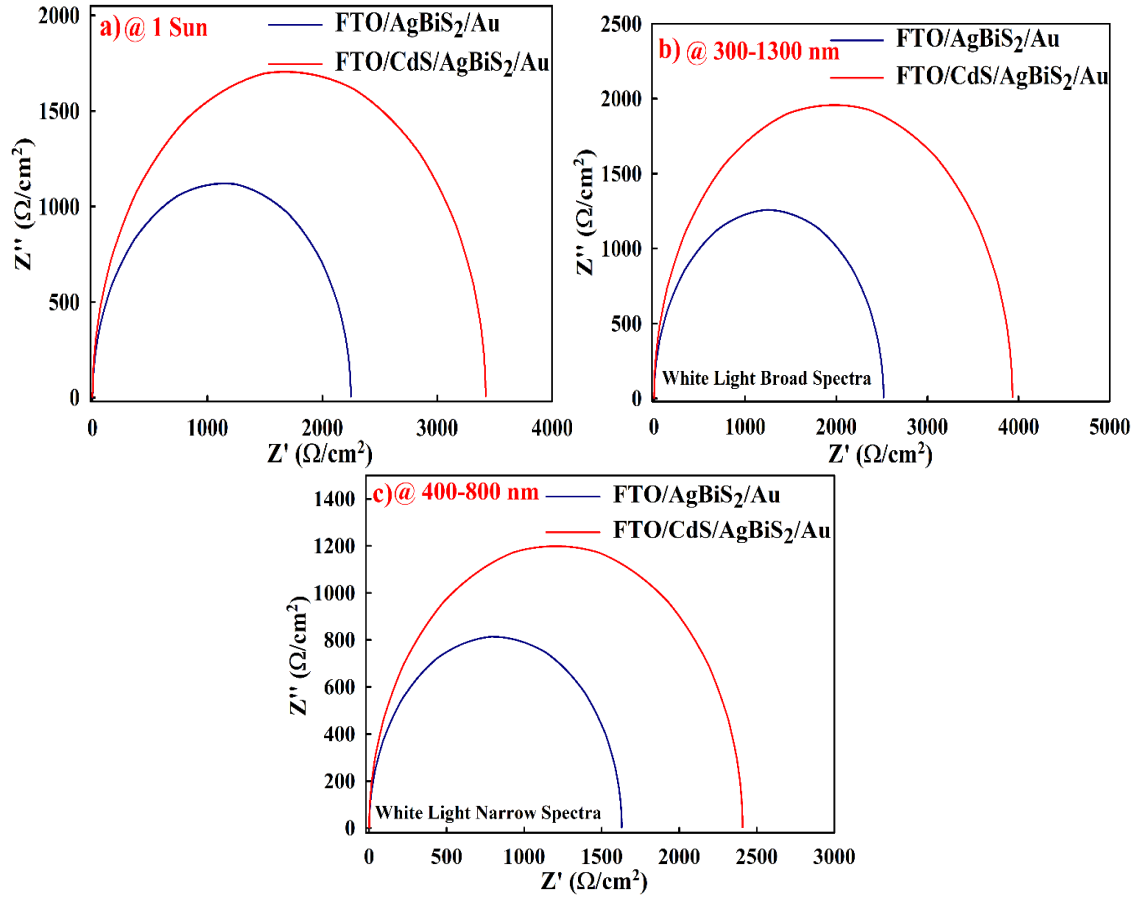
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Figure 7 Nyquist plots of D0 and D1 under (a) 1 Sun, (b) 300–1300 nm and (c) 400–800 nm illumination.

The photovoltaic parameters obtained under standard AM1.5G illumination for both configurations are summarized in Table 2. The ETL-free device D0 yields $V_{OC} = 0.917$ V, $J_{SC} = 30.885$ mA/cm², FF = 82.31% and a power conversion efficiency of 23.32%. The introduction of the CdS buffer in D1 leaves V_{OC} essentially unchanged at 0.917 V and slightly increases the fill factor to 83.64%, corresponding to a relative gain of +1.6%. However, J_{SC} drops significantly from 30.885 to 27.478 mA/cm², corresponding to a relative reduction of 11.0%. The resulting efficiency decreases to 21.06%, representing an absolute loss of 2.26% and a relative reduction of 9.7% with respect to D0. This outcome reveals a clear trade-off. The CdS buffer produces a modest improvement in the fill factor, but the associated reduction in short-circuit current density dominates the overall device response and leads to a lower power conversion efficiency. The nearly unchanged V_{OC} suggests that the CdS layer has a limited influence on the overall voltage-generating mechanism under the simulated conditions, while the slight enhancement of FF may be associated with the modified interfacial band alignment at the CdS/AgBiS₂ boundary. These results support the interpretation that CdS acts as an interfacial modifier whose net contribution to AgBiS₂-based photovoltaic performance depends critically on the balance between its optical, transport and interfacial effects [23].

Considered together, the J–V, EQE, spectral responsivity, conductance and impedance results form a coherent physical description of the two device configurations. The CdS buffer contributes to the device operation through two distinct sets of effects. On one hand it produces a modified band alignment at the front interface, which may be associated with the marginal improvement of the fill factor observed for D1. On the other hand it

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introduces additional short-wavelength optical attenuation and modifies the electrical response of the front region, both of which contribute to the systematic reduction of J_{SC} observed under all illumination conditions studied.

Conclusions

Two AgBiS₂-based photovoltaic architectures were compared by SCAPS-1D simulations, an ETL-free configuration (FTO/AgBiS₂/Au) and a CdS-containing counterpart (FTO/CdS/AgBiS₂/Au). The introduction of the CdS buffer left the open-circuit voltage essentially unchanged at 0.917 V and produced a modest improvement in fill factor from 82.31% to 83.64%, while the short-circuit current density decreased from 30.885 to 27.478 mA/cm². Impedance and conductance analyses consistently showed a larger and more complex electrical response for the CdS-containing device under all illumination conditions studied, which is consistent with a coupled contribution of short-wavelength optical attenuation and modified interfacial transport at the CdS/AgBiS₂ boundary. The thickness-resolved results further indicated that the CdS buffer contributes constructively only within a narrow thickness range and becomes increasingly detrimental as its thickness grows. These findings identify CdS as an interfacial modifier rather than a universally beneficial electron transport layer for AgBiS₂ solar cells and support the ETL-free FTO/AgBiS₂/Au architecture as a viable route for low-cost and Cd-free thin-film photovoltaic applications.

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Impact of ALD-Deposited ZnO Interlayer on the Dielectric Response and Electric Modulus of Al/p-Si Junctions

^{1*}A. KARACA

^{1*}*Department of Physics, Faculty of Arts and Sciences, Yozgat Bozok University, Yozgat 66000, Türkiye.*

Abstract

In this study, Al/ZnO/p-Si heterojunction structures were fabricated by depositing a 5 nm ZnO interlayer on p-type Si (100) substrates via atomic layer deposition, followed by thermal evaporation of Al top contacts. Frequency- and voltage-dependent dielectric and electrical characteristics were systematically examined through admittance spectroscopy across 1 kHz–1 MHz and –2 to +2 V. Capacitance–voltage and conductance–voltage measurements revealed pronounced low-frequency dispersion, attributed to interface trap states at the ZnO/p-Si junction that respond to the AC signal only at lower frequencies. Derived dielectric parameters, including effective complex permittivity components, loss tangent, and electric modulus, indicated a dielectric response consistent with Maxwell–Wagner-type interfacial polarization alongside trap-assisted relaxation. Cole–Cole analysis revealed a broadened distribution of relaxation times, which can be attributed to defect-mediated relaxation dynamics, plausibly associated with hopping processes within the ultrathin ALD-grown ZnO layer. These findings offer critical insight into the interfacial charge dynamics and relaxation behavior of ZnO/p-Si heterostructures, underscoring the importance of understanding interfacial polarization and defect dynamics for the design and optimization of sub-10 nm oxide-based heterojunction devices.

Keywords: Atomic layer deposition (ALD), ZnO/p-Si heterojunction, Admittance spectroscopy, Dielectric, Interface states.

Corresponding authors: abdullah.karaca@bozok.edu.tr

1. Introduction

Heterojunctions based on transition metal oxide interlayers integrated onto single-crystal silicon substrates represent a highly effective device architecture for modern electronic and optoelectronic technologies [1]. Among various binary oxides, zinc oxide (ZnO) is an exceptional candidate due to its wide direct bandgap, high exciton binding energy, robust chemical stability, and favorable energy band alignment when paired with p-type silicon [2,3]. However, the operational performance of such heterostructures is heavily dictated by the physical quality and thickness uniformity of the interfacial layer [4,5]. Traditional deposition techniques frequently introduce pinhole pathways, non-uniform film thickness, and uncontrolled trap distributions that intensify unwanted carrier recombination [6]. In this context, atomic layer deposition (ALD) stands out as an advanced synthesis route that utilizes self-limiting surface chemical reactions to achieve precise thickness control, yielding pinhole-free, highly conformal thin oxide interlayers with structural homogeneity [7,8].

Evaluating the dynamic electrical and dielectric properties of these heterojunctions under alternating current (AC) electric fields is essential for understanding their internal charge transport mechanisms and barrier dynamics [9]. Admittance spectroscopy serves as a powerful non-destructive analytical approach to probe how charge carriers and localized states respond across varying bias voltages and signal frequencies. Under small-signal AC modulation, the overall device response is governed by the kinetic behavior of interface trap states located at the oxide-semiconductor junction. At lower frequencies, these interface traps can capture and emit charge carriers in phase with the applied signal, leading to noticeable capacitance dispersion. As the perturbation frequency escalates, the trap emission rates cannot keep pace with the rapidly oscillating field, causing a freeze-

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out effect where the contribution of slower interface states is progressively suppressed, leaving a response increasingly dominated by faster dielectric and bulk processes. In particular, the presence of interface states at the ZnO/p-Si boundary can give rise to anomalous dispersion in the low-frequency regime, while bulk defects within the oxide layer, such as oxygen vacancies, contribute to relaxation processes that are analyzed in depth for ALD-grown ZnO films [10,11]. Despite extensive research on thicker oxide interlayers, a detailed understanding of the dynamic dielectric response and charge relaxation kinetics across sub-10 nm ALD-grown oxide barriers remains incomplete.

The present study systematically investigates the frequency- and voltage-dependent electrical and dielectric characteristics of Al/ZnO/p-Si heterojunction structures featuring an ultrathin 5 nm ZnO interlayer deposited via atomic layer deposition. Through admittance spectroscopy conducted across a broad frequency spectrum (1 kHz to 1 MHz) and bias voltage window (−2.0 V to +2.0 V), capacitance–voltage and conductance–voltage characteristics demonstrated pronounced low-frequency dispersion attributed to interface trap states. Furthermore, derived dielectric parameters—including complex permittivity components, loss tangent, dynamic AC conductivity, and complex electric modulus—suggested dielectric behaviors consistent with Maxwell–Wagner-type interfacial polarization and trap-assisted relaxation processes, while Cole–Cole arc evaluations verified distributed relaxation times associated with defect-mediated hopping conduction through localized defect states, plausibly attributed to oxygen vacancies, within the 5 nm ZnO layer. These findings not only provide a detailed picture of the interfacial charge dynamics and relaxation behavior of ZnO/p-Si heterostructures but also highlight the importance of controlling the ALD-grown interfacial layer and its defect population in determining the dielectric response. The results underscore the critical role of interfacial polarization and defect dynamics in governing the AC electrical response of ultrathin oxide-based heterojunctions.

2. Experimental details

The fabrication of the Al/ZnO/p-Si heterojunction structures commenced with single-side polished p-type Si (100) wafers featuring a carrier concentration of $7.3 \times 10^{15} \text{ cm}^{-3}$. The substrates were sectioned into $1 \times 2 \text{ cm}^2$ chips and systematically cleaned by sequential ultrasonic agitation in acetone, deionized water, and isopropanol. To strip the native oxide (SiO_2) layer, the clean Si substrates were immersed in a dilute $\text{HF:H}_2\text{O}$ (1:10) solution for 30 seconds, followed by thorough rinsing in deionized water and dry nitrogen blow-drying. Low-resistance rear Ohmic contacts were established by thermally evaporating a 150 nm-thick aluminum (Al) film onto the unpolished back side, followed by thermal annealing at 450°C in a nitrogen atmosphere for a brief duration. Subsequently, a thin 5 nm ZnO interlayer was deposited onto the polished front surface of the p-Si substrates using a Savannah S300 Atomic Layer Deposition (ALD) platform at a substrate temperature of 200°C . A calibrated growth rate of 2 Å per cycle was applied to deposit the ZnO thin films, where the nominal thickness of 5 nm corresponds to 25 ALD cycles. The morphological integrity and smooth surface pattern of the ALD-grown ZnO films on p-Si were verified in a separate study reported by Yildiz et al. [12]. Finally, 100 nm-thick Al top Schottky contacts were thermally deposited through a shadow mask containing circular apertures, yielding an active device area of $7.85 \times 10^{-3} \text{ cm}^2$.

The dynamic electrical response and interfacial dielectric properties of the fabricated Al/ZnO/p-Si heterojunction diodes were investigated using admittance spectroscopy ($Y = G + j\omega C$), as shown in Fig. 1. Parallel capacitance (C) and conductance (G) characteristics were simultaneously recorded as a function of DC bias voltage spanning from −2.0 V to +2.0 V (in 0.05 V increments) under small-signal AC perturbation. The test frequency was swept across a broad range from 1 kHz to 1 MHz at room temperature. The complex dielectric permittivity ($\epsilon^* = \epsilon' - j\epsilon''$), dielectric loss tangent ($\tan\delta$), dynamic AC conductivity (σ_{ac}), and complex electric

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modulus ($M^* = M' + jM''$) were systematically derived from the experimental admittance data using fundamental geometric relations.

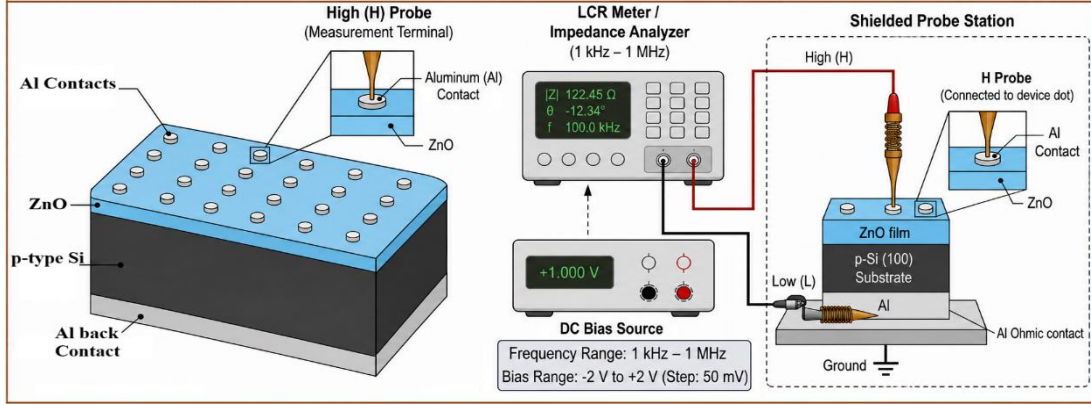


Figure 1 Schematic device structure and impedance measurement setup for ZnO/p-Si heterojunction.

3. Results and discussion:

The frequency- and bias-dependent admittance spectroscopy characteristics of the fabricated Al/ZnO/p-Si heterojunction diodes were systematically analyzed using the fundamental mathematical relations summarized in Table 1.

Figure 2a displays the capacitance–voltage (C – V) profiles recorded across a frequency range of 1 kHz to 1000 kHz within a bias window of -2.0 V to $+2.0$ V. A pronounced frequency dispersion is observed, particularly in the positive bias region (0.0 V to $+2.0$ V). At low test frequencies (1 kHz to 20 kHz), the capacitance increases rapidly with bias voltage, forming a broad peak near $+0.5$ V with a maximum of 1.58×10^{-8} F at 1 kHz. This low-frequency accumulation behavior originates from interface trap states localized at the ALD-ZnO/p-Si junction, which possess relaxation times fast enough to follow the small-signal AC perturbation ($\omega=2\pi f$, Table 1, Eq. 1). Conversely, as the frequency increases to 1000 kHz, the capacitance drops to $\sim 1.14 \times 10^{-9}$ F due to the inability of interface states to respond to fast signal oscillations [13,14].

To evaluate the uncompensated acceptor concentration and built-in potential (V_{bi}), Mott–Schottky ($1/C^2$ – V) analysis was performed in the depletion regime (-2.0 V to 0 V) using Table 1, Eq. 4. As shown in Figure 2b, linear fits at high frequencies (500 kHz and 1000 kHz) suppress trap contributions, yielding negative slopes that are consistent with the p-type character of the Si substrate. The linear regression equations are $y=-11.89x-9.37$ at 500 kHz and $y=-10.76x-4.86$ at 1000 kHz, corresponding to voltage axis intercepts ($V_0 = -V_{intercept}$) of 0.79 V and 0.45 V, respectively. Accounting for the thermal voltage correction term ($V_{bi} = V_0 + kT/q$, where $kT/q \approx 0.026$ V at room temperature), the built-in potential (V_{bi}) values were determined as 0.81 V (at 500 kHz) and 0.48 V (at 1000 kHz). The observed frequency-dependent shift in V_{bi} reflects deep-level trap modulation and spatial barrier height fluctuations at the thin 5 nm ALD-grown ZnO interface [15,16].

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Table 1 Fundamental relations for admittance, dielectric, conductivity, and impedance analysis of Al/ZnO/p-Si heterojunction diodes.

Eq. No:	Equation	Relation
1	$w = 2\pi f$	Angular frequency
2	$Y = G + j\omega C$	Complex admittance
3	$K = \frac{d}{\varepsilon_0 A}$	Geometric factor
4	$\frac{1}{C^2} = \frac{2}{q\varepsilon_s\varepsilon_0 A^2 N_A} (V_{bi} - V - \frac{kT}{q})$	Mott-Schottky relation
5	$\phi_B = V_{bi} + \frac{kT}{q} \ln(\frac{N_V}{N_A})$	Barrier height
6	$\frac{G_p}{\omega} = \frac{\omega C_i^2 G}{(G^2 + \omega^2(C_i - C)^2)}$	Parallel conductance
7	$\tau_{it} = \frac{1}{2\pi f_{max}}$	Trap relaxation time
8	$\varepsilon' = C \cdot K$	Real permittivity
9	$\varepsilon'' = \frac{G \cdot K}{\omega}$	Imaginary permittivity
10	$\varepsilon^* = \varepsilon' - j\varepsilon''$	Complex permittivity
11	$\tan \delta = \frac{G}{\omega C}$	Loss tangent
12	$\sigma_{ac} = \omega\varepsilon_0\varepsilon'' = G \cdot d/A$	AC conductivity
13	$M' = \frac{\varepsilon'}{\varepsilon'^2 + \varepsilon''^2}$	Real modulus
14	$M'' = \frac{\varepsilon''}{\varepsilon'^2 + \varepsilon''^2}$	Imaginary modulus
15	$M^* = \frac{1}{\varepsilon^*} = M' + jM''$	Complex modulus
16	$Z' = \frac{G}{G^2 + \omega^2 C^2}$	Real impedance
17	$Z'' = -\frac{\omega C}{G^2 + \omega^2 C^2}$	Imaginary impedance

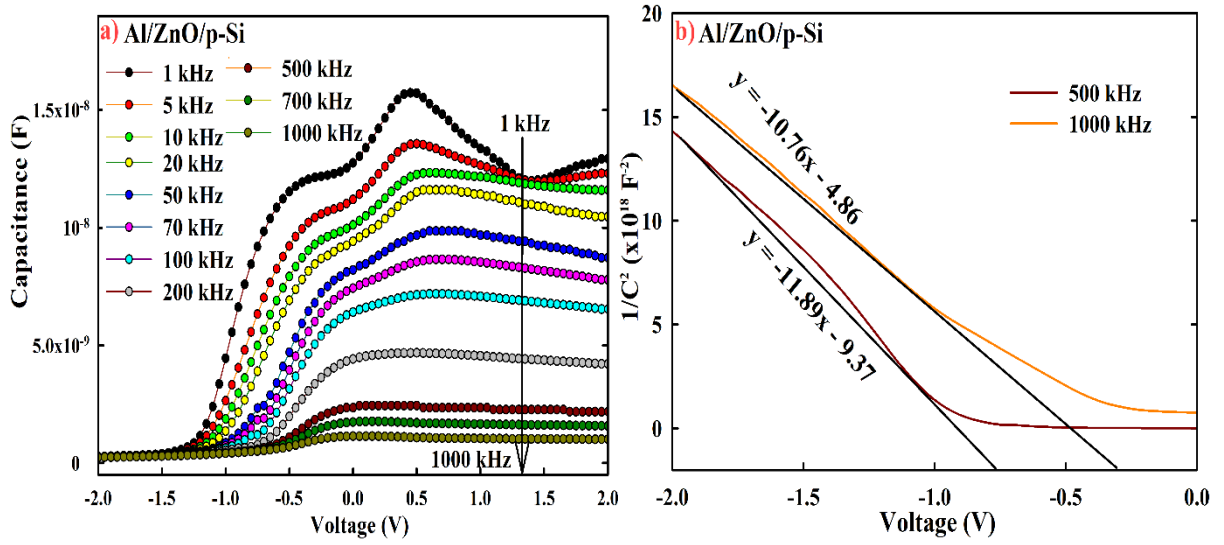


Figure 2 a) Capacitance–voltage and b) inverse capacitance–voltage characteristics of Al/ZnO/p-Si heterojunction at different frequencies.

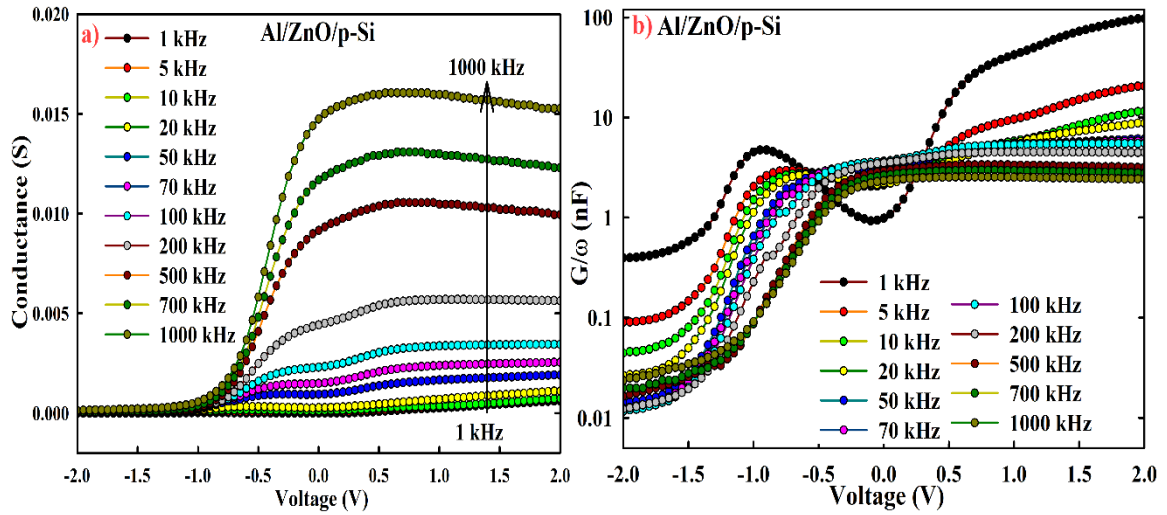


Figure 3 Frequency-dependent conductance characteristics of Al/ZnO/p-Si heterojunction.

Figure 3a depicts the bias-dependent conductance (G – V) characteristics, where G increases systematically with both frequency and forward bias, reaching a maximum of $\sim 0.015 \text{ S}$ at 1000 kHz. This rise is associated with enhanced carrier transport and increased defect-assisted conduction across the 5 nm ALD-ZnO interlayer under forward bias and high-frequency excitation. The normalized conductance (G/ω – V) curves in Figure 3b reveal a prominent loss peak at low frequencies (1 kHz) centered near -0.9 V and $+0.5 \text{ V}$, which systematically suppresses as frequency increases, confirming energy dissipation mediated by interface trap states (D_{it}) that cannot follow high-frequency AC perturbations (Table 1, Eq. 6). Correspondingly, the voltage-dependent series resistance (R_s) profiles shown in Figure 4, evaluated via the real part of complex impedance, demonstrate a strong frequency dispersion where R_s drops precipitously from $\sim 2.7 \times 10^5 \Omega$ at 1 kHz to a stable baseline of $\sim 60 \Omega$ at 1000 kHz in the depletion region [17,18]. The characteristic peaks observed in $R_s(V)$ near the depletion-

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to-accumulation transition region (-0.8 V to $+0.5$ V) gradually flatten at higher frequencies, proving that low-frequency admittance is heavily distorted by interface state restructuring, whereas high-frequency modulation significantly reduces the contribution of slower interface-state processes, thereby approaching the true bulk resistance of the Al/ZnO/p-Si heterojunction.

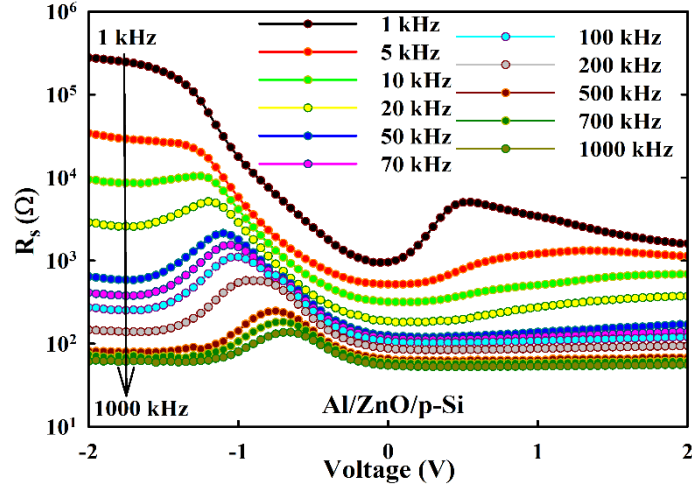


Figure 4 Frequency-dependent series resistance (R_s) of Al/ZnO/p-Si heterojunction as a function of applied voltage.

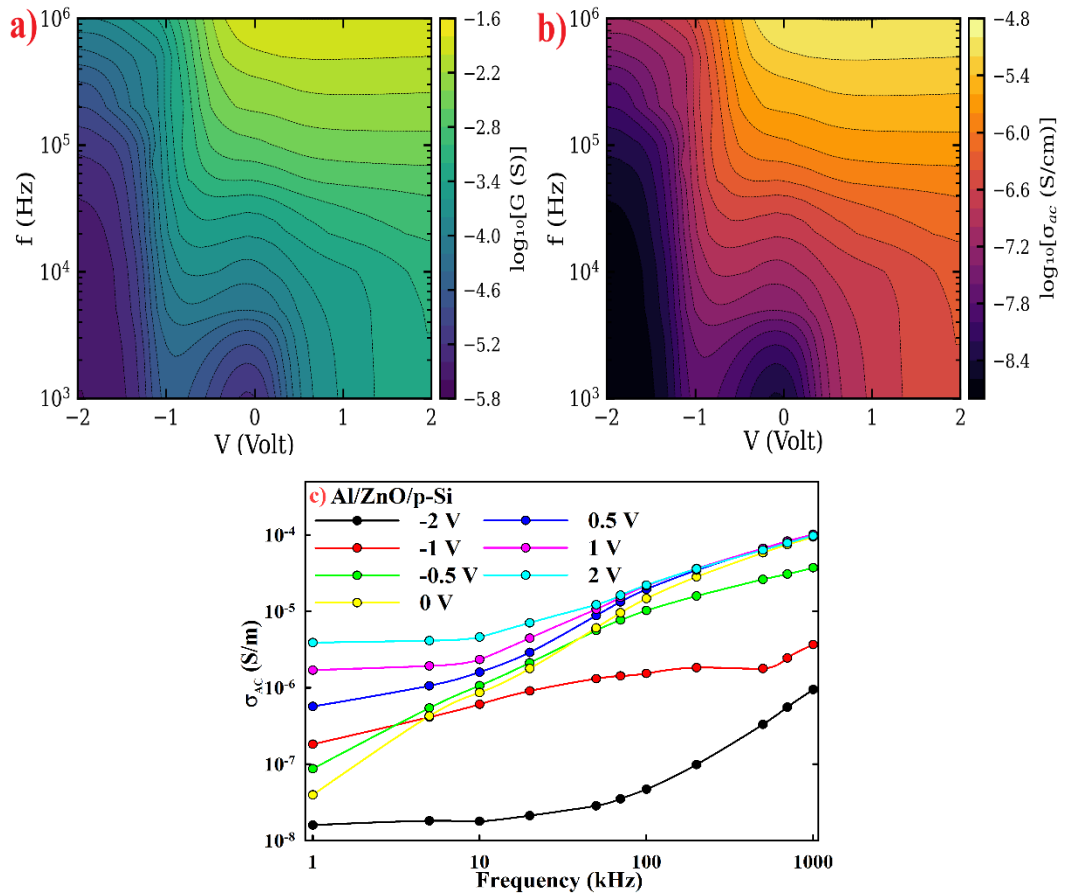


Figure 5 Voltage- and frequency-dependent DC and AC conductivity of Al/ZnO/p-Si heterojunction.

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To comprehensively map the dynamic charge transport kinetics, 2D contour representations of the conductance ($\log_{10}G$) and dynamic AC conductivity ($\log_{10}\sigma_{ac}$) as functions of bias voltage (-2.0 V to $+2.0$ V) and frequency (1 kHz to 1 MHz) are depicted in Figures 5a and 5b, respectively. Both contour maps clearly illustrate that minimum conductance and conductivity values ($\log_{10}\sigma_{ac} \approx -8.4$ S/cm) occur under strong reverse bias at low frequencies, whereas forward bias and high-frequency excitation trigger a dramatic enhancement in carrier transport, reaching maximum conduction states ($\log_{10}\sigma_{ac} \approx -4.8$ S/cm). Figure 5c details the frequency dispersion of σ_{ac} at selected bias voltages, evaluated via Table 1, Eq. 12. At low frequencies (<10 kHz), σ_{ac} remains nearly frequency-independent, representing the low-frequency quasi-DC transport contribution (σ_{dc}). However, at higher frequencies (>10 kHz), σ_{ac} increases monotonically following Jonscher's universal power law ($\sigma_{ac} \propto \omega^s$). The sub-linear frequency exponent ($0 < s < 1$) observed across all bias levels is consistent with a correlated barrier hopping (CBH) mechanism, where localized charge carriers hop between defect-induced localized states—plausibly related to oxygen vacancies—over potential barriers modulated by the applied small-signal AC field [19-21].

The bias- and frequency-dependent complex dielectric permittivity components (ϵ' , ϵ'') and loss tangent ($\tan\delta$), evaluated using Table 1, Eqs. 8, 9, and 11, are presented in Figure 6. As observed in Figure 6a, the real permittivity (ϵ') reaches maximum values (~ 10) under accumulation bias at 1 kHz and systematically decreases with increasing frequency down to ~ 0.82 at 1 MHz. It should be noted that these ϵ' values represent the effective dielectric response of the entire heterojunction structure rather than the intrinsic permittivity of the 5 nm ZnO layer alone, as the measured capacitance incorporates series contributions from the oxide barrier, the p-Si depletion region, and interface states. This dispersion can be phenomenologically described within the framework of Maxwell–Wagner–Sillars (MWS) interfacial polarization and Koops' two-layer model, where charge accumulation at the ALD-ZnO/p-Si heterointerface and depletion space-charge dynamics govern the low-frequency dielectric response, whereas space charges freeze out at higher perturbation frequencies [22,23]. Correspondingly, the imaginary permittivity (ϵ'' , Figure 6b) and loss tangent ($\tan\delta$, Figure 6c) display prominent relaxation peaks in the depletion region (around -0.9 V), which attenuate at higher frequencies as interface traps lose their ability to follow the AC signal, while the increase in $\tan\delta$ under strong forward bias at high frequencies is governed by parasitic series resistance dissipation. To suppress low-frequency electrode polarization artifacts and emphasize relaxation processes that are less affected by electrode polarization, the complex electric modulus formalism ($M^* = M' + jM''$) was analyzed using Table 1, Eqs. 13–15, as shown in Figure 7. As depicted in Figure 7a, the real modulus (M') exhibits higher values under reverse bias (depletion regime) and approaches zero in the accumulation region, displaying an opposite trend to ϵ' due to the inverse permittivity relationship ($M^* = 1/\epsilon^*$). The imaginary modulus profiles (M'' , Figure 7b) reveal characteristic relaxation peaks in the transition region (-0.7 V to -0.8 V) that vary systematically with test frequency. The presence and systematic dispersion of the M'' peaks are consistent with localized relaxation processes and provide evidence for a significant contribution from short-range charge dynamics at the ALD-ZnO/p-Si interface.

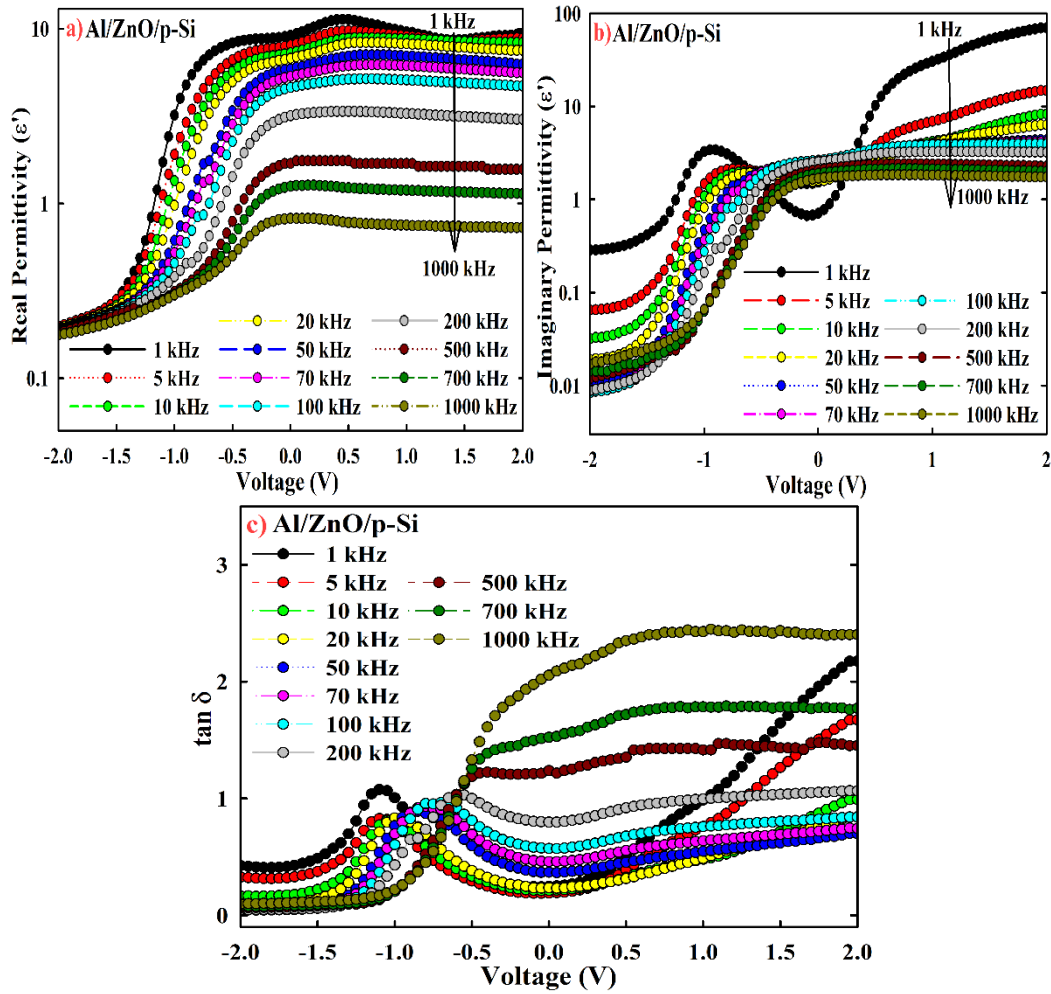
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Figure 6 Voltage- and frequency-dependent dielectric properties (ϵ' , ϵ'' , and $\tan \delta$) of Al/ZnO/p-Si heterojunction.

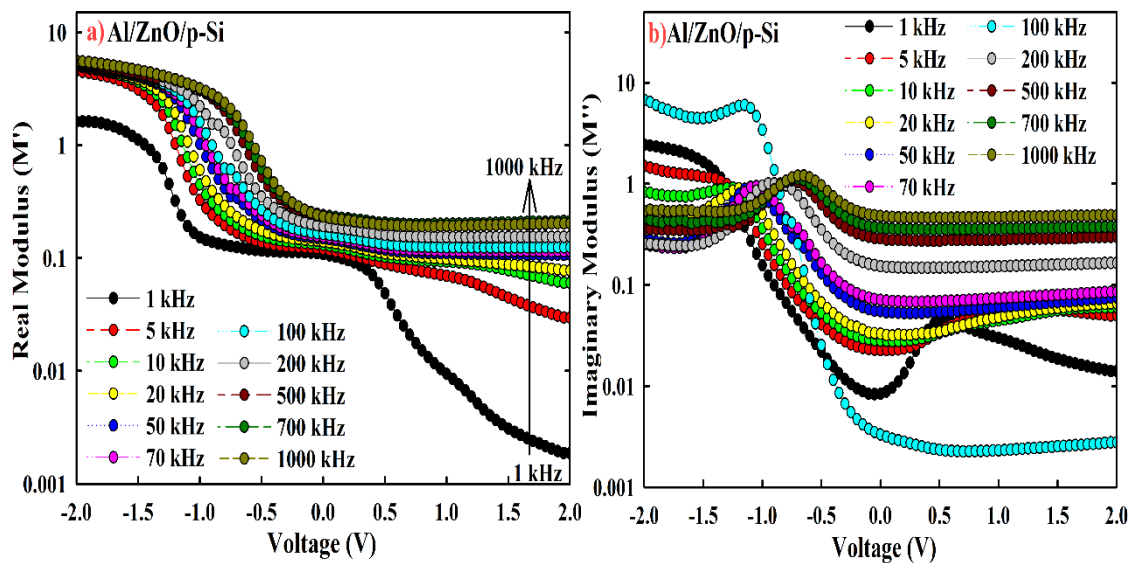


Figure 7 Voltage- and frequency-dependent real (M') and imaginary (M'') electrical modulus of Al/ZnO/p-Si heterojunction.

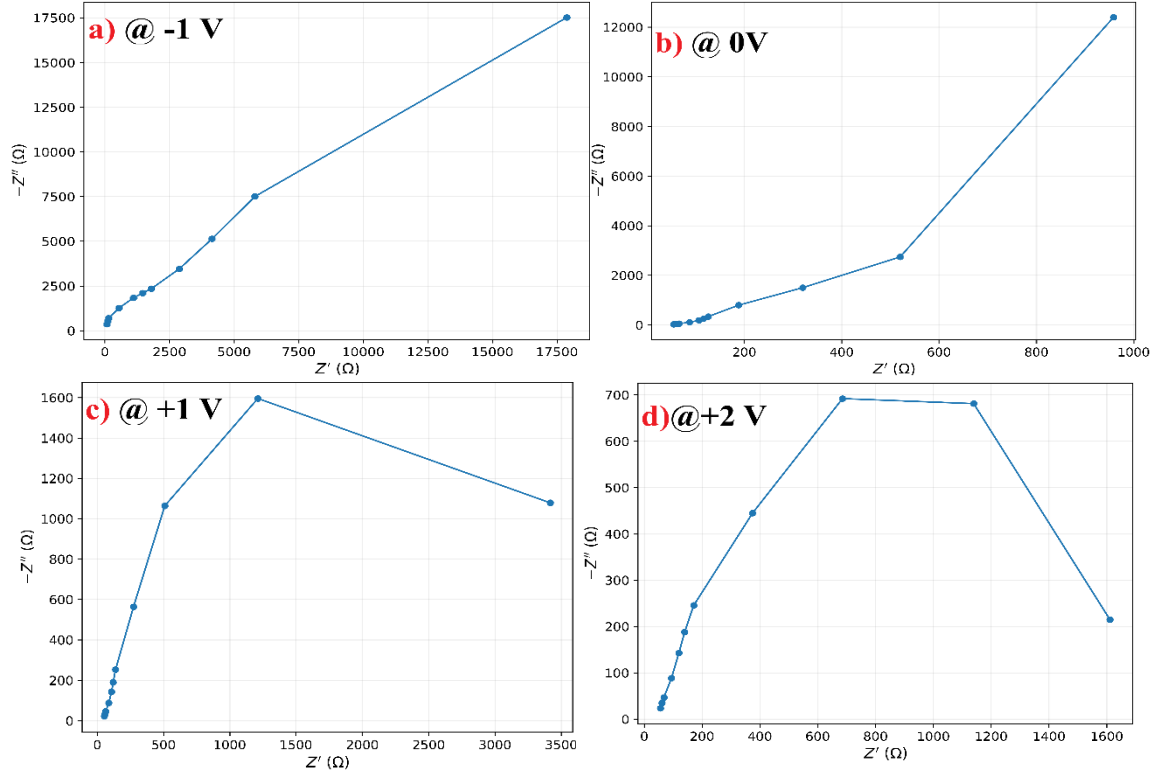
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Figure 8 Nyquist impedance spectra ($-Z''$ vs. Z') of Al/ZnO/p-Si heterojunction measured at different applied voltages

Table 2 Frequency-dependent electrical parameters of Al/ZnO/p-Si heterojunction.

Frequency (f)	C (F)	G (S)	ϵ'	ϵ''	M'	M''	$\tan \delta$	$\sigma_{ac}(S/cm)$
1 kHz	1.28×10^{-8}	1.14×10^{-5}	9.20	1.30	0.107	0.0151	0.141	7.26×10^{-10}
10 kHz	1.01×10^{-8}	2.42×10^{-5}	7.26	0.276	0.137	0.0052	0.038	1.54×10^{-9}
100 kHz	6.41×10^{-9}	1.22×10^{-4}	4.61	0.139	0.217	0.0065	0.030	7.77×10^{-9}
1 MHz	1.14×10^{-9}	1.58×10^{-3}	0.82	0.181	1.163	0.2567	0.221	1.01×10^{-7}

To further elucidate the interfacial charge transport dynamics and equivalent circuit behavior, complex impedance spectra (Nyquist plots, $-Z''$ vs. Z') measured under applied bias voltages are depicted in Figures 8a–d, with the key parameters summarized in Table 2. Under reverse (-1 V) and zero-bias (0 V) conditions (Figs. 8a and 8b), the spectra display large, incomplete capacitive arcs characterized by high real (Z') and imaginary ($-Z''$) impedance values, reflecting a wide depletion region and a high junction polarization resistance (R_p). Upon transitioning to forward bias ($+1.0$ V and $+2.0$ V, Figs. 8c and 8d), the internal potential barrier shrinks, promoting barrier-limited carrier injection and trap-assisted hopping conduction across the thin ALD-ZnO interlayer. Consequently, the Nyquist radii contract dramatically, evolving into defined depressed semicircular arcs [24]. The depression of these arcs signifies a clear deviation from ideal Debye relaxation, which is attributed to localized state distributions, spatial barrier height fluctuations, and structural micro-inhomogeneities inherent to atomic layer deposited thin oxide interfaces [25]. For a rigorous quantitative assessment at 0 V, the relaxation time calculated directly from the peak frequency of the imaginary impedance spectrum yields $\tau_{peak} = 1.592 \mu s$. Concurrently, non-linear least-squares fitting of the experimental data using the empirical Cole–Cole impedance

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model yields a characteristic relaxation time of $\tau = 1.649 \mu\text{s}$, a broadness parameter of $\alpha=0.643$, and a high coefficient of determination $R^2 = 0.986$. The fractional exponent ($\alpha = 0.643 < 1$) quantitatively confirms a distribution of relaxation times associated with multi-channel hopping processes via defect levels, likely originating from oxygen vacancies, at the ALD-ZnO/p-Si boundary. Remarkably, the high degree of proximity between the independently evaluated relaxation time constants ($\tau_{peak} = 1.592 \mu\text{s}$ and Cole–Cole $\tau = 1.649 \mu\text{s}$) provides an independent consistency check for the extracted characteristic relaxation time, supporting the interpretation that defect-mediated interfacial relaxation makes a substantial contribution to the observed AC response in the Al/ZnO/p-Si heterojunction.

Conclusions

In conclusion, the dynamic electrical, dielectric, and interfacial relaxation kinetics of Al/ZnO/p-Si heterojunction structures featuring an ultrathin ALD-grown ZnO interlayer were systematically established via admittance spectroscopy (1 kHz–1 MHz, –2 V to +2 V). Pronounced low-frequency capacitance and conductance dispersion confirmed the active participation of interface trap states, while effective complex permittivity and electric modulus analyses revealed dielectric relaxation kinetics consistent with Maxwell–Wagner-type interfacial polarization alongside trap-assisted relaxation processes. Furthermore, complex impedance and Cole–Cole evaluations revealed a distributed relaxation mechanism ($\alpha=0.643$) associated with defect-mediated charge transport, consistent with a correlated barrier hopping (CBH) mechanism via localized defect states plausibly associated with oxygen vacancies, supported by the physical consistency between the derived relaxation times ($\tau_{peak} = 1.592 \mu\text{s}$ vs. Cole–Cole $\tau = 1.649 \mu\text{s}$), which provides an independent consistency check for the extracted characteristic relaxation time. Overall, these findings demonstrate that ALD oxide barriers afford precise control over interfacial polarization and defect dynamics, providing fundamental insights into interfacial polarization, trap dynamics, and charge transport essential for optimizing ultrathin oxide-semiconductor junction architectures.

Acknowledgments

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First report on the green synthesis of silver nanoparticles using *Magnolia grandiflora* leaf extract as a sustainable biogenic reducing agent

R. Sanayeva¹, E. Kasapoglu², M. B. Yücel^{3*}

¹*Department of Physics, Institute of Natural and Applied Science, Akdeniz University, Antalya 07058, Türkiye*

²*Department of Physics, Faculty of Science, Sivas Cumhuriyet University, Sivas 58140, Türkiye*

^{3*}*Department of Physics, Faculty of Science, Akdeniz University, Antalya 07058, Türkiye*

Abstract

Silver nanoparticles (AgNPs) exhibit distinctive nanoscale optical properties arising from localized surface plasmon resonance (LSPR), making them promising for plasmonic, sensing, photonic, and optoelectronic applications. In this study, AgNPs were synthesized via a simple and environmentally sustainable green route using an aqueous extract of shade-dried *Magnolia grandiflora* leaves as a biological reducing and stabilizing medium. A 0.1 mM AgNO₃ solution was added dropwise to a 1% (w/v) leaf extract maintained at 70 °C under continuous stirring, and nanoparticle formation was evaluated by UV–Vis absorption spectroscopy over 350–700 nm without sample dilution. The original leaf extract showed no distinct absorption maximum in the investigated visible region, whereas the AgNP-containing solution exhibited a pronounced and broad absorption band centered at approximately 440 nm. The emergence of this band was attributed to the LSPR of metallic silver nanostructures and provides clear spectroscopic evidence of AgNP formation. The LSPR maximum was slightly red-shifted relative to previously reported values of approximately 417–425 nm for *Magnolia grandiflora*-mediated AgNPs. This shift, together with the broad plasmonic profile, may reflect differences in nanoparticle characteristics, interparticle interactions, surface-bound phytochemicals, and the local dielectric environment; however, these contributions cannot be distinguished by UV–Vis spectroscopy alone. The results demonstrate that aqueous *Magnolia grandiflora* leaf extract provides an effective and sustainable platform for producing silver nanostructures with a well-defined plasmonic response. Further structural and morphological characterization will enable correlation of the observed LSPR behavior with the physicochemical properties of the synthesized AgNPs.

Keywords: Silver nanoparticles (AgNPs), Green synthesis, Localized surface plasmon resonance (LSPR)

Corresponding author: myucel@akdeniz.edu.tr

1. Introduction

Nanoparticles (NPs) have attracted considerable attention because of their nanoscale dimensions, high surface-to-volume ratios, and size-dependent physicochemical properties, which provide a wide range of potential applications in physics, materials science, environmental technologies, energy, and biomedicine [1]. Among metallic NPs, AgNPs are particularly important due to their distinctive optical response, high electrical and thermal conductivity, and electromagnetic properties [2]. One of their most characteristic physical features is LSPR, which originates from the collective oscillation of conduction electrons induced by incident electromagnetic radiation. The strong plasmonic response of AgNPs makes these nanostructures particularly attractive for applications in optical sensing, surface-enhanced Raman spectroscopy (SERS), photonics, optoelectronics, and advanced sensor technologies. In addition, their well-established antimicrobial activity has stimulated considerable interest in biomedical and environmental applications [3].

Conventional physical and chemical methods for AgNP synthesis may involve high energy consumption, costly processes, and potentially hazardous reagents. Green synthesis has therefore emerged as an environmentally sustainable alternative in which biological materials can serve as reducing and stabilizing agents [1-3]. Plant

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extracts are particularly attractive for this purpose because naturally occurring phenolic compounds, flavonoids, and other phytochemicals may participate in the reduction of Ag^+ ions to metallic Ag^0 and subsequently contribute to NP capping and stabilization [4].

Magnolia is a promising biological source for AgNP synthesis because of its phytochemical composition and reported antioxidant properties [5-7]. In particular, phytochemical studies have demonstrated the presence of various flavonoids, including derivatives of apigenin, luteolin, quercetin, kaempferol, and isorhamnetin, in different organs of several Magnolia species.

Previous work by Okafor et al. [3] demonstrated the feasibility of synthesizing AgNPs using an aqueous *Magnolia grandiflora* leaf extract and monitoring NP formation by UV–Vis spectroscopy, confirming the suitability of this plant species for biological AgNP synthesis.

In the present study, an aqueous extract prepared from shade-dried *Magnolia grandiflora* leaves was used for the green synthesis of AgNPs. NP formation was investigated by UV–Vis absorption spectroscopy, with particular emphasis on the characteristic LSPR behavior of the resulting silver nanostructures. The main objective was to evaluate *Magnolia grandiflora* leaf extract as a simple and sustainable biological medium for AgNP synthesis and to investigate the optical and electronic responses of the synthesized nanostructures.

2. Experimental details

The *Magnolia grandiflora* leaves used in this study and the experimental procedure are illustrated in Fig. 1. Fresh *Magnolia grandiflora* leaves were collected in Döşemealtı, Antalya, Türkiye, washed twice with tap water and subsequently twice with distilled water to remove surface impurities, and then shade-dried for approximately two months. The dried leaves were ground using an electric grinder (Arzum AR1034). A 1% (w/v) aqueous leaf extract was prepared by dispersing 2.0 g of the ground leaves in 200 mL of distilled water, followed by heating at 70 °C under continuous hot plate magnetic stirring at 500 rpm for 30 min. After cooling to room temperature, the extract was first filtered through cheesecloth and subsequently through quantitative filter paper (Filter-Lab 1244) and stored at 4 °C until use. For the green synthesis of AgNPs, 15 mL of the prepared leaf extract was maintained at 70 °C under continuous stirring at 500 rpm, and 0.1 mM AgNO_3 solution was added dropwise. The addition was stopped upon observation of a distinct color change, corresponding to a total AgNO_3 volume of 3.4 mL. The resulting AgNP-containing solution was allowed to cool to room temperature, protected from light by wrapping the sample container with aluminum foil, and stored under dark conditions until characterization. The optical response of the synthesized AgNPs was investigated using a THORLABS CCS Series (CCS100/M) optical spectrometer (350–700 nm), and the samples were measured directly without dilution.

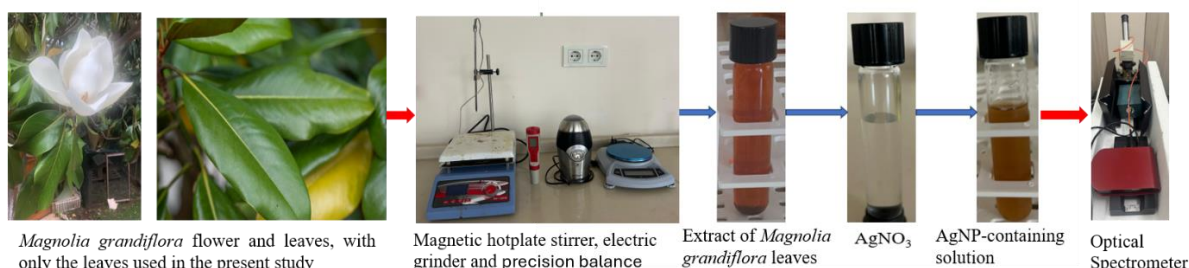


Figure 1 Experimental workflow for preparation of the aqueous *Magnolia grandiflora* leaf extract and green synthesis of AgNPs

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3. Results and discussion:

As shown in Fig. 2, UV–Vis spectroscopy confirmed AgNP formation, revealing a broad LSPR band at approximately 440 nm, which was absent in the original *Magnolia grandiflora* leaf extract. Compared with the 417–425 nm range reported by Okafor et al. [3], the observed red shift may be associated with differences in nanoparticle characteristics, aggregation, surface chemistry, or synthesis conditions.

Phytochemicals present in *M. grandiflora* extract may facilitate the reduction of Ag^+ to Ag^0 and contribute to nanoparticle stabilization. However, complementary techniques such as AFM, SEM, or TEM are required to determine particle size and morphology.

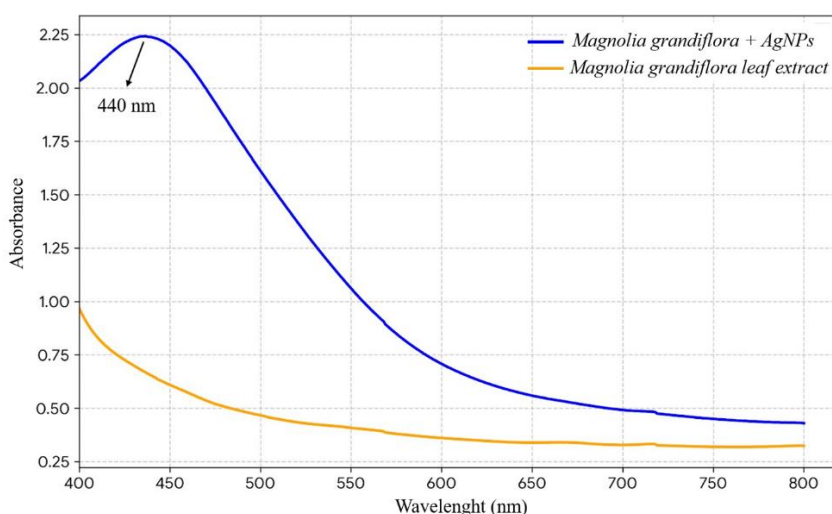


Figure 2 UV–Vis absorption spectra of the aqueous extract prepared from shade-dried *Magnolia grandiflora* leaves and the AgNP-containing solution recorded without sample dilution over the wavelength range of 400–800 nm. The pronounced absorption band centered at approximately 440 nm is attributed to the localized surface plasmon resonance (LSPR) of the synthesized silver nanoparticles.

Conclusions

AgNPs were successfully synthesized through a simple green approach using an aqueous extract prepared from shade-dried *Magnolia grandiflora* leaves. The plant extract provided a biological reaction medium capable of promoting the reduction of Ag^+ ions and the formation of silver nanostructures under relatively mild synthesis conditions.

UV–Vis spectroscopy revealed a pronounced absorption maximum at approximately 440 nm, which was absent in the original leaf extract and is attributed to the localized surface plasmon resonance of the synthesized AgNPs. The emergence of this characteristic plasmonic response provides strong optical evidence for AgNP formation.

The observed LSPR maximum is slightly red-shifted relative to the approximately 417–425 nm range previously reported for *Magnolia grandiflora*-mediated AgNP synthesis [3]. This difference may originate from variations in nanoparticle characteristics, surface chemistry, aggregation state, local dielectric environment, or experimental synthesis conditions. However, the individual contributions of these factors cannot be distinguished solely by UV–Vis spectroscopy.

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Overall, the present results demonstrate that aqueous *Magnolia grandiflora* leaf extract provides a simple and environmentally sustainable biological platform for producing AgNPs with a characteristic plasmonic response. Further structural, morphological, elemental, and surface characterization will be required to establish detailed correlations between the synthesis conditions and the physicochemical properties of the resulting nanostructures. Such investigations may further clarify their potential for plasmonic, sensing, photonic, optoelectronic, environmental, and biomedical applications.

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Effect of Sputtering Pressure on Surface Morphology and Magnetic Domain Evolution of DC Magnetron-Sputtered Ni₅₂Mn₃₃Ga₁₅ Thin Films Deposited on Glass Substrates

G. Durak Yüzüak^{1,*}, E. Yüzüak²

¹ Rare Earth Elements Application and Research Center, Munzur University, Tunceli, Turkey

² Department of Energy Systems Engineering, Recep Tayyip Erdoğan University, Rize, Turkey

Abstract

In this study, 100 nm thick Ni₅₂Mn₃₃Ga₁₅ thin films were deposited on glass substrates by DC magnetron sputtering under Ar working pressures of 4–15 mTorr, while all other deposition parameters were kept constant. The surface morphology and the magnetic domain evolution were investigated by atomic force microscopy (AFM) and magnetic force microscopy (MFM), respectively. The surface roughness was quantitatively evaluated using the arithmetic average roughness (R_a), the root mean square roughness (R_q), and the maximum height (R_z).

The AFM results revealed that increasing the sputtering pressure significantly increased the surface roughness, with R_a rising from 1.5 nm at 4 mTorr to 5.8 nm at 15 mTorr, accompanied by corresponding increases in R_q and R_z . Three-dimensional AFM images confirmed the transition from smooth and compact surfaces to coarse island-like morphologies with increasing pressure, which was attributed to the reduced adatom mobility during film growth.

The MFM measurements showed that the magnetic domain configuration also depended on the sputtering pressure. While the films deposited at low pressures exhibited weak magnetic contrast, intermediate pressures produced more distinct magnetic domains. At higher pressures, the increased surface roughness resulted in less uniform magnetic domain distributions, suggesting enhanced domain-wall pinning and local magnetostatic variations. The close agreement between the AFM and MFM observations demonstrates that the sputtering pressure effectively controls both the surface evolution and the nanoscale magnetic behavior. These findings provide useful insight into the optimization of Ni-Mn-Ga Heusler alloy thin films for magnetic and spintronic applications.

Keywords: Ni-Mn-Ga Heusler alloy; DC magnetron sputtering; atomic force microscopy (AFM); magnetic force microscopy (MFM); surface roughness; magnetic domains; sputtering pressure; thin films.

Corresponding author: gizemdurakyuzuak@munzur.edu.tr

1. Introduction

Ferromagnetic Heusler alloys have attracted significant attention owing to their multifunctional properties, including magnetic shape memory behavior, high spin polarization, a large magnetocaloric effect, and an excellent magnetic response [1]. Among them, Ni-Mn-Ga alloys are considered one of the most promising smart materials for applications in microelectromechanical systems (MEMS), magnetic actuators, sensors, spintronic devices, and energy harvesting technologies. The continuous demand for miniaturized magnetic devices has stimulated extensive research on Ni-Mn-Ga thin films, because their properties can be effectively tailored by controlling the deposition conditions during film growth [2–4].

DC magnetron sputtering is one of the most versatile techniques for fabricating Ni-Mn-Ga thin films, owing to its excellent compositional control, uniform deposition, and compatibility with large-area coatings. However, the physical properties of sputtered films are highly sensitive to the deposition parameters, particularly to the working pressure. During sputtering, the working pressure determines the collision frequency between the

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sputtered atoms and the Ar gas atoms, thereby controlling the kinetic energy and the surface mobility of the adatoms arriving at the substrate [4]. At low working pressures, energetic atoms experience fewer collisions and diffuse more efficiently on the substrate surface, resulting in relatively smooth and dense films. In contrast, increasing the working pressure reduces the kinetic energy of the arriving atoms, suppresses surface diffusion, and promotes island-like growth accompanied by increased surface roughness. Consequently, the working pressure becomes a key parameter governing the evolution of the thin-film morphology.

The surface morphology of ferromagnetic thin films plays an important role in determining their local magnetic behavior. Differences in the nanoscale topography influence the magnetic anisotropy, the exchange coupling, the magnetostatic interactions, and the domain-wall pinning, all of which affect the formation of magnetic domains [5]. Therefore, knowledge of the surface morphology and of the evolution of the magnetic domains is essential for optimizing the properties of magnetic thin films for functional applications. Atomic force microscopy (AFM) is a widely used technique for investigating the nanoscale surface morphology, since it provides high-resolution three-dimensional topographical information. Apart from the qualitative imaging of surfaces, AFM allows a quantitative evaluation of roughness parameters, such as the arithmetic average roughness (R_a), the root mean square roughness (R_q), and the maximum surface height (R_z). The R_a parameter describes the average deviation of the surface profile from the mean plane; R_q is more sensitive to large height fluctuations, because it is calculated from the squared deviations; and R_z describes the vertical distance between the highest peaks and the deepest valleys within the scanned area. Together, these parameters enable a comprehensive description of the surface evolution under different deposition conditions. Complementary to AFM, magnetic force microscopy (MFM) enables the direct imaging of magnetic domain structures by detecting the local magnetic force gradients between a magnetized probe and the sample surface, which makes it a powerful tool for correlating the surface morphology with the local magnetic behavior.

Although numerous studies have reported the structural and magnetic properties of Ni-Mn-Ga thin films, systematic investigations correlating the sputtering pressure with the nanoscale surface morphology and the magnetic domain evolution remain relatively limited. Therefore, the present study focuses specifically on the evolution of the surface topography and of the magnetic domain structures. $\text{Ni}_{52}\text{Mn}_{33}\text{Ga}_{15}$ thin films were deposited on glass substrates by DC magnetron sputtering at working pressures ranging from 4 to 15 mTorr, while all other deposition parameters were kept constant. The influence of the sputtering pressure on the surface morphology was quantitatively evaluated by AFM through the R_a , R_q , and R_z roughness parameters, and the corresponding magnetic domain evolution was investigated by MFM.

2. Experimental details

$\text{Ni}_{52}\text{Mn}_{33}\text{Ga}_{15}$ thin films were deposited onto commercial glass substrates by DC magnetron sputtering using a 2-inch $\text{Ni}_{52}\text{Mn}_{33}\text{Ga}_{15}$ alloy target. Prior to deposition, the glass substrates were ultrasonically cleaned sequentially in acetone, ethanol, and deionized water, and were then dried with nitrogen gas in order to remove surface contaminants. The base pressure of the deposition chamber was maintained at approximately 3×10^{-5} Torr before the sputtering gas was introduced.

High-purity argon (99.999%) was used as the sputtering gas with a constant flow rate of 30 sccm. The sputtering power was fixed at 50 W, while the substrate was kept at room temperature throughout the deposition process. In order to investigate the influence of the working pressure on the surface morphology and the magnetic domain evolution, the argon working pressure was systematically varied from 4 to 15 mTorr (4, 6, 8, 10, 12, and 15 mTorr), while all other deposition parameters were kept unchanged. The deposition time was fixed at 30 min, resulting in a film thickness of approximately 100 nm for all samples.

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The surface morphology of the deposited films was characterized using an AFM (Park Systems) operated in tapping mode. All topographical images were acquired over a scan area of $1 \times 1 \mu\text{m}^2$. In addition to the two-dimensional topographic images, three-dimensional surface reconstructions were generated in order to visualize the evolution of the surface features with increasing sputtering pressure. The surface roughness was quantitatively evaluated using three standard roughness parameters: R_a , R_q , and R_z . The R_a parameter represents the arithmetic mean of the absolute height deviations from the mean surface and is commonly used to describe the average surface roughness, whereas R_q , which is calculated from the squared height deviations, is more sensitive to isolated peaks and valleys. The R_z parameter corresponds to the vertical distance between the highest peak and the deepest valley within the scanned area.

The magnetic domain structures were investigated by MFM using a CoCr-coated magnetic probe operated in lift mode. The measurements were carried out with a lift height of 50 nm, which allowed the magnetic interaction between the tip and the sample surface to be detected while minimizing the influence of topographical artifacts. All MFM images were recorded over the same $1 \times 1 \mu\text{m}^2$ scan area used for the AFM measurements, in order to enable a direct comparison between the surface morphology and the magnetic domain distribution. The combined AFM and MFM analyses were employed to evaluate the influence of the sputtering pressure on both the nanoscale surface topography and the corresponding magnetic domain evolution of the $\text{Ni}_{52}\text{Mn}_{33}\text{Ga}_{15}$ thin films.

3. Results and discussion

The influence of the sputtering pressure on the surface morphology of the $\text{Ni}_{52}\text{Mn}_{33}\text{Ga}_{15}$ thin films was investigated, and the corresponding two-dimensional topographical images are presented in Figs. 1 and 2. The AFM observations clearly indicate that the surface morphology strongly depends on the working pressure applied during the sputtering process. At a working pressure of 4 mTorr, the deposited film exhibited a relatively smooth and compact surface with uniformly distributed nanoscale features. The limited height variation indicates that the sputtered atoms arrived at the substrate with relatively high kinetic energy, which allowed efficient surface diffusion and the formation of a dense microstructure. Increasing the pressure to 6 mTorr slightly increased the surface irregularity, but the film was still characterized by a relatively homogeneous morphology. At 8 mTorr, the surface became considerably rougher and larger surface asperities were formed. A similar trend was observed at 10 mTorr, where the topographical images revealed more pronounced hill-like structures distributed over the film surface. A further increase of the pressure to 12 and 15 mTorr led to the development of coarse surface features with larger height fluctuations and a less homogeneous morphology. These results indicate that increasing the sputtering pressure progressively modifies the thin-film growth mechanism.

The morphological evolution can be understood in terms of the decrease in the adatom kinetic energy with increasing working pressure. At low pressures, the sputtered atoms undergo only a few collisions with Ar atoms and therefore retain sufficient kinetic energy to migrate over the substrate surface before being incorporated into the growing film. As the working pressure increases, the number of gas-phase collisions increases and the kinetic energy of the arriving species decreases, which suppresses surface diffusion and favors localized nucleation. Neighboring nuclei can therefore no longer coalesce completely, which gives rise to irregular, island-like surface structures. This growth behavior is consistent with the Volmer–Weber growth mechanism and with the Thornton structure zone model, both of which predict an increasing surface roughness with decreasing adatom mobility [6,7].

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In order to quantitatively evaluate the influence of the sputtering pressure on the surface evolution, the R_a , the R_q , and the R_z were calculated from the AFM images. The obtained values are summarized in Table 1. All three roughness parameters increase systematically with increasing sputtering pressure. The R_a increases from 1.5 nm at 4 mTorr to 5.8 nm at 15 mTorr, which corresponds to an almost fourfold increase. A similar trend is observed for R_q , which increases from 2.1 nm to 6.3 nm, indicating that large surface height fluctuations become increasingly dominant at higher working pressures. Likewise, R_z rises continuously from 1.8 nm to 6.9 nm, confirming the development of deeper valleys and higher surface peaks.

The relation between R_a and R_q also provides useful information regarding the surface profile. Since R_q is calculated from the squared height deviations, it is more sensitive to isolated protrusions and depressions than R_a . The fact that R_q exceeds R_a for the film deposited at the highest working pressure suggests that the surface of this film contains pronounced individual asperities rather than uniformly distributed roughness. Similarly, the continuous increase in R_z indicates that extreme topographical features become increasingly significant as the deposition pressure increases. These quantitative results are in good agreement with the AFM observations and confirm that the working pressure is one of the primary parameters controlling the nanoscale surface evolution of sputtered Ni-Mn-Ga thin films. The films deposited at 4 and 6 mTorr exhibit relatively smooth surfaces with shallow height variations, which indicates efficient lateral growth and good surface continuity. As the pressure increases to 8 and 10 mTorr, the surface becomes increasingly corrugated and localized hill-like features begin to dominate the morphology. The largest vertical height variations are observed for the films deposited at 12 and 15 mTorr, where coarse surface asperities and irregular topographical features are clearly visible.

Table 1 Surface roughness parameters (R_a , R_q , and R_z) obtained from the AFM measurements of $\text{Ni}_{52}\text{Mn}_{33}\text{Ga}_{15}$ thin films deposited under different sputtering pressures.

Working Pressure (mTorr)	R_a (nm)	R_q (nm)	R_z (nm)
4	1.5	2.1	1.8
6	1.9	2.7	1.9
8	2.9	4.2	2.8
10	3.1	4.0	3.7
12	4.9	5.6	4.9
15	5.8	6.3	6.9

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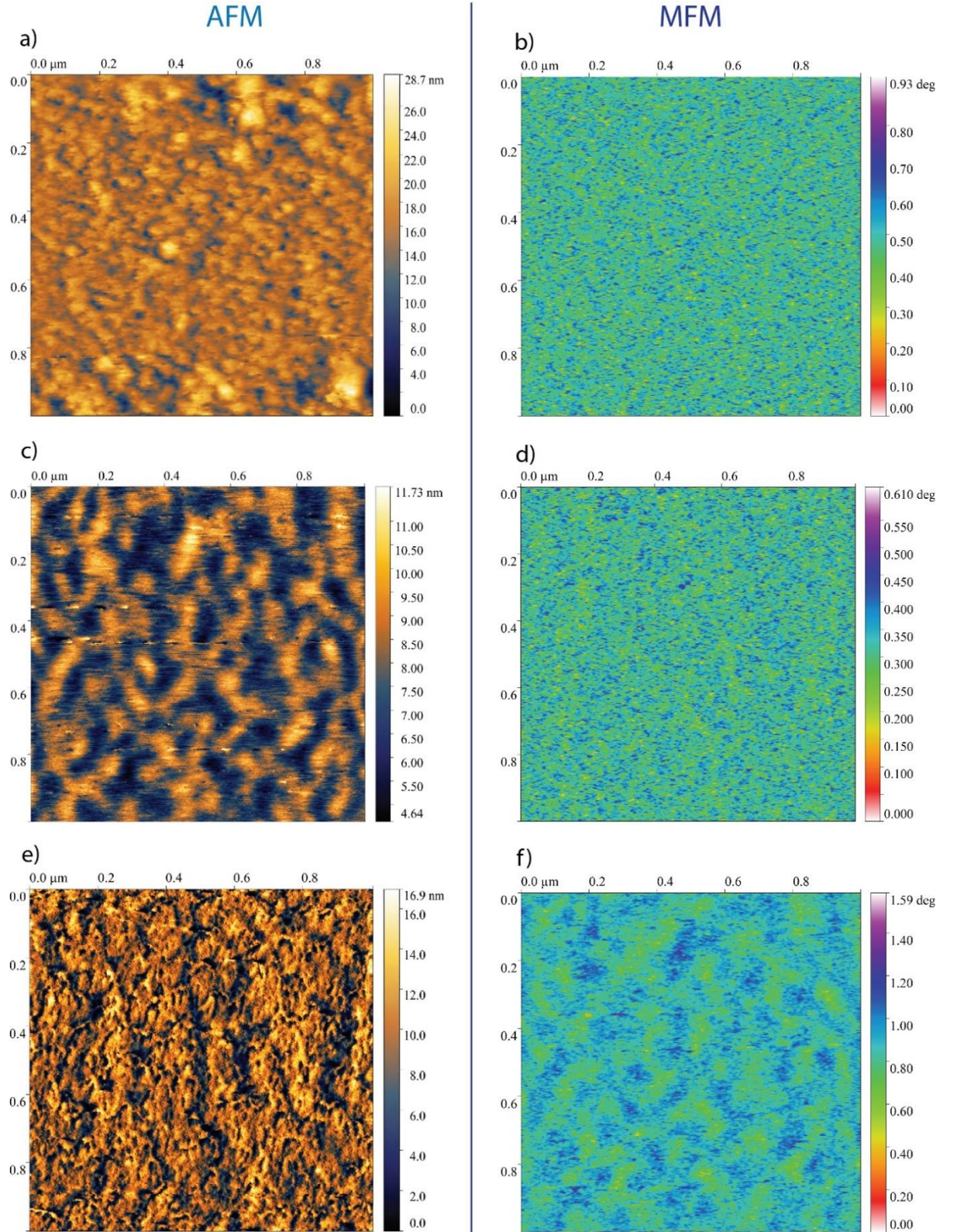


Figure 1 AFM topography and corresponding MFM images of $\text{Ni}_{52}\text{Mn}_{33}\text{Ga}_{15}$ thin films deposited at working pressures of 4, 6, and 8 mTorr. The AFM images reveal the evolution of the surface morphology, while the corresponding MFM images illustrate the pressure-dependent changes in the magnetic domain distribution.

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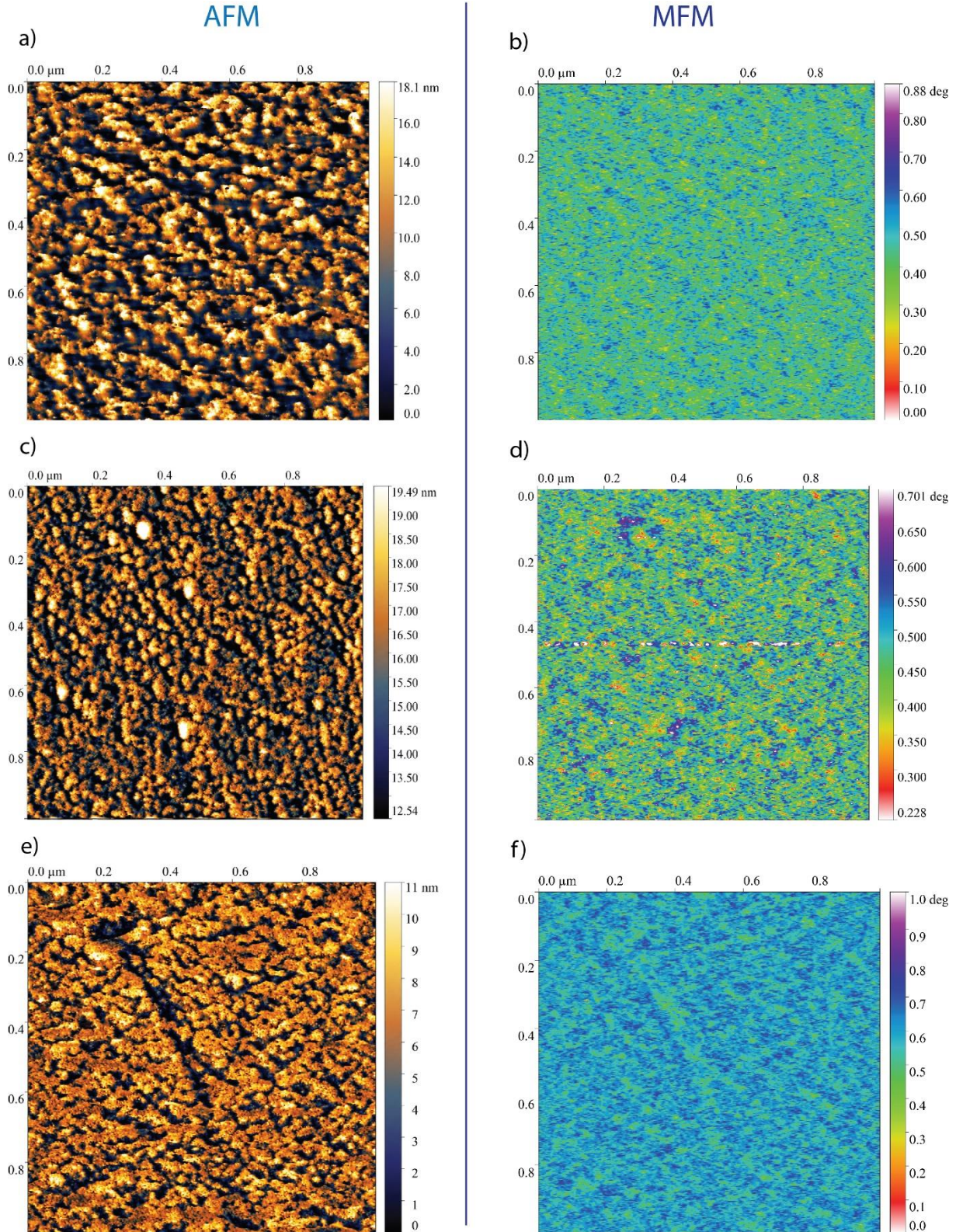


Figure 2 AFM topography and corresponding MFM images of $\text{Ni}_{52}\text{Mn}_{33}\text{Ga}_{15}$ thin films deposited at working pressures of 10, 12, and 15 mTorr. Increasing the sputtering pressure leads to more pronounced surface asperities and to corresponding modifications in the magnetic domain contrast.

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The progressive increase in the surface roughness observed in the three-dimensional AFM images (Fig. 3) supports the quantitative roughness analysis discussed above. The reduced kinetic energy of the sputtered atoms at higher working pressures suppresses adatom migration, thereby limiting grain coalescence and promoting localized vertical growth. Consequently, the surface evolves from a relatively compact morphology to a rougher structure characterized by larger height fluctuations. The magnetic domain structures of the deposited $\text{Ni}_{52}\text{Mn}_{33}\text{Ga}_{15}$ thin films were examined by MFM, and the corresponding images are shown in Figs. 1 and 2. The MFM images demonstrate that the magnetic response varies considerably with the sputtering pressure. At 4 mTorr, only a weak magnetic contrast was observed, which suggests relatively uniform stray magnetic fields over the scanned region. The magnetic contrast was more pronounced for the films deposited at 6 and 8 mTorr, indicating the gradual formation of localized magnetic domains.

The magnetic contrast was most pronounced for the film deposited at 10 mTorr, where the bright and dark regions were more clearly defined. This behavior points to a better-defined magnetic domain configuration and may indicate an improved local magnetic ordering. However, when the sputtering pressure was further increased to 12 and 15 mTorr, the magnetic contrast became less uniform and exhibited fragmented magnetic features across the scanned area. The observed changes can be associated with the modifications in the surface morphology. Local variations in the magnetostatic energy and in the magnetic anisotropy induced by surface irregularities govern the formation and the stability of the magnetic domains. Moreover, rough surfaces increase the number of pinning sites, which hinders the motion of the domain walls and produces more complex magnetic configurations. Therefore, the MFM observations indicate that the evolution of the magnetic domains is closely related to the topographical characteristics of the deposited films.

A comparison of the AFM and MFM images reveals a clear correlation between the surface morphology and the magnetic domain evolution. The films deposited at low sputtering pressures possess relatively smooth surfaces, which are associated with a weaker magnetic contrast. As the working pressure increases, a moderate roughness enhances the local magnetic contrast, which suggests that changes in the surface topography influence the distribution of the local magnetic stray fields. At higher sputtering pressures, the significant increase in roughness leads to a more heterogeneous magnetic behavior. The coarse surface features can generate local variations in magnetic anisotropy and in magnetostatic interactions, thereby increasing the number of potential domain-wall pinning sites. The magnetic domain configuration becomes less uniform as the surface roughness increases. These results demonstrate that the working pressure simultaneously controls the surface growth kinetics and the magnetic microstructure of the films, as summarized schematically in Fig. 4. The decrease in adatom mobility at higher pressures modifies the film topography, which in turn affects the distribution of the magnetic domains through variations in the local magnetic interactions. Thus, the sputtering pressure can be considered an effective processing parameter for tuning the surface morphology and the magnetic domain properties of Ni-Mn-Ga thin films.

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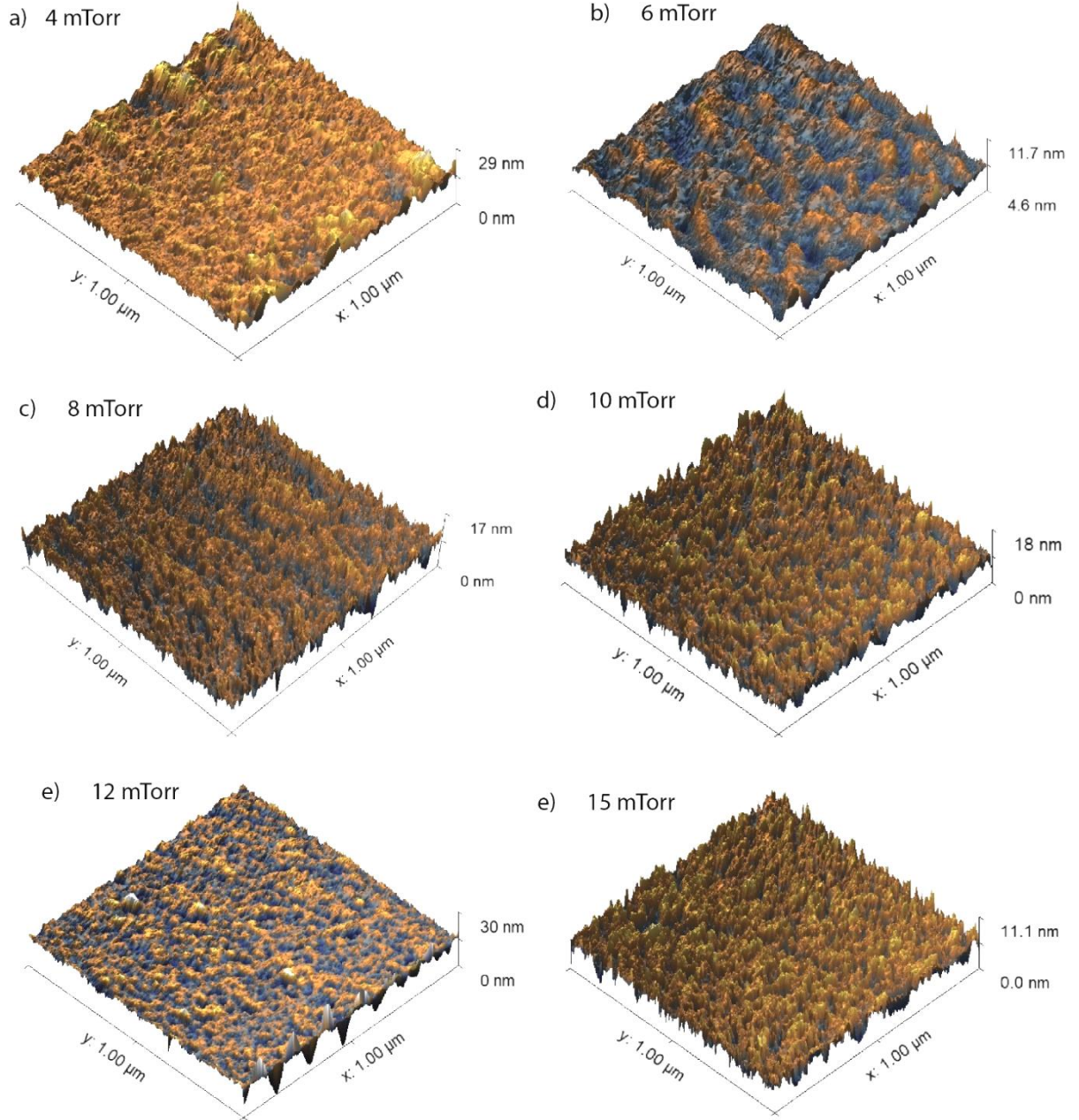


Figure 3 Three-dimensional AFM surface reconstructions of $\text{Ni}_{52}\text{Mn}_{33}\text{Ga}_{15}$ thin films deposited at different sputtering pressures (4–15 mTorr), illustrating the progressive increase in the surface height variation and in the roughness with increasing working pressure.

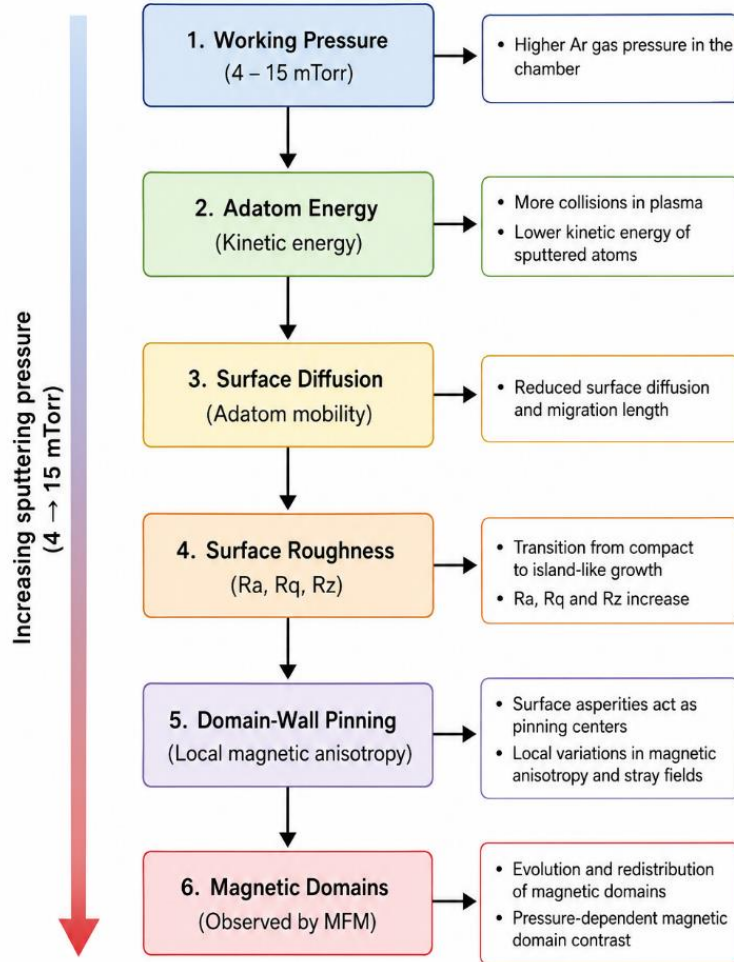


Figure 4 Proposed mechanism illustrating the effect of the sputtering pressure on the surface morphology and the magnetic domain evolution of $\text{Ni}_{52}\text{Mn}_{33}\text{Ga}_{15}$ thin films.

4. Conclusions

In this study, the effect of the sputtering pressure on the surface morphology and the magnetic domain evolution of DC magnetron-sputtered $\text{Ni}_{52}\text{Mn}_{33}\text{Ga}_{15}$ thin films deposited on glass substrates was investigated by AFM and MFM analyses. The working pressure was varied between 4 and 15 mTorr, while all other deposition parameters were kept constant. The AFM results revealed that the surface morphology strongly depends on the sputtering pressure. Increasing the working pressure gradually increased the surface roughness, with the arithmetic average roughness (R_a) increasing from 1.5 to 5.8 nm, accompanied by corresponding increases in the R_q and R_z values. The three-dimensional AFM images further confirmed the transformation from relatively smooth and compact surfaces at low working pressures to coarse island-like structures with pronounced height fluctuations at higher pressures. This morphological evolution is explained in terms of the reduced kinetic energy and the limited surface diffusion of the sputtered atoms caused by the enhanced gas-phase collisions. The magnetic domain distribution was also influenced by the deposition pressure, as shown by the MFM observations. The magnetic contrast was found to evolve together with the surface morphology, which reveals a close correlation between the nanoscale topography and the local magnetic behavior. The films deposited at intermediate sputtering pressures

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showed a relatively well-defined magnetic contrast, whereas the increased surface roughness at higher pressures led to more heterogeneous magnetic domain distributions, which is attributed to enhanced domain-wall pinning and local magnetostatic variations.

The combined AFM and MFM analyses demonstrate that the sputtering pressure is an effective parameter for simultaneously controlling the nanoscale surface morphology and the magnetic domain evolution of $\text{Ni}_{52}\text{Mn}_{33}\text{Ga}_{15}$ thin films. The results presented in this work provide useful guidance for optimizing the deposition conditions of Ni-Mn-Ga Heusler alloy thin films intended for future magnetic, spintronic, and microelectromechanical device applications.

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Green Synthesis of Pure and Boron-Doped TiO₂ Nanoparticles Synthesized via Sambucus nigra Extract and Photocatalytic Degradation of Tetracycline

T. Öztürk*, B. Gül

Department of Physics, Faculty of Science, Selçuk University, 42130, Konya, Türkiye

Abstract

In this study, pure and boron (B)-doped titanium dioxide (TiO₂) nanoparticles were successfully produced using elderberry (*Sambucus nigra*) plant extract via green synthesis. Unlike traditional chemical reduction methods, this approach eliminates the need for high temperatures and toxic reagents, offering an environmentally friendly and cost-effective production protocol. The structural, morphological, and optical properties of the synthesized nanomaterials were analyzed using X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), and Fourier Transform Infrared Spectroscopy (FTIR) techniques, respectively. The photocatalytic performance of the produced nanoparticles was tested by the photodegradation of tetracycline antibiotic under ultraviolet (UV) light, which triggers the development of antibiotic-resistant bacteria (ARB) when released into the environment. A comparison of the obtained results shows that boron-doped TiO₂ exhibits more effective photocatalytic activity. These results demonstrate that photocatalysts obtained through green synthesis offer a sustainable alternative for removing pharmaceutical waste from water.

Keywords: TiO₂, Boron, Green Synthesis, *Sambucus Nigra*

***Corresponding author:** teomanozturk@selcuk.edu.tr

1. Introduction

Fresh water accounts for only 2.5% of the water on the Earth's surface, and most of it is found in glaciers. Due to increasing population, industrialization, and climate change, these limited resources are rapidly becoming polluted and depleted. Various strategies, such as filtration, osmosis, membrane therapy, ozonation, and photocatalysis, have been developed in the literature to treat polluted water. Photocatalysis means light-activated catalysts and their reaction mechanisms. This topic gained significant momentum following the pioneering study by Fujishima and Honda [1] on TiO₂-mediated water splitting under UV illumination. Although alternative semiconductor metal oxides such as ZnO, CuO, and SnO₂ are widely investigated, TiO₂ continues to be the most preferred photocatalyst owing to its chemical stability, non-toxicity, abundance, and accessibility. Although photocatalysis is commonly used in water treatment, it is also widely applied in areas such as CO₂ reduction and hydrogen production. Another interesting application of photocatalysis is in antibiotic degradation. While antibiotics are beneficial to humans and animals, antibiotics released into water threaten aquatic and terrestrial ecosystems. When released into these environments without treatment, antibiotics can cause mutations in bacteria's genes, leading to the emergence of antibiotic-resistant bacterial strains [2]. Traditional TiO₂ synthesis methods (sol-gel, sulfate, or high-temperature chloride treatments) require harsh chemicals like sulfuric acid or extreme temperatures (~1000 °C). These methods are harmful and costly, and also lead to the formation of secondary products. Recently, the production of TiO₂ using green synthesis has attracted considerable attention as a cost-effective, eco-friendly alternative [3]. In this method, plant extracts are used. The phytochemicals found in these plant extracts are used as reducing agents in the reduction of precursor materials.

In this present work, pristine and boron (B)-doped titanium dioxide (TiO₂) nanoparticles were eco-friendly synthesized using elderberry (*Sambucus nigra*) plant extract. The structural, morphological, and optical properties of the synthesized nanomaterials were characterized using X-ray Diffraction (XRD), Scanning Electron

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Microscopy (SEM), and Fourier Transform Infrared Spectroscopy (FTIR) techniques, respectively. The photocatalytic efficiency of the produced nanoparticles was evaluated by the photodegradation of tetracycline antibiotic under ultraviolet (UV) illumination. Comparative results showed that B-doping enhances the photocatalytic activity of TiO₂. These findings have shown that photocatalysts synthesized via green methods offer a viable and sustainable approach for the removal of pharmaceutical pollutants from water [4].

2. Experimental details

Sambucus nigra herbs were collected from the Kütahya region. The collected herbs were dried. The dried herbs were washed with pure water. Then, they were spread on filter paper and left to dry in sunlight at room temperature. The dried herbs were then ground using a blender. 10 grams of the ground sample were weighed and left to steep in 200 ml of pure water at 80 °C for 10 minutes. Separately, 3.4 mL of titanium tetraisopropoxide (TTIP) and 16 mL of ethanol were added to each of two separate beakers and mixed on a magnetic stirrer at 500 rpm for 20 minutes. Pure TiO₂ was synthesized by adding one TTIP mixture dropwise into a solution of 16.8 mL ethanol and 6 mL acetic acid. For boron-doped TiO₂, 1 wt% boric acid was added to the ethanol-acetic acid solution before introducing the TTIP mixture dropwise under identical stirring conditions. The obtained solutions were combined with the Sambucus nigra extract at a 1:1 (v/v) volume ratio. Then this mixture was dried at 80 degrees. The dried materials were annealed in an ash furnace at 500 degrees.

3. Results and discussion:

Structural characterization of the obtained nanoparticles was performed using XRD and the XRD patterns were demonstrated in Fig.1. The characteristic diffraction peaks observed in both samples at approximately 25.2°, 37.9°, 48.2°, 54.1°, 55.2° and 62.8° were affiliated with planes (101), (004), (200), (105), (211) and (204) respectively, belonging to the anatase crystal phase of TiO₂. This shows that boron doping does not alter the basic crystal structure of TiO₂. This indicates that boron ions are incorporated into the titanium dioxide crystal lattice and that the amount of boron is less than the detection limit of the device.

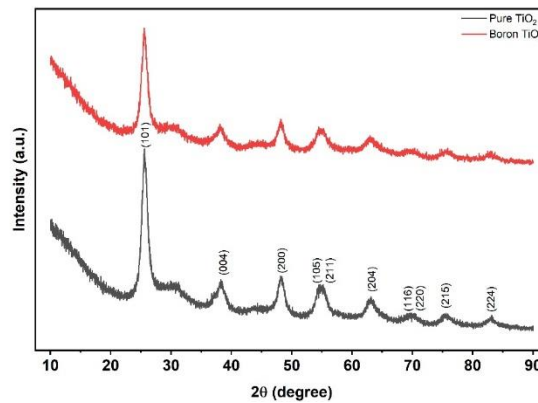


Figure 1 XRD analysis of pure and Boron doped TiO₂ photocatalysts.

The surface morphology of the synthesized photocatalysts were examined using SEM and the obtained images were shown in Fig.2. Both images were acquired at a magnification of 50 kX. While the pure TiO₂ exhibits a uniform microstructural arrangement with low surface roughness, the boron-doping leads to a prominent modification in surface morphology, characterized by increased micro-roughness and localized nanoparticle

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agglomeration. In photocatalytic applications, the increased surface roughness and defect formation observed in B-doped TiO_2 are advantageous, as they provide a higher density of active sites for the adsorption of target pollutants and enable enhanced photon absorption under light irradiation.

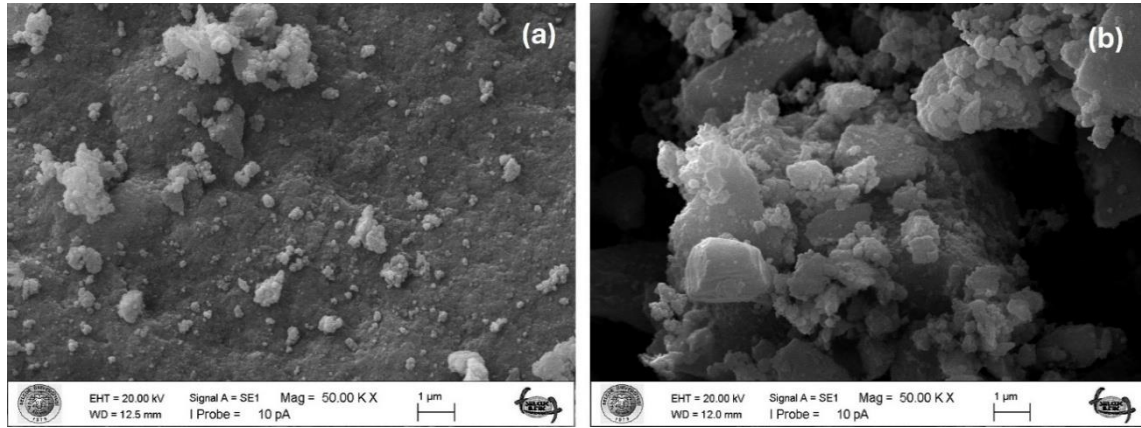


Figure 2 SEM analysis of pure (a) and Boron doped (b) TiO_2 photocatalysts.

The FTIR spectra of the synthesized pure and B-doped TiO_2 nanoparticles were measured in the 4000-500 cm^{-1} range are illustrated in Fig.3. The broad absorption band observed between 3200 and 3500 cm^{-1} , along with the weak peak at approximately 1630 cm^{-1} , corresponds to the stretching and bending vibrations of surface-adsorbed hydroxyl groups (-OH) and water molecules (H-O-H), respectively [5]. The strong absorption below 900 cm^{-1} is attributed to the characteristic Ti-O and Ti-O-Ti framework stretching vibrations [6]. Notable differences are observed in the 1000-1400 cm^{-1} region for the B-doped sample; specifically, the emerging features around 1050-1200 cm^{-1} and 1380 cm^{-1} confirm the presence of B-O stretching and B-O-Ti bonds [7-8]. These structural modifications verify the successful substitution of boron into the TiO_2 lattice structure via the Sambucus nigra mediated synthesis route.

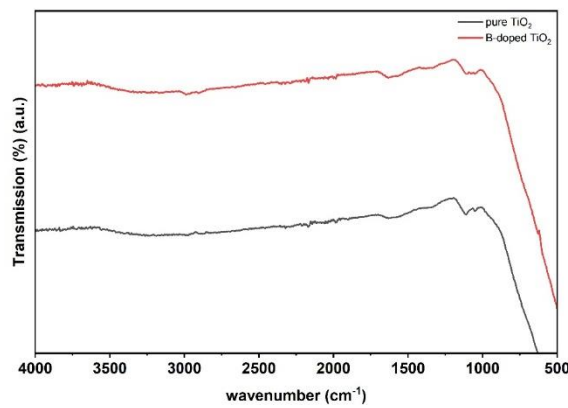


Figure 3 FTIR spectra of pure (a) and Boron doped (b) TiO_2 photocatalysts.

The photocatalytic activity of pure and B-doped TiO_2 photocatalysts was determined by the degradation of tetracycline solution under UV light irradiation for 120 minutes, and the absorption spectra are given in the Fig.4. The degradation rates (C_t/C_0) were evaluated under light irradiation as a function of time, as depicted in

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Fig.5a. Prior to illumination, the suspension was stirred in the dark for 30 minutes to establish adsorption-desorption equilibrium between the photocatalyst surface and the tetracycline solution. During the dark phase, both samples exhibited a minor concentration reduction corresponding to approximately 6% physical adsorption. Upon light exposure, continuous degradation was observed for both photocatalysts; however, B-TiO₂ displayed better photocatalytic efficiency compared to pure TiO₂. After 120 min of total reaction time, the degradation rate reached 45.3% for B-TiO₂, whereas pure TiO₂ achieved a degradation efficiency of 39.5%. The enhanced photocatalytic activity of the boron-doped sample can be attributed to the suppressed recombination rate of photogenerated electron-hole (e⁻/h⁺) pairs and the introduction of localized structural defect states within the TiO₂ lattice. Additionally, kinetic rate constants were calculated via Langmuir-Hinshelwood pseudo-first-order kinetic model, expressed as $-\ln(C_t/C_0) = kt$, where k represents the apparent kinetic constant [9]. The plot of $-\ln(C_t/C_0)$ versus time (t) is shown in Fig.5b. Kinetic constants are determined from the slope of the linear regression fit of the data. Kinetic rate constants were found 0.0453 min⁻¹ and 0.0545 min⁻¹ for the pure TiO₂ and B-doped TiO₂ photocatalysts, respectively. So that, kinetic value of the B-TiO₂ is 16.8% higher than pure TiO₂ nanoparticles. This kinetic rate enhancement confirms that boron doping effectively promotes the formation of reactive oxygen species by accelerating interfacial charge transfer and delaying the recombination of photo-generated charge carriers.

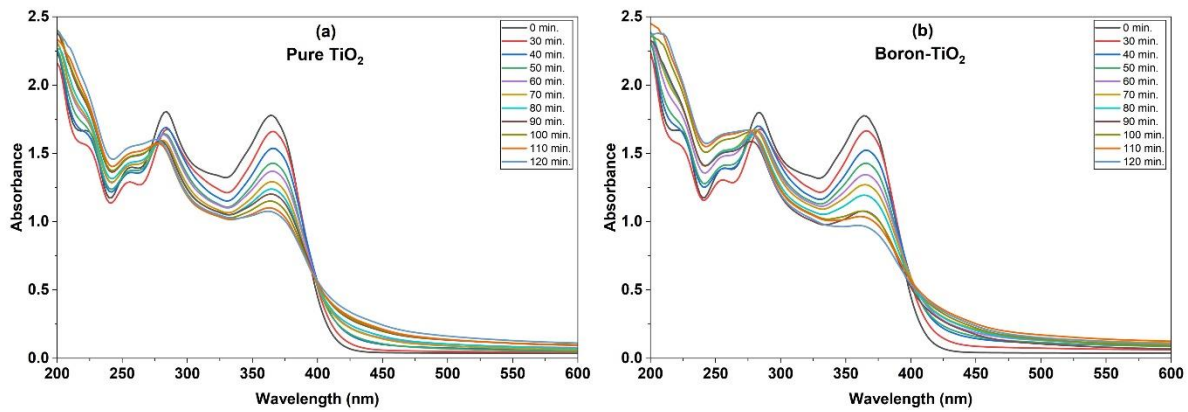


Figure 4 Absorbance spectra of the tetracycline degradation with using **a)** pure and **b)** boron doped TiO₂ photocatalysts.

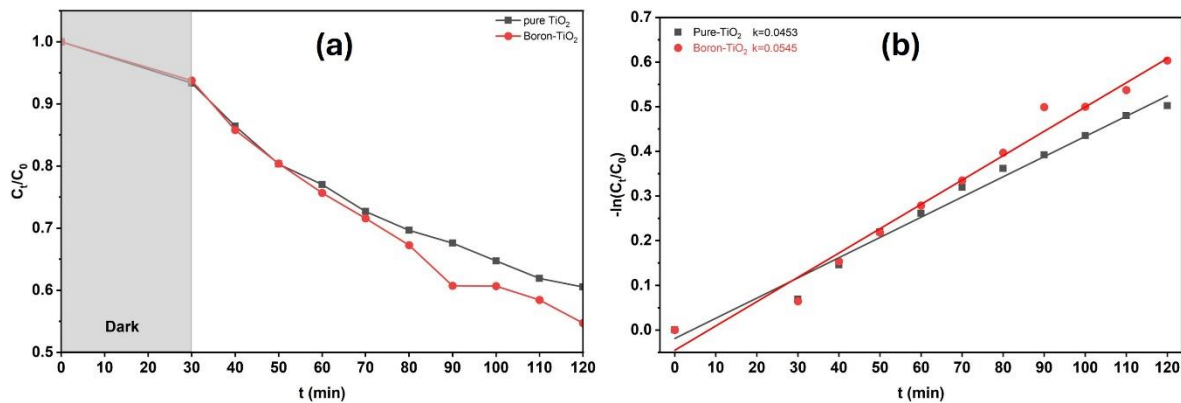


Figure 5 (a) Degradation rate of the pure and B-doped TiO₂ photocatalysts and (b) variation of $-\ln(C_t/C_0)$ of time.

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Conclusions

In this report, pure and B-TiO₂ nanoparticles were synthesized by a facile and green method using Sambucus Nigra flowers extract. The XRD results show that anatase phase was obtained. SEM image of B-TiO₂ depicts a more porous structure than the pure TiO₂. FTIR spectra verify the successful substitution of B into the TiO₂ lattice structure. The photocatalytic activities of the photocatalysts were investigated under UV light irradiation with the degradation of tetracycline antibiotic. B-TiO₂ exhibited a better performance than the pure one.

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Improving the Performance of PEO and PEGMEMA-Based Solid Electrolytes with Environmentally Friendly DOBHTP Plasticizer for Solid-State Lithium Batteries

E.Yildiz^{1,2*}, V.Chandra², A. Magasinski², W. Fu², G. Yushin²

¹Cukurova University, Department of Chemistry, Faculty of Arts&Science, Adana, Türkiye

²Georgia Institute of Technology, School of Materials Science and Engineering, Atlanta, USA

Abstract

In this study, an environmentally friendly, phthalate-free plasticizer, commercial DOBHTP, was incorporated into polyethylene oxide (PEO) and poly(ethylene glycol) monomethyl ether monomethacrylate (PEGMEMA)- based flexible solid macromolecules to fabricate solid-state lithium battery electrolytes. Compared to conventional commercial plasticizers such as diisononyl phthalate (DINP) and di-2-ethylhexyl phthalate (DEHP), DOBHTP demonstrated superior plasticizing efficiency, accelerated processing desiccation, and a reduced melting temperature. When blended with the PEO/lithium-salt matrix, the rapid thermal transition of the DOBHTP commercial mixture significantly lowered processing energy consumption. Electrochemical characterization of the resulting membranes (thicknesses of 100 μm and 132 μm) was conducted via cyclic voltammetry. These findings indicate that the integration of DOBHTP into PEO-based solid electrolytes is a highly promising strategy for optimizing electrochemical performance.

Keywords: Plasticizer, Solid State Lithium Battery (SSLB), Polyethylene Oxide (PEO), electrolyte

Corresponding authors: eeyildiz@cu.edu.tr

1. Introduction

Flexible lithium-ion battery production is a cutting-edge area of research and development aimed at creating batteries that maintain their performance while being bendable, and stretchable to various shapes. Improvements in encapsulation materials, electrodes, advanced binders, gel-solid electrolytes and manufacturing techniques can be modified to increase the flexibility of lithium-ion batteries. Conductive polymers such as heteroatom-free polyacetylene (PAC), polyaniline (PANI), N-heteroatom-containing polypyrrole (PPy), poly (3,4-ethylenedioxythiophene) (PEDOT), and poly (3,4-ethylenedioxythiophene) polystyrene sulfonate are modified for this aim¹⁻⁵.

The facile and scalable one-pot preparation method of a gel polymer electrolyte (GPE) based on highly safe polyethylene glycol dimethyl ether (PEGDME) plasticizer in a poly (vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) polymer matrix, LiTFSI: lithium bis-(trifluoromethanesulfonyl) imide to obtain all-solid-state lithium battery in Figure 1, (ASSLB)⁶.

Plasticizers reduce the glass transition temperature of polymers, giving them the ability to stretch under ambient conditions. Dioctylterephthalate (DOTP), diisononyl phthalate (DINP) and di-2-ethylhexyl phthalate (DEHP) polymers are used for this purpose⁷⁻⁸.

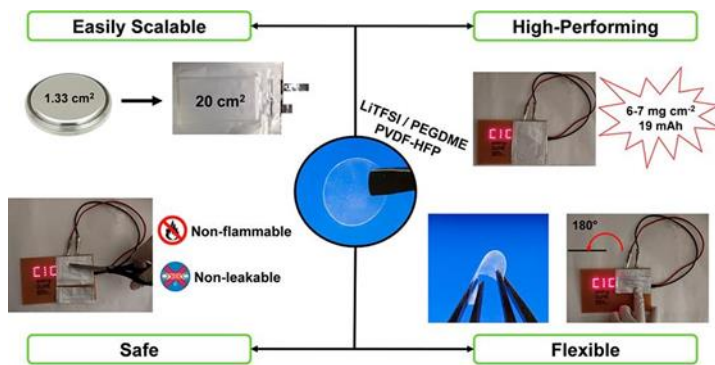


Figure 1 The facile and scalable one-pot preparation method of GPE for rechargeable lithium metal batteries⁶

DOBHTP was chosen as a phthalate-free plasticizer, a commercially available and environmentally friendly polymer that provides better efficiency, better drying time, and lower fusion temperatures compared to DINP and DEHP. It is compatible with plastic in a shorter time. Fast fusion performance contributes to reduced temperature and energy savings in the production process for flexible solid electrolyte, polyethylene oxide (PEO), in this work. In addition, PEGMEMA is known to exhibit stability at low operating potential. This makes the cycling of lithium titanate half-cells a viable option. The reason for preferring PEGMEMA Solid Polymer Electrolytes (SPE) is that it exhibits a lower degree of crystallinity compared to pure PEO SPE, and this value decreases further with the addition of LiTFSI salt⁹.

2. Experimental details

2.1. PEO with DOBHTP in Solid Electrolyte

To produce solid-state lithium batteries, we first verified that the plasticizer was compatible with the electrolyte. Accordingly, DOBHTP was used as the plasticizer to enhance the flexibility of the PEO-based solid electrolyte matrix containing Li salt.

Before using the glovebox, a molecular sieve was used to remove water from DOBHTP. PEO-based polymer, Li salt and DOBHTP are mixed in an 8:1:1 (w:w%) composition ratio to prepare the polymer electrolyte film in a glove box under N₂ gas (Fig. 2). DOBHTP was used after being kept in a molecular sieve.

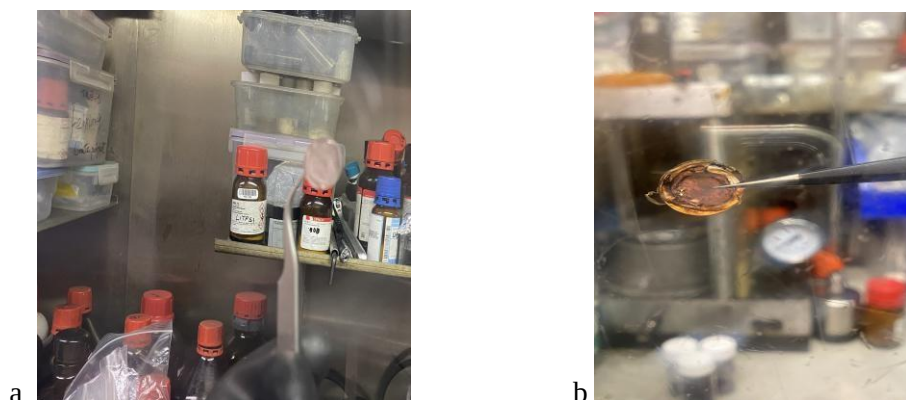


Figure 2 Electrolyte form before (a), and after 60 °C CV application, opened coin cell (b).

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Membrane preparation:

The polymer electrolyte was prepared by mixing LiTFSI (99.95%, anhydrous, Sigma Aldrich) and polyethylene oxide (molecular weight: 600 g.mol⁻¹, Sigma Aldrich). The LiTFSI/PEO ratio was 1:20. The powder mixture was completely dissolved in acetonitrile (ACN, 99.8%, anhydrous, Sigma Aldrich) and stirred with a magnetic stirrer for several hours. Then, the plasticizer was added at a concentration of 20% by weight. The LiTFSI-PEO-DOBHTP solution was then cast onto a Teflon template. After complete evaporation of the acetonitrile, the substrate was transferred to a vacuum chamber for drying at room temperature for 6 hours. The membranes, obtained as 3/4-inch diameter discs, were used to assemble CR2032 flat tablet cells (Fig. 2 a).

2.2. Assembly the Battery

Electrochemical cells are assembled by using fabricated and chosen compositions using 2,032 stainless steel coin cell setups. Stainless steel (SS), Li and SS/SS compositions as half cells were carried out.

Battery Making:

Electrochemical tests were conducted on CR2032 coin cells assembled with a lithium negative electrode (99.9%, MSE, 0.4 mm thick). The cells were operated at 60°C using an MITS Arbin Workstation. Before electrochemical measurements, all cells were conditioned for 12 hours at 60°C in open-circuit mode.

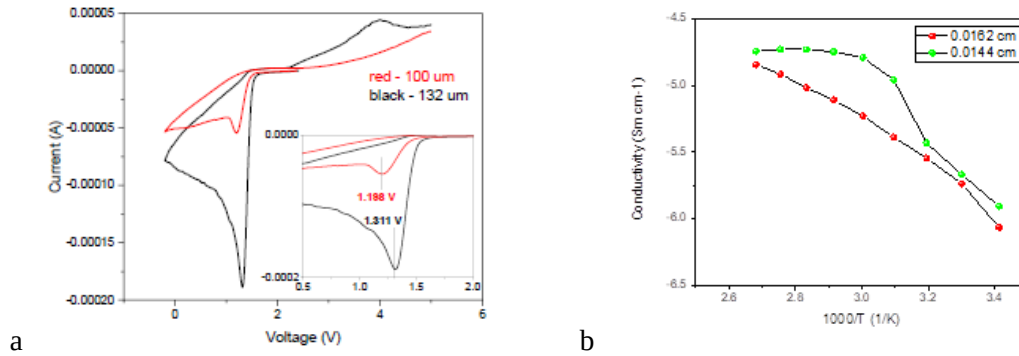
2.3. PEGMEMA with DOBHTP in Solid Electrolyte

The same method was used for the second electrolyte, poly (ethylene glycol) monomethyl ether monomethacrylate (PEGMEMA) instead of PEO with/without DOBHTP.

3. Results and discussion

The initial-cycle current response provides key insights into the electrochemical stability and Li interaction of the electrolyte membrane. The distinct peak around 1.2–1.3 V corresponds to the reduction of the plasticizer, a common initial redox event in solid polymer electrolyte (SPE) systems. Furthermore, membrane thickness plays a critical role; the thinner (100 µm) sample exhibited a higher current density than the thicker (132 µm) one. This is attributed to lower ionic resistance and more efficient Li⁺ transport in the thinner membrane, leading to a more pronounced electrochemical reaction. The reduction peaks at ~1.19 V and ~1.31 V are likely associated with the formation of a preliminary SEI-like layer and the stabilization of the polymer matrix at the electrode interface in Fig.3 a.

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CR2032, SS//membrane//Li-foil coin cell. The peak at 1.2-1.3 V corresponds to the electrochemical activity of the plasticizer. Voltage range: -0.2 – 5 V, scan rate: 0.2 mV/s

Figure 3 Cyclic voltammetry of DOBHTP-doped electrolytes with different thicknesses (100 μm and 132 μm , a). Conductivity vs $1000/T$ (b)

Both membrane thicknesses exhibit a temperature-dependent rise in ionic conductivity (as $1000/T$ decreases), with the thinner membrane (0.0144 cm) consistently achieving superior conductivity values, particularly at higher temperatures (Fig3. b).

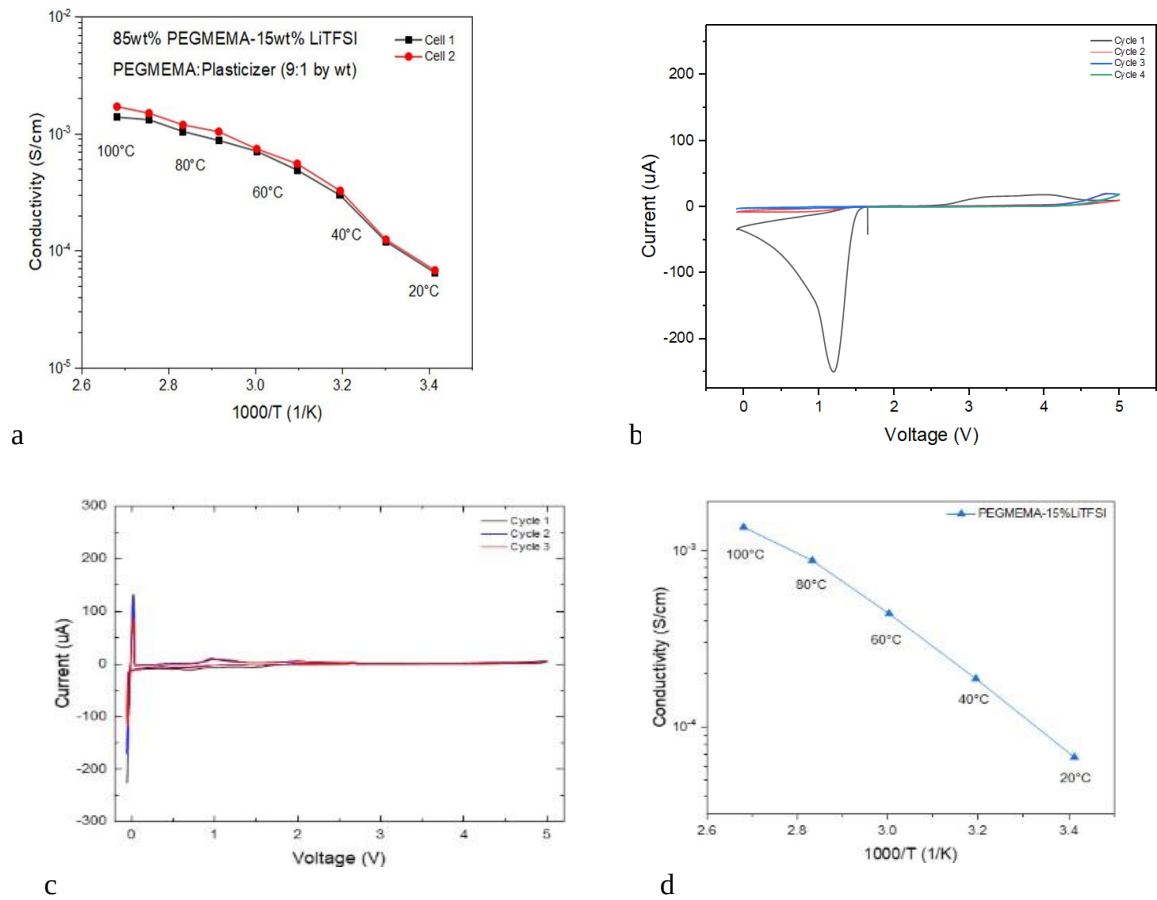


Figure 4 PEGMEMA-DOBHTP CV (a), Conductivity (b), without DOBHTP (c,d)

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PEGMEMA–DOBHTP (a,b) and the PEGMEMA without DOBHTP (c,d) have similar current scale and very similar conductivities, but their CV shapes differ slightly. Panels (a) and (c) the peak magnitudes are comparable; however, (a) shows a broader cathodic feature in the first cycle, whereas (c) is mostly flat with only sharp spikes near 0 V, indicating limited redox activity in both cases with only a modest shape change when DOBHTP is added. The conductivity curves (b) and (d) follow almost the same Arrhenius trend and values from 100 to 20 °C, meaning that DOBHTP does not significantly change the bulk ionic conductivity, and any differences are within experimental variation in Figure 4.



Figure 5 DOBHTP-PEGMEMA, after CV test at 60°C, opened coin cell

After at 60°C CV test, opening the cells for both electrolytes, it was observed that their color changed from transparent to brown due to secondary reactions caused by DOBHTP oxidation or LiPF₆ hydrolysis (Fig. 2 b and Fig. 5).

Conclusions

In conclusion, the incorporation of DOBHTP as a plasticizer in PEO-based solid electrolytes offers a promising strategy for improving the performance of solid-state lithium batteries. While the material system demonstrates encouraging bulk transport behavior, the results also reveal that interfacial compatibility with lithium metal remains a major limitation. This indicates that ionic conductivity alone is not sufficient to guarantee practical battery performance, and that the stability of the electrolyte/electrode interface must be addressed to fully realize the benefits of the plasticized membrane.

The experimental findings suggest that DOBHTP can enhance the flexibility and ionic transport properties of the PEO matrix; however, the poor compatibility with lithium metal, as reflected in EIS measurements, highlights the need for further interface engineering. Future work should therefore focus on improving interfacial stability, reducing interfacial resistance, and optimizing the balance between polymer flexibility and electrochemical performance. Such efforts are essential for translating the advantages of DOBHTP-modified PEO

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electrolytes that are vastly superior to the PEGMEMA system into high-performance, sustainable solid-state lithium batteries.

Overall, DOBHTP represents a promising and environmentally attractive approach for developing greener polymer electrolytes. Its phthalate-free nature and compatibility with PEO-based systems make it a valuable candidate for advancing sustainable solid-state battery technology, provided that interfacial challenges are effectively resolved.

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DFT and TD-DFT Investigation of the OLED Properties of a Triazole-Based MoleculeZ. Ş. Turhan¹, M. Beytur², and E. Yıldız³¹*Department of Biochemistry, Faculty of Arts and Sciences, Iğdır, Türkiye*²*Department of Chemistry, Faculty of Arts and Sciences, Kars, Türkiye*³*Department of Chemistry, Faculty of Arts and Sciences, Adana, Türkiye***Abstract**

Triazoles are important compounds with potential for use in organic light-emitting diodes (OLEDs). Triazole-based ligands can play important roles in energy transfer mechanisms. This property also has a positive effect on the energy efficiency of phosphorescent materials used in OLEDs. Triazole-containing complexes generally provide higher light and quantum efficiencies, thereby increasing the energy efficiency of OLED technologies. In this study, the OLED behavior of the molecule 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one was determined following the determination of quantum chemical parameters via DFT and TD-DFT calculations.

The three-dimensional ground-state (S_0) geometries of the molecule were optimized using the Gaussian 09W software package and the B3LYP hybrid functional. To determine their electronic and optoelectronic properties, E_{HOMO} , E_{LUMO} , E_{gap} , dipole moment (μ), polarization (α), hyperpolarization (β), electron/hole rearrangement energies (λ_e , λ_h), adiabatic/vertical ionization potentials (IP_a , IP_v), adiabatic/vertical electron affinities (EA_a , EA_v), chemical hardness (η) and softness (σ) values, and boundary orbital shapes were obtained; subsequently, the energies of the molecules under investigation in the S_0 , S_1 , and T_1 states, the oscillator force (f), and the transition energy (E_{ex}) were calculated at the TD-DFT level. Based on the results obtained, the emission values and TADF parameters of the studied molecules were determined. The OLED behaviors were investigated using the parameters obtained in this study. It was determined that the material cannot be used as an HTL, ETL, or direct emitter but is suitable as a host material; based on the results, recommendations were made to improve the efficiency of the OLED device, and an example design was presented.

Keywords: Triazole, DFT, OLED**Corresponding authors:** zeynep.turhan@igdir.edu.tr**1. Introduction**

Organic light-emitting diodes (OLEDs) are devices composed of a series of organic thin films placed between two electrodes. Although each organic layer performs a function within the device, these devices emit light when an external voltage is applied [1]. This phenomenon, known as electroluminescence (EL), occurs when hole and electron charge carriers pumped from electrodes form electron-hole pairs—called excitons—within organic semiconductors moving under an electric field [2-5].

Unlike early electroluminescent devices, modern OLED devices feature a multilayer structure in which electrical energy is directly converted into light via organic semiconductors. A typical OLED architecture consists of an anode, a hole injection layer (HIL), a hole transport layer (HTL), an emissive layer (EML), an electron transport layer (ETL), an electron injection layer (EIL), and a cathode. During device operation, electrons and holes are injected from the cathode and anode, respectively. The recombination of these charge carriers leads to efficient light generation [6].

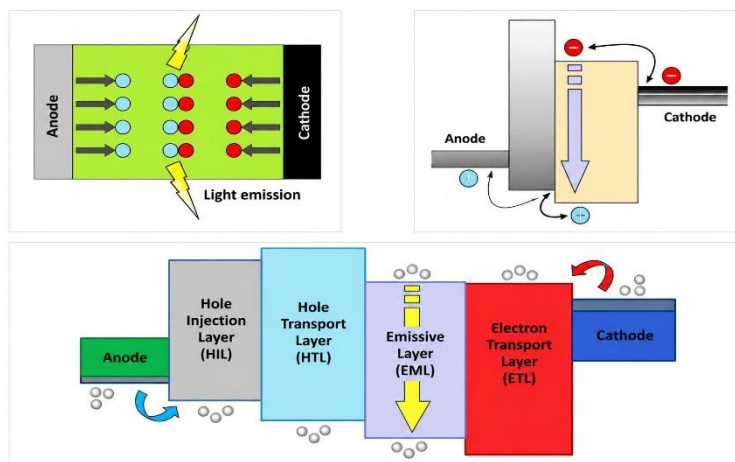


Figure 1 Single-layer, Double-layer, and Multi-layer OLEDs [5].

Current OLED research addresses not only high luminous efficiency but also charge balance, exciton confinement, energy level alignment, and operational stability. While only the singlet fraction—approximately one-quarter of electrically generated excitons—can be directly utilized via fluorescence in conventional fluorescent OLEDs due to spin statistics, phosphorescence and TADF mechanisms enable the utilization of triplet excitons as well. In TADF design, minimizing the energy gap between the S1 and T1 states and accelerating reverse intersystem crossing (RISC) are of critical importance. Current assessments emphasize that, while maintaining a very small ΔE_{ST} value is crucial for successful TADF systems, factors beyond ΔE_{ST} —such as the nature of the excited states, spin-orbit coupling, and molecular rigidity—must also be taken into account [7,8].

Due to the fundamental role of organic molecules in light-emitting material technologies, detailed examination of the behavior of these devices with quantum chemical parameters is very important in terms of scientific contribution. Understanding the electronic, optical and transport properties of the molecule to be used for OLED applications is also critical for device performance. These parameters are obtained through both DFT and TD-DFT calculations. These methods allow for the prediction of a material's potential OLED performance. In OLEDs, the recombination of holes and electrons brings the light-emitting organic layer into an excited state. Light emission occurs upon the transition from the excited state back to the ground state [7]. The wavelength of the emitted light is related to the exciton energy. Therefore, it is possible to change the color of the light by altering the molecular structure. Furthermore, the quantity of emitted photons is directly dependent on the number of excitons generated. Consequently, the emitted light can be made brighter by increasing the probability of electron-hole recombination.

In OLED devices, the accurate alignment of the HOMO and LUMO energy levels of the materials used is crucial for controlling charge flow and balancing charges within the light-emitting layer. Controlling the transport and recombination of electrons and holes are key factors influencing the overall efficiency and performance of the OLED. HOMO and LUMO energy levels represent the energy levels where electrons and holes can be accommodated within specific molecular orbitals. The appropriate alignment of the HOMO and LUMO levels of the materials in the light-emitting layer facilitates the effective recombination of charge carriers, thereby potentially contributing to increased light emission [9]. The energy levels of the electrodes and organic layers are defined using the same unit: the electronvolt (eV).

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Since anodes and cathodes are typically made of metallic materials, they do not possess HOMO and LUMO orbitals; therefore, their energy levels are referred to as the Fermi level. These energy levels are characterized by the work function. For OLED devices, a high anode work function and a low cathode work function are desirable. For electrons and holes to move effectively between organic layers and electrodes, the energy levels of these layers must be sufficiently close to one another. This difference in energy levels between different layers is defined as an energy barrier [7]. For example, the HOMO level of MEH-PPV (Poly[2-methoxy-5-(2'-ethylhexyloxy)-1,4-phenylene vinylene]), used as the light-emitting layer in an OLED, is 5.3 eV, and its LUMO level is 3.0 eV. The work function of ITO (indium tin oxide), commonly used as an anode material, is 4.7 eV. This indicates that the energy barrier between ITO and MEH-PPV is quite large. This energy barrier can be balanced by employing additional organic or inorganic layers between these layers. For example, PEDOT:PSS (poly(3,4-ethylenedioxythiophene) polystyrene sulfonate) (HOMO: 5.1 eV, LUMO: 2.2 eV) is an organic material frequently used as an HTL in hole injection layers [7].

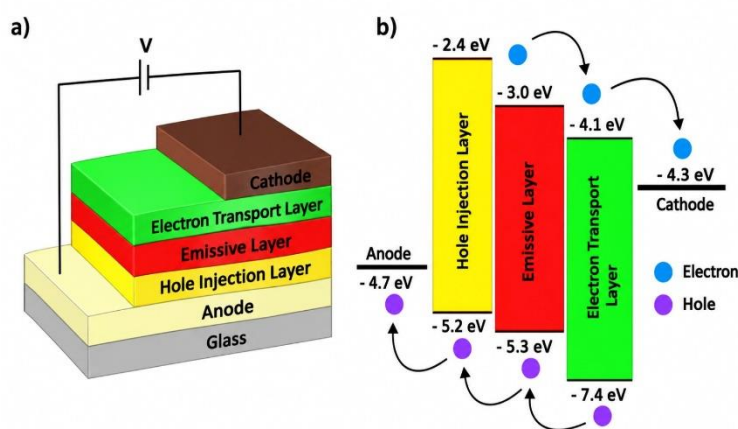


Figure 2 OLED structure and exciton formation [10]

1,2,4-Triazole derivatives are notable building blocks in OLED material chemistry. The electron-withdrawing nature of the five-membered heteroaromatic 1,2,4-triazole ring—which contains three nitrogen atoms—enables the enhancement of electron transport, hole-blocking, and charge-transfer properties. It has been reported in the literature that structures containing 1,2,4-triazole can be used—particularly as electron-transporting and blocking materials—due to their wide energy gap, deep HOMO level, high triplet energy, and thermal stability [11, 12]. Furthermore, the triazole scaffold can be utilized not only in transport layers but also in host and light-emitting structures. Combining the electron-withdrawing triazole unit with electron-donating groups or with various π -bridge systems enables such as carbazole that its tuning of the molecule's electronic and photophysical properties and the development of structures exhibiting bipolar character. Thanks to these properties, triazole derivatives are versatile molecular systems that can contribute to improving charge balance and recombination processes in OLEDs [13]. Therefore, the theoretical investigation of the HOMO/LUMO energy levels, singlet and triplet excitation energies, and charge-transport properties of the new triazole ligands to be synthesized offers a rational approach to determining which function electron transport, blocking, host, or light-emitting material is most suitable for these compounds within an OLED structure.

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The aim of this study is to evaluate the quantum chemical parameters of the 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one compound and to reveal the potential of the structure in question for use as an HTL, ETL, emitter, TADF emitter, or host/co-host material.

2. Materials and Methods

2.1. Molecular Structure

In the study, the 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one ligand shown in Figure 3 was used. The molecule consists of a 1,2,4-triazol-3-one core, a propyl substituent, and a conjugated imine linkage containing a phenyl group. The presence of nitrogen and carbonyl centers allows for the heterogeneous distribution of electron density across the molecule and the formation of a distinct molecular dipole.

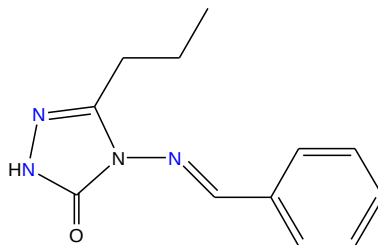


Figure 3 2D molecular drawing of the 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one molecule.

2.2. Quantum Chemical Calculations

The geometries of all ligands in their three-dimensional ground state (S_0) were optimized using the Gaussian 09W [14] software package and the hybrid functional B3LYP [15]. B3LYP consists of Becke's three-parameter exchange functional (B3) [16] and the non-local correlation functional developed by Lee, Yang, and Parr (LYP) [17]. The basis set used for all atoms was selected as 6-311G for geometry optimizations. The basis set used for all atoms was selected as 6-311G for geometry optimizations.

Vibrational analyses were performed for the compound using the same basis set employed in the corresponding geometry optimizations. Normal mode analysis was applied to the $3N-6$ vibrational degrees of freedom, where N represents the number of atoms in the molecule [18].

To determine electronic and optoelectronic properties, values for E_{HOMO} , E_{LUMO} , E_{gap} , dipole moment (μ), polarizability (α), hyperpolarizability (β), electron/hole reorganization energies (λ_e , λ_h), adiabatic/vertical ionization potentials (IP_a , IP_v), adiabatic/vertical electron affinities (EA_a , EA_v), chemical hardness (η) and softness (σ), as well as frontier orbital shapes, were obtained. Subsequently, the energies of the investigated molecule in the S_0 , S_1 , and T_1 states, as well as the oscillator strength (f) and transition energy (E_{ex}), were calculated at the TD-DFT level. Based on the obtained results, the emission values and TADF parameters of the investigated molecule were determined [19].

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The theoretically obtained results were evaluated, and the potential suitability of specific layers for OLEDs was assessed. Finally, the suitability of TADF or NIR materials as candidates for organic light-emitting diodes was also examined.

2.3. Evaluation of OLED Behaviors

In an OLED device, the anode must have a high work function, while the cathode must have a low work function. In this study, the anode and cathode were selected based on the literature. The work function of ITO (indium tin oxide), which is commonly used as the anode, is 4.7 eV. The Mg:Ag alloy was selected as the cathode material. The work function of the cathode is 3.7 eV [20]. However, since interface dipoles, chemical interactions, and film morphology can alter energy alignment at actual organic/electrode interfaces, the calculated injection barriers have been treated as first-approximation values.

3. Results and discussion:

The values of E_{HOMO} , E_{LUMO} , E_{gap} , dipole moment (μ), polarizability (α), hyperpolarizability (β), electron/hole reorganization energies (λ_e , λ_h), chemical hardness (η), ΔE_{ST} , oscillator strength (f), and transition energy (E_{ex}) were calculated from the optimized structure of the 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one ligand and are summarized in Table 1.

Table 1 Calculated quantum chemical parameters for 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one

Parameters	Values
E_{HOMO}	-6.206 eV
E_{LUMO}	-1.971 eV
E_{gap}	4.235 eV
Dipole Moment (μ)	4.877 Debye
Polarization (α)	169.286×10^{-24} esu
Hyperpolarization (β)	0.715×10^{-30} esu
$\lambda_{\text{abs}} (S_0 \rightarrow S_1)$	330.85 nm
$E_{\text{ex}} (S_1)$	3.748 eV
$E_{\text{ex}} (T_1)$	2.593 eV
f	0.235
$\Delta E_{\text{ST}} (\text{B3LYP/de})$	1.155 eV
λ_h	0.281 eV
λ_e	0.361 eV

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The OLED behaviors of 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one were investigated by evaluating its calculated parameters individually. First, it can be inferred whether the ligand would serve as a hole-transporting material (HTL), electron-transporting material (ETL), host, or emitter (light-emitting material).

In the case of forward biasing an OLED (i.e., the anode is positive and the cathode is negative), holes and electrons are injected and transported from the anode material to the highest occupied molecular orbital (HOMO) energy level of the HTL, and from the cathode material to the lowest unoccupied molecular orbital (LUMO) energy level of the ETL, respectively [7].

The HOMO value of the material determines hole injection in the OLED. The HOMO energy value must be aligned with the work functions of the HTL and the electrode. The closer the molecule's HOMO energy level is to the anode's work function (ϕ_{anode}), the lower the barrier. Consequently, hole injection becomes easier, resulting in a more efficient device with a lower operating voltage. The hole injection barrier (ϕ_h) is calculated using Equation 1 [21,22].

$$\phi_h = |E_{HOMO}| - \phi_{anode} \quad (1)$$

The EHOMO value of 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one is not close to the work function of 4.7 eV. The hole barrier value is high (~1.51 eV). This value indicates that hole injection may be difficult. Consequently, it cannot directly accept holes from ITO and is unsuitable for use as an HTL. It can be suggested that a strong donor group be added or the conjugated system be extended to raise the HOMO value that is, to make it less negative.

The EHOMO value of 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one is not close to the work function of 4.7 eV. The hole barrier value is high (~1.51 eV). This value indicates that hole injection may be difficult. Consequently, it cannot directly accept holes from ITO and is unsuitable for use as an HTL. It can be suggested that a strong donor group be added or the conjugated system be extended to raise the HOMO value that is, to make it less negative.

The LUMO value of the material determines electron injection in the OLED. The LUMO energy value must be aligned with the ETL and electrode work functions. The closer the molecule's LUMO energy level is to the cathode's work function ($\phi_{cathode}$), the lower the barrier. Consequently, electron injection is facilitated, and better charge balance is achieved. The electron injection barrier (ϕ_e) is calculated using Equation 2 [22,23].

$$\phi_e = \phi_{katode} - |E_{LUMO}| \quad (2)$$

The ELUMO value of 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one is not close to the work function of 3.7 eV. The electron barrier value is high (~1.73 eV). This value indicates that electron transport would be difficult and charge balance would be disrupted, making it unsuitable for use as an ETL. Alignment can be achieved by tuning the energy levels through the use of substituent groups; specifically, the LUMO energy level can be shifted to a more negative value by adding an acceptor group.

The HOMO/LUMO energy levels and the associated calculated injection barriers indicate that the direct acceptance of electrons and holes from the electrodes by the 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one compound is energetically unfavorable. This suggests that the molecule may not adequately support charge carrier injection and transport within a neat EML, thereby potentially limiting the electron-hole recombination efficiency. Consequently, given its current molecular structure, the compound appears to have limited utility as both a charge carrier and a single-component emitter in the EML.

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To enhance OLED efficiency, electrode and interlayer modifications aimed primarily at reducing the electron injection barrier can be implemented. In this context, using metals with lower work functions such as Ca or Ba instead of the existing cathode can facilitate electron injection from the cathode into the organic layer. Similarly, the insertion of electron injection layers (EILs) such as LiF, Cs₂CO₃, PEI/PEIE, or alkali metal fluorides between the cathode and the organic layer can lower the effective work function by creating an interface dipole and improve electron injection. In addition, selecting an electron transport layer (ETL) with a LUMO energy level that is more favorably aligned with the cathode can contribute to reducing the electron injection barrier and improving charge balance. If the molecule is intended for use as an emitter and a charge carrier within the EML, structural modifications can be applied. While the addition of electron-donating groups can raise the HOMO level and facilitate hole injection, electron-withdrawing groups can lower the LUMO level to a lower energy state, thereby improving electron injection. Thus, through functional group modifications, it is possible to aim for a more favorable alignment of HOMO–LUMO energy levels with the electrode and transport layers, a balancing of charge injection and transport, and, consequently, an enhancement of OLED performance.

The HOMO-LUMO energy gap (E_{gap}) for the compound was determined to be 4.235 eV, indicating that the molecule possesses a wide-bandgap structure. This wide energy gap suggests that the molecule is electronically more stable and may have a limited tendency for charge transport. In TD-DFT calculations, the transition energy (E_{ex}) for the first singlet excited state was calculated as 3.748 eV, and the corresponding absorption wavelength (λ_{abs}) as 330.85 nm. This result indicates that the compound's primary electronic absorption lies in the UV region. The oscillator strength (f) of 0.235 for the transition in question indicates that the transition is electric-dipole allowed and exhibits moderate absorption intensity. However, since the value of 330.85 nm represents the absorption wavelength, this result should not be directly interpreted as the emission wavelength. Similarly, the f value provides information regarding the probability of the molecule's absorption associated with the relevant electronic transition. When the obtained results are evaluated collectively, it can be stated that the compound's electronic structure exhibits a distinct excitation character in the UV region; furthermore, should the aim be to achieve more favorable optical properties in the visible region, the molecular structure could be modified by increasing conjugation or by incorporating suitable donor and acceptor groups.

As for the dipole moment, it determines the polar nature of the molecule in OLEDs and how it aligns within the film. It influences whether charge carriers (λ_{h} and λ_{e}) become localized on the molecule. A value of 4.877 D indicates a moderately polar structure; while this can be advantageous regarding orientation within the device, optimizing host-guest compatibility may be necessary.

Polarizability (α) and hyper polarizability (β) values play a significant role in light propagation, NLO applications, electronic conduction, and energy transfer. The α value of 169.286×10^{-24} esu can be considered moderate; however, the molecule's deformation in an electric field is insufficient. While it supports charge transport and exciton stability and contributes to interactions within the film careful consideration is required. It has a slight effect on light propagation, though this is not critical for OLEDs. Its direct contribution to light emission (via the β value) is minor, yet it contributes to light-matter interaction, exciton stabilization, and photon extraction efficiency. The β value is in the moderate-to-low range at 0.715×10^{-30} ; this is favorable in terms of light-matter interaction.

The λ_{h} and λ_{e} values determine the efficiency and voltage state of the OLED device. λ_{h} determines the hole carrier movement and λ_{e} determines the electron carrier movement. Convection energy values are desired to be small. Molecules with low values exhibit rapid, easy charge transport and higher mobility. The λ_{h} and λ_{e} values are 0.281 eV and 0.361 eV, respectively. Both hole and electron reorganization energies can be considered moderate. These results indicate that hole transport is difficult, and electron transport is slightly more difficult.

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This indicates that they cannot serve as the transport layer; however, since λ values are not critical when acting as a host, it can be said that exciton transfer remains possible.

The ΔE_{ST} value is crucial for the evaluation of TADF OLEDs. It is calculated using Equation 3 [24].

$$\Delta E_{ST} = E_{T1} - E_{S1} \quad (3)$$

As a result of the calculation, ΔE_{ST} was determined to be 1.15 eV. This energy difference is one of the most distinct findings of the study regarding TADF. Much smaller singlet-triplet energy differences ($\Delta E_{ST} \leq 0.5$ eV) are targeted for an efficient thermal RISC process [24]. Therefore, the compound's current molecular structure does not appear suitable as a TADF emitter. However, this result does not imply that the triazole core cannot be used in TADF design. D-A designs that spatially separate donor and acceptor orbitals can lower the exchange energy, thereby reducing ΔE_{ST} . In the derivatives of the compound, while the triazole moiety is retained as an acceptor-type core, the attachment of donor groups—such as carbazole, diphenylamine, or similar—via a suitable π -bridge could be investigated in the next stage of molecular design. However, such modifications must not excessively lower the triplet energy; otherwise, the host properties could be compromised [8, 25].

The most notable result of the study regarding OLEDs is the compound's triplet energy of $T_1 = 2.593$ eV. Triplet energies in the range of approximately 2.0–2.1 eV have been reported in the literature for the red phosphorescent emitter Ir(MDQ)₂(acac) [26,27]. Therefore, the T_1 level of the compound is approximately 0.59 eV higher than the triplet level of the red-phosphorescent guest, and this difference creates an advantageous energy window for confining triplet excitons on the guest.

In phosphorescent OLED hosts, ensuring that the host's T_1 energy is higher than the dopant's T_1 energy is a fundamental criterion for preventing the back-transfer of triplet excitons formed on the dopant to the host and for confining the excitons to the emissive guest. In this regard, the compound's T_1 energy of 2.593 eV provides a suitable energy reserve for a red phosphorescent guest [12,27].

However, the T_1 energy alone is insufficient to definitively classify the compound as a “good host.” A good PhOLED host also requires suitable HOMO/LUMO energy levels, a balance between electron and hole transport, high thermal and morphological stability, an appropriate glass transition temperature, adequate film-forming capability, and host-guest compatibility. Therefore, in light of the available data, the most cautious and scientifically robust statement is that the compound is a promising high-triplet host or co-host candidate for red PhOLEDs [12,28].

Conclusions

Through comprehensive DFT and TD-DFT quantum chemical calculations, this study demonstrates the potential of 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one for OLED applications, revealing a wide-bandgap character with HOMO, LUMO, and energy gap values of -6.206 eV, -1.971 eV, and 4.235 eV, respectively.

Based on the energy level alignment with ITO and Mg:Ag electrodes, the estimated injection barriers are approximately 1.51 eV for holes and 1.73 eV for electrons. Therefore, the use of 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one as an HTL in direct contact with ITO or as an ETL directly accepting electrons from the cathode does not appear suitable. The calculated $S_0 \rightarrow S_1$ transition for 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one is 330.85 nm and 3.748 eV. This result indicates an absorption transition in the

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UV region; however, the current calculations alone are insufficient to determine the emission maximum or the photoluminescence quantum yield. This limits its use as an efficient emitter.

In terms of charge transport dynamics, the calculated reorganization energies ($\lambda_h = 0.281$ eV and $\lambda_e = 0.361$ eV) indicate that hole transport is intramolecularly more favorable than electron transport. The singlet-triplet gap of 1.155 eV, calculated at the B3LYP level, indicates that 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one is not suitable as a TADF emitter in its current form.

The most significant result of the study regarding OLEDs is the high T_1 energy of 2.593 eV exhibited by 4-(benzylideneamino)-5-propyl-2,4-dihydro-[1,2,4]triazol-3-one. The energy difference of approximately 0.59 eV between this compound and Ir(MDQ)₂(acac), which has a triplet energy of about 2.0 eV is advantageous for confining triplet excitons to the red-phosphorescent guest. Therefore, evaluating the compound as a high-triplet host/co-host candidate for red phosphorescent emitters such as Ir(MDQ)₂(acac) rather than as a direct emitter or a simple transport material is a more robust conclusion that aligns with the literature [26-28].

In conclusion, while the investigated 1,2,4-triazol-3-one derivative is unsuitable for TADF emitters, its high T_1 energy makes it a promising scaffold for red PhOLED hosts. Future design efforts should focus on fine-tuning frontier orbitals and charge transport via donor/acceptor modifications without compromising T_1 energy. Overall, DFT and TD-DFT approaches serve as a robust platform for rationally predicting and optimizing key optoelectronic properties prior to synthesis.

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Experimental Investigation of Curvature-Induced Performance Changes in Flexible Photovoltaic Modules under Simultaneous Outdoor Measurements

Salih Öztürk*, Ali Yüce

Department of Electrical and Electronics Engineering, Malatya Turgut Özal University, Malatya 44100, Turkey

Abstract

Flexible photovoltaic (FPV) modules are well suited for non-planar surfaces and building integration, but mechanical bending causes internal stresses. While there are indoor (laboratory) studies on flexible photovoltaic panels, comprehensive experimental measurements under outdoor conditions are still rare. This study aims to investigate the performance difference between a flat panel and a curved panel under the same environmental conditions to fill this gap. An Arduino-based data acquisition module was used to continuously record the experimental data under the same ambient conditions by varying the bending angle of one panel while keeping the other constant. To examine the effect of the internal stress due to curvature, current-voltage characteristics and power fluctuations were measured simultaneously.

Keywords: Flexible photovoltaic modules, Curvature effects, Outdoor measurements, Electrical performance, Solar energy

Corresponding authors: salih6001@gmail.com

1. Introduction

Flexible photovoltaic (FPV) modules have an advantageous structure thanks to their lightweight nature, mechanical flexibility, and adaptability to non-planar surfaces [1-3]. Unlike conventional flat photovoltaic panels, flexible photovoltaic panels provide the opportunity to be integrated into irregular geometries thanks to their curved structures. [4,5] Flexible photovoltaic panels have advantages in terms of integration into irregular geometries; however, their curved structures cause bending-induced internal stress and lead to losses in energy efficiency [6].

Although many studies have investigated the behavior of photovoltaic panels in a laboratory environment, comprehensive experimental evaluations under outdoor conditions remain limited. [7-9]. Despite significant advances in simulating and testing flexible photovoltaics in laboratory environments, measurements under real outdoor operating conditions will fully reveal the energy performance of flexible photovoltaics [10-13].

This study presents an analysis of the performance variations between a flat panel and a flexible photovoltaic panel subjected to simultaneous outdoor measurements. A flexible panel with an adjustable bending angle and a flat panel were positioned under identical environmental conditions, and their current-voltage (I-V) and power characteristics were monitored simultaneously. The findings will serve as a guide for evaluating the efficiency of flexible photovoltaic systems in real outdoor environments and calculating stress-induced energy losses.

2. Experimental details

In this study, performance variations of flexible photovoltaic (FPV) modules resulting from mechanical curvature were evaluated using specially designed rigid mounting fixtures with predetermined arc angles (R).

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These fixtures securely fixed flexible modules at specific arc angles to ensure uniform stress distribution across the active photovoltaic area, while a side-by-side outdoor testing platform was deployed to eliminate spatial discrepancy variables among the configurations.

An Arduino-based data logger was integrated into the experimental platform to continuously record electrical parameters such as current, voltage, and power. Data collected at different bending angles on different days were continuously recorded using the data logger.

3. Results and discussion:

The following graph fig.1 shows the current-voltage (I-V) characteristics of a typical silicon PV cell operating under normal conditions. [14]

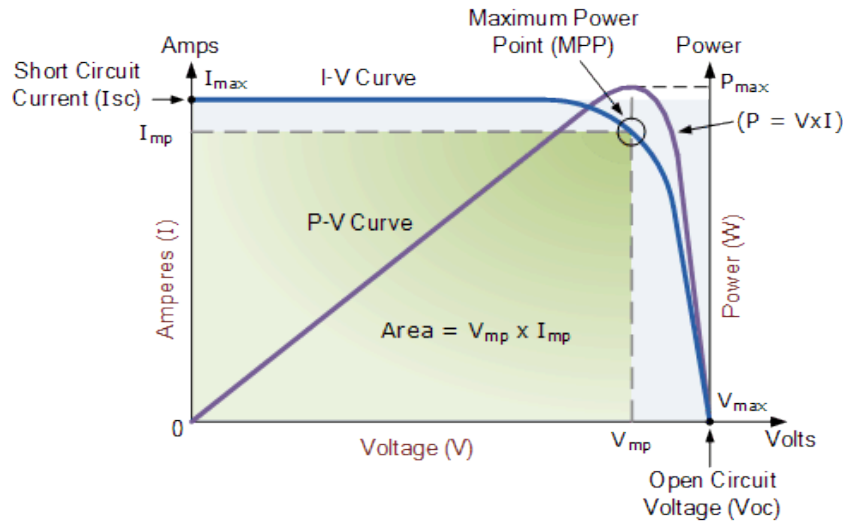


Figure 1 Solar Cell I-V Characteristic Curve

The definitions shown in *Fig.1* are explained below.

Open-Circuit Voltage (V_{oc}): The maximum voltage measured across a solar panel terminals when no load is connected (the circuit is open and the current is zero). [15]

Short-Circuit Current (I_{sc}): The maximum current produced by a solar cell or panel when its terminals are short-circuited together (the voltage is zero). [16]

Current at Maximum Power (I_{mp}): The current delivered by a solar cell or panel when it is operating at its maximum power point (MPP). [17]

Voltage at Maximum Power (V_{mp}): The voltage delivered by a solar cell or panel when it is operating at its maximum power point (MPP). [17]

Maximum Power Point (MPP): The optimal operating point on a solar panel's I-V curve where the product of voltage and current is at its maximum, producing the highest possible electrical power (P_{max}) [18]

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The flat panel and curved panel platform established for simultaneous outdoor measurements is shown in fig.2. The simultaneous outdoor measurements revealed clear performance variations in the flexible photovoltaic modules as a function of the induced arc angle (R). As the modules were subjected to sharper bending curvatures, internal mechanical stresses affected the current-carrying conductors, significantly altering the series resistance and directly impacting key electrical parameters such as short-circuit current (I_{sc}), open-circuit voltage (V_{oc}), and maximum power (P_{max}). Specifically, increased curvature led to a progressive degradation in overall energy efficiency.

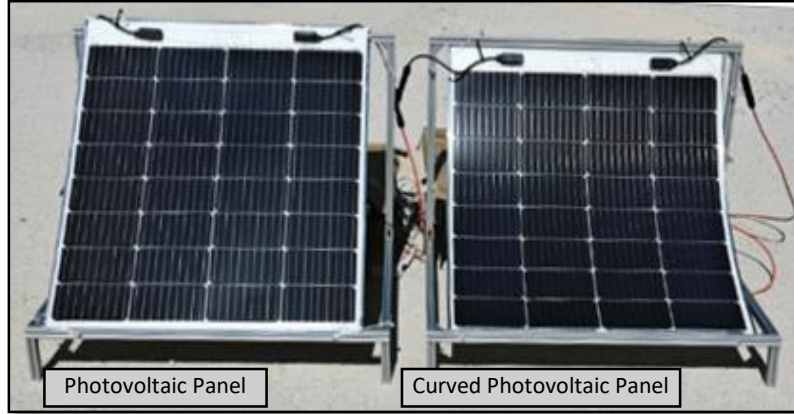


Figure 2 PV Panel and CPV Panel

Furthermore, the simultaneous analysis of electrical outputs recorded using a dedicated datalogger confirmed that curvature-induced mechanical deformation introduces immediate electromechanical losses during outdoor operation and provided guidelines for analyzing the electrical losses of flexible solar panels. The datalogger, specially designed to record current, voltage, power, and temperature data, is presented in fig.3.



Figure 3 Arduino-based real-time data acquisition unit.

In the experimental setup, the flexible photovoltaic panel, tested at various arc angles, is connected to an MPPT charge regulator that regulates the energy. The MPPT circuit connection diagram is presented in fig.4. A solar gel battery is integrated into the system to ensure system stability and energy flow, and a rheostat is included at the output to test load characteristics and operating points.

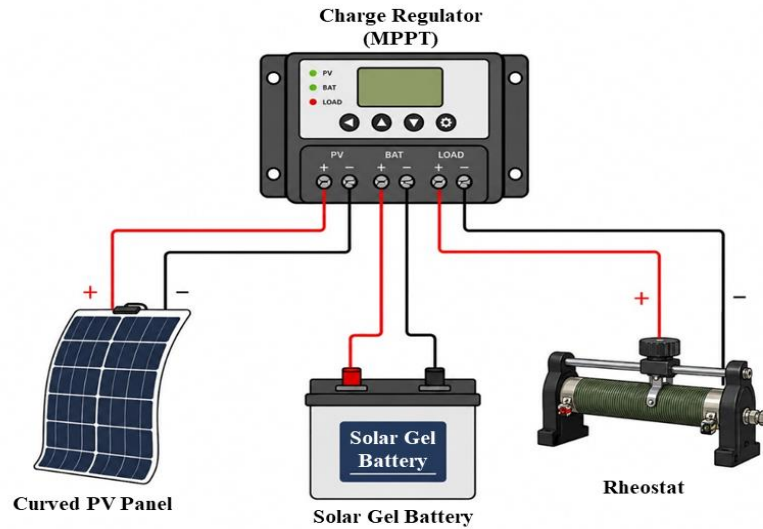


Figure 4 Experimental setup diagram.

The data measured for the flat panel under identical outdoor conditions are presented in table 1, while the data for the 30° curved panel are given in table 2.

Table 1 Outdoor operational test results and electrical performance parameters of the photovoltaic (PV) module.

Curve (°)	Time (Hour)	Temperature (°C)	Voltage (Volt)	Current (Ampere)	Power (Watt)
0	10:00	34,69	16,77	4,00	67,01
0	11:00	39,81	18,41	3,77	69,46
0	12:00	42,19	16,65	4,81	80,07
0	13:00	37,31	16,33	4,96	80,96
0	14:00	41,38	16,55	4,44	73,48
0	15:00	37,56	16,80	3,70	62,13
0	16:00	37,06	16,24	2,74	44,44
0	17:00	33,53	16,56	1,82	30,14

Table 2 Outdoor operational test results and electrical performance parameters of the curved photovoltaic (CPV) module, Curve = 30°.

Curve (°)	Time (Hour)	Temperature (°C)	Voltage (Volt)	Current (Ampere)	Power (Watt)
30	10:00	36,00	12,52	4,14	51,89
30	11:00	42,00	12,79	4,88	62,41
30	12:00	45,88	12,89	5,18	66,76
30	13:00	40,50	12,92	5,18	66,88
30	14:00	43,81	12,92	4,66	60,20
30	15:00	39,00	12,79	3,92	50,16
30	16:00	39,31	12,55	2,74	34,35
30	17:00	34,12	12,38	1,78	22,04

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The data for both the flat panel and the 30° curved panel throughout the day were recorded using the specially designed datalogger. It was observed that the measured power was lower in the morning hours, partly due to low solar irradiance. As noon approached, an increase in the measured power was observed. In the afternoon, along with the decrease in solar irradiance, a drop in the measured power was observed. While the power output of the flat panel was 80.96 W at 13:00, that of the 30° curved panel was 66.88 W at 13:00. Throughout the day, the flat panel generated more power than the 30° curved panel.

The data measured for the flat panel under identical outdoor conditions on a different day are presented in table 3, while the data for the 60° curved panel are given in table 4.

Table 3 Outdoor operational test results and electrical performance parameters of the photovoltaic (PV) module.

Curve (°)	Time (Hour)	Temperature (°C)	Voltage (Volt)	Current (Ampere)	Power (Watt)
0	10:00	48,20	15,92	4,44	70,69
0	11:00	48,56	16,12	4,64	74,80
0	12:00	49,20	16,18	4,82	77,99
0	13:00	45,38	15,84	4,88	77,30
0	14:00	44,38	15,94	4,44	70,77
0	15:00	44,94	15,99	3,85	61,56
0	16:00	37,94	16,97	2,66	45,14
0	17:00	34,00	15,75	1,55	24,41

Table 4 Outdoor operational test results and electrical performance parameters of the curved photovoltaic (CPV) module, Curve = 60°.

Curve (°)	Time (Hour)	Temperature (°C)	Voltage (Volt)	Current (Ampere)	Power (Watt)
60	10:00	46,63	12,10	5,12	61,95
60	11:00	48,65	12,44	5,25	65,31
60	12:00	48,26	12,51	5,14	64,30
60	13:00	47,06	12,57	5,18	65,11
60	14:00	43,75	12,57	4,81	60,46
60	15:00	46,19	12,55	4,07	51,07
60	16:00	39,63	12,38	2,81	34,79
60	17:00	33,50	12,23	1,41	17,24

As observed from table 3 and table 4, the experimental data measured throughout the day indicate that the flat panel generated more power than the 60° curved panel. While the power output of the flat panel was 77.30 W at 13:00, that of the 60° curved panel was 65.11 W at 13:00. The flat panel generated more power than the 60° curved panel.

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The data measured for the flat panel under identical outdoor conditions on a different day are presented in table 5, while the data for the 90° curved panel are given in table 6.

Table 5 Outdoor operational test results and electrical performance parameters of the photovoltaic (PV) module.

Curve (°)	Time (Hour)	Temperature (°C)	Voltage (Volt)	Current (Ampere)	Power (Watt)
0	10:00	33,47	17,12	3,21	54,95
0	11:00	39,50	17,04	4,36	74,38
0	12:00	37,56	17,26	4,59	79,17
0	13:00	36,75	18,63	3,85	71,66
0	14:00	39,63	18,87	3,18	60,04
0	15:00	41,88	18,36	3,18	58,41
0	16:00	34,31	16,41	3,26	53,41
0	17:00	33,12	16,28	2,29	37,28

Table 6 Outdoor operational test results and electrical performance parameters of the curved photovoltaic (CPV) module, Curve = 90°.

Curve (°)	Time (Hour)	Temperature (°C)	Voltage (Volt)	Current (Ampere)	Power (Watt)
90	10:00	34,24	12,21	3,42	41,75
90	11:00	38,19	12,50	4,36	54,56
90	12:00	39,38	12,67	4,81	60,93
90	13:00	40,25	12,77	4,96	63,29
90	14:00	43,81	12,74	4,76	59,40
90	15:00	44,75	12,67	3,92	49,68
90	16:00	38,81	12,43	2,74	34,02
90	17:00	34,46	12,28	1,78	21,85

Similarly, the measured power was lower during the morning hours when solar irradiance was low. As solar irradiance increased around noon, the measured power also increased. Comparing table 5 and table 6, it was observed that the flat panel generated more power than the 90° curved panel throughout the day. While the power output of the flat panel was 71.66 W at 13:00, that of the 90° curved panel was 63.29 W at 13:00. The flat panel generated more power than the 90° curved panel.

The data measured for the flat panel under identical outdoor conditions on a different day are presented in table 7, while the data for the 120° curved panel are given in table 8.

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Table 7 Outdoor operational test results and electrical performance parameters of the photovoltaic (PV) module.

Curve (°)	Time (Hour)	Temperature (°C)	Voltage (Volt)	Current (Ampere)	Power (Watt)
0	10:00	33,13	16,44	3,92	64,45
0	11:00	43,81	16,58	4,51	74,81
0	12:00	49,44	16,65	4,66	77,59
0	13:00	45,06	18,24	3,77	68,77
0	14:00	47,94	15,89	4,51	71,66
0	15:00	41,19	16,36	3,63	59,38
0	16:00	41,25	16,60	2,81	46,65
0	17:00	36,00	16,80	1,65	27,72

Table 8 Outdoor operational test results and electrical performance parameters of the curved photovoltaic (CPV) module, Curve = 120°.

Curve (°)	Time (Hour)	Temperature (°C)	Voltage (Volt)	Current (Ampere)	Power (Watt)
120	10:00	33,13	12,23	3,33	40,73
120	11:00	34,44	12,43	3,77	46,86
120	12:00	44,88	12,57	4,29	53,95
120	13:00	41,44	12,65	4,29	54,27
120	14:00	44,69	12,60	3,77	47,53
120	15:00	38,50	12,40	2,89	35,78
120	16:00	41,31	12,26	1,92	23,57
120	17:00	34,34	12,15	1,10	13,37

When comparing table 7 and table 8, the data measured under identical environmental conditions indicate that the flat panel generated more power than the 120° curved panel. While the power output of the flat panel was 68.77 W at 13:00, that of the 120° curved panel was 54.27 W at 13:00. The flat panel generated more power than the 120° curved panel.

Upon examining the experimental data, it was observed that under identical environmental conditions, the flat panel generated more power compared to the curved panel. Furthermore, as the curvature increased, the generated power was observed to decrease. The generated power exhibits a decreasing trend with increasing curvature. The graph illustrating this decreasing trend based on the analyzed data is presented in fig.5.

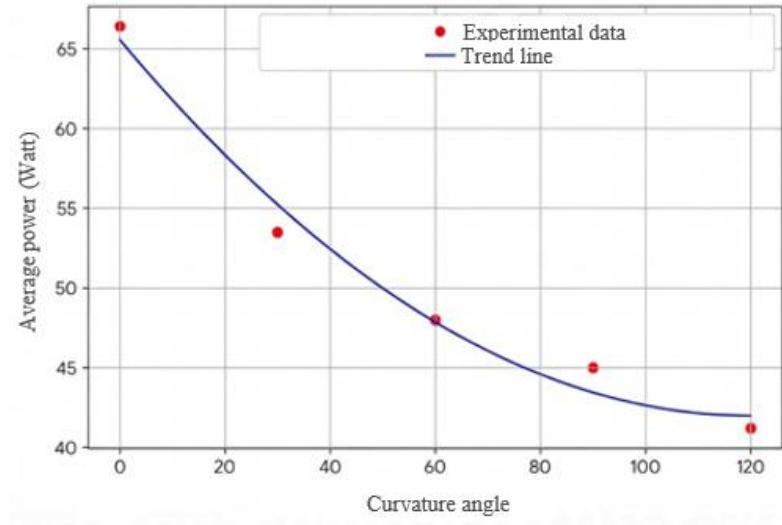


Figure 5 Flexible PV panel curvature angle and power graph.

As shown in fig.5, the relationship between the curvature angle (θ) and the average power (P_{avg}) of the flexible photovoltaic module can be mathematically expressed by a second-order polynomial regression model. The established regression model is given as:

$$P(\alpha, R) = 0,0007\alpha^2 - 0,2704\alpha + 0,0819R + 11,5048 \quad (1)$$

The curve demonstrates a distinct descending trend as the bending angle increases, further validating the curvature-induced power losses. The root mean squared error of the established regression model is $\approx 5 \text{ W}$.

Conclusions

The simultaneous outdoor measurements clearly demonstrated that mechanical curvature and its associated internal stress significantly impact the electrical performance of flexible photovoltaic modules. Across all tested bending angles (30°, 60°, 90°, and 120°), the curved panels experienced progressive reductions in operating voltage and maximum power output compared to the reference flat panel. For instance, at peak solar irradiation hours (at 13:00), the maximum power output was 66.88 W for the 30° bent panel, whereas it was 80.96 W for the flat panel. At 13:00, while the maximum power was 54.27 W at 120° bending, it was 68.77 W for the flat panel. These findings confirm that curvature-induced mechanical stress leads to a distinct performance degradation.

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