

Structural and Optical Properties of Zn_2SnO_4 Thin Films for Enhanced Photovoltaic Performance

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Abstract

Today, the development of inexpensive, non-toxic and highly transparent oxide semiconductors is very crucial for the sustainable growth of next-generation photovoltaic technologies owing to their efficient charge transport properties and higher thermal stability. The present study involves fabrication and characterization of a transparent thin-film heterojunction comprising of Zn_2SnO_4 and NiO hetero-partners, synthesized by a unique combinatorial approach. The phenomena of carrier injection, directional transportation, generation/recombination, and their extraction are rigorously analyzed through band alignment engineering. The growth of all-oxide p-n heterojunction with Al/p-NiO/n-ZTO/ITO device architecture demonstrated a sound J-V response in the dark with an ideality factor of ~ 2.58 , turn on voltage of ~ 1.44 V, a series resistance of ~ 2.8 Ω . A type-II band alignment is perceived for the proposed heterojunction with improved electrical conduction, yielding a built-in-potential of ~ 0.54 V across the hetero-interface. Under 1-sun illumination, the thin-film heterojunction solar cell demonstrates an open circuit voltage of ~ 0.62 V, short circuit current density of ~ 15.4 mA cm^{-2} , fill factor of $\sim 31\%$, and power conversion efficiency of $\sim 2.95\%$. The realization of low-cost and environmentally benign oxide-based thin-film heterojunction would open new avenues for sustainable and high-performance photovoltaic applications.

1 Introduction

Rapidly growing population together with their rising energy demands that have long relied on conventional fossil fuels has led to the swift depletion of these finite resources and intensified severe environmental concerns globally [1]. These challenges have driven researchers to pursue clean, sustainable, and economically viable renewable energy resources. Under these circumstances, highly-transparent oxide semiconductors have emerged as promising class of materials due to their tunable optical band gap, strong absorption of visible light, high electrical conductivity and superior optical transparency [2, 3]. To date, indium tin oxide (ITO) has been extensively studied as transparent conducting oxide (TCO) and widely employed in optoelectronic device applications. However, issues related to indium scarcity, material cost, and long-term stability have motivated researchers to explore other potential alternates [4]. In this context, zinc tin oxide (Zn_2SnO_4) has gained substantial attention in recent years as a transparent ternary alloy due to its high electron mobility up to ~ 30 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$, direct tunable optical band gap (typically ~ 3.2 to 4.1 eV) and excellent optical transmittance of $\sim 85\%$ across the visible spectrum [5, 6]. The n-type conductivity and low electrical resistivity of ZTO make it as an ideal electron transport material particularly for optoelectronic and photovoltaic applications. So far, various experimental approaches have been explored for the deposition of ZTO films. In general, as-deposited Zn_2SnO_4 film is generally amorphous and/or nanocrystalline in nature. However, optimized post-deposition annealing can induce a phase transformation from the amorphous state to a polycrystalline structure [7]. Ho et al. used RF magnetron sputtering to synthesize ZTO films on glass substrates by incorporating high-purity ZnO and SnO_2 targets. The as-deposited films were subsequent annealed in vacuum and in air at temperatures ranging from 200 to 600°C for 60 min [8]. This study presented a comparative analysis based on annealing conditions to acquire highly crystalline ZTO films with preferential crystal growth. An extremely transparent (93.4%) ZTO film across the 400 – 900 nm spectral range is reported elsewhere [9]. Kumar et al, incorporated flash evaporation technique to obtain of ZTO films by varying Zn-content. It is revealed that the ZTO films with an equal ZnO: SnO_2 weight ratio demonstrated the optimum electrical properties at an annealing temperature of 450°C for 1 h under vacuum. ZTO films exhibited a lowest resistivity of $\sim 1.12 \times 10^{-3}$ $\Omega\cdot\text{cm}$, carrier density of $\sim 2.96 \times 10^{20}$ cm^{-3} , and higher carrier mobility of ~ 18.8 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ [5]. Furthermore, atomic layer deposition (ALD) technique was also employed to deposit high crystalline ZTO films by varying the Sn-content to explore the morphological, structural, and electronic characteristics of zinc stannate thin films for the practical

implementation of thin-film transistors (TFTs) [9]. Sol-gel spin-coating technique has also been used to synthesize ZTO film as a channel layer for the fabrication of TFT. The study evaluates how different metal electrodes influence contact resistance for device performance [10]. In this framework, Sharanu et al investigated the photocatalytic degradation studies for spin-coated $\text{ZnO-Zn}_2\text{SnO}_4$ (ZTO) thin films using methyl orange (MO) dye under UV light irradiation. As-grown ZTO films were annealed at 500 °C to improve crystallinity and phase purity [11]. The impact of air-annealing on the physio-chemical properties of $\text{Zn}_2\text{SnO}_4\text{-ZnO}$ nanostructured films were also studied elsewhere [12].

ZTO-based heterojunctions have been widely used in numerous applications such as ultraviolet (UV) photodetectors, gas sensors, thin-film transistors (TFTs), and photovoltaic solar cells with the desired heterostructure design. In this framework, Hao et al. adopted co-precipitation method for the growth of zinc tin oxide (ZTO) where post annealing was performed to tune its structural and electrical transport properties. ZTO/ SnO_2 heterostructure exhibited favorable gas-sensing characteristics [13]. Moreover, Cruz et al reported SILAR method to synthesize ZTO thin films for water splitting and photocatalytic CO_2 reduction in clean fuel generation systems [14]. The solution-processed ZTO/ITO heterojunction was proposed by Huang et al in order to co-relate mobility and stability for TFT-applications. Ta-doped ZTO films have been coated on ITO at a speed of 2000 r/min for 30 s, followed by post-annealing annealed at 500°C for 1 h [15]. The fabrication of UV-photodetector based on $\text{CsPbCl}_3/\text{Zn}_2\text{SnO}_4$ heterojunction on a flexible PET substrate via spin-coating method is reported by Hu et al. The pairing of ZTO with perovskite layer improved the phenomenon of charge separation and transportation owing to its high electron mobility and compatible band alignment [16]. J-V characteristics of n-ZTO/p-Si heterojunction exhibited a good rectifying behavior with reduced barrier height by increasing ZTO thickness. The fabricated n-ZTO/p-Si heterojunction demonstrated a turn on voltage of 2.35V, barrier height of 0.25 eV, ideality factor of 2.2, and reverse saturation current of 0.81 μA [17]. Recent experimental and theoretical investigations have demonstrated the significant potential of ZTO in fabricating thin-film heterojunction solar cells, where ZTO functions as a transparent conducting oxide (TCO) layer, offering excellent optical transparency and electrical conductivity [18–20]. ZTO-based solar cell (CIGS/ZTO and ZTO/i-ZnO) demonstrated a power conversion efficiency of $\sim 24.7\%$, theoretically calculated through numerical simulations [21]. Nanowire-based $\text{SnO}_2/\text{Zn}_2\text{SnO}_4$ heterostructure was synthesized by one-pot synthesis approach for solar energy conversion [22]. The ZTO based heterostructure demonstrated a photovoltaic response with an open circuit voltage of 0.59 V, a short circuit current density of 10.98 mA/cm^2 , fill factor of 73.0, and power conversion efficiency of 4.72%. Later on, same research group proposed composite-based SnO_2/ZTO heterostructure through solvothermal synthesis route to demonstrate its potential as a photoanode as well as a gas-sensing material. The ZTO based heterostructures demonstrated promising photovoltaic characteristics with an open circuit voltage of 0.71 V, a short circuit current density of 9.83 mA/cm^2 , fill factor of 70.3, and power conversion efficiency of 4.91% [23]. The similar heterojunction (ZTO- SnO_2) was fabricated using a two-step synthesis process followed by calcination for photovoltaic applications, yielding a V_{oc} of ~ 706 mV, J_{sc} of 2.85 mA/cm^2 with PCE of $\sim 1.29\%$ [24]. Moreover, ZTO film was also investigated as an efficient electron transport layer (ETL) for composite $\text{ZnO}/\text{Zn}_2\text{SnO}_4$ solar cell via spray pyrolysis. The fabricated solar cell demonstrated an enhanced photocurrent of ~ 19.71 mA/cm^2 with PCE of 12.03% under AM 1.5 solar light 100 mW/cm^2 [25]. Zinc stannate (ZTO) and nickel oxide (NiO) films were synthesized by the sol-gel method to obtain a transparent heterojunction, achieving a maximum rectification ratio of 11.7 and an on/off current ratio of 18.3 at a bias voltage of 5 V [26]. Previous studies have focused to investigate ZTO ternary alloy as buffer layer or electron transport layers (ETLs) for UV-photodetection [21, 27]. Herein, a simple and cost-effective two-step synthesis route is employed to obtain high quality n-type Zn_2SnO_4 (ZTO) thin-films as a transparent window layer for solar cell

application. A comprehensive review of the available literature indicates that, seldom systematic investigations have been reported so far, regarding fabrication of all-oxide thin-film ZTO/NiO p-n heterojunction emphasizing band alignment engineering for enhanced carrier transport properties.

2 Experimental section

2.1 Preparation of thin films

Highly transparent ZTO/NiO thin-film heterojunction was fabricated on quartz glass, Si and ITO substrates following two-step thermal evaporation and subsequent thermal oxidation process. The substrates were ultrasonically cleaned with organic solvents (i.e., acetone and ethanol), rinsed in deionized water for 05 minutes to remove surface contaminants and blow-dried using nitrogen (N_2) gas. Initially, ZnSn precursors (in similar weight ratio) were kept in tungsten crucible and placed into vacuum chamber and different substrates were mounted on the substrate holder at a distance of approximately 18–19 cm from source material. Pre-deposition was performed around 15–20 minutes to remove volatile impurities of source material. As-deposited films were subsequently heat-treated in tube furnace at 500 °C for 1 hr for their complete thermal oxidation. Similarly, a metallic Ni-film was deposited over the ZTO layer by thermal evaporation and then heat-treated for its complete oxidation under the same working conditions to convert it into p-type NiO. Finally, a thin layer of aluminium was deposited as top-metallic contact by thermal evaporator through shadow masking. The comprehensive detail of experimental plan for fabricating p-n heterojunction with structural design Al (as front electrode)/NiO/ZTO/ITO (as back contact) is highlighted in Fig. 1.

2.2 Characterization tools

The elemental and phase identification of the deposited films were analyzed using a powder X-ray diffractometer (D8 Advance, Bruker). Structural and morphological properties were thoroughly investigated using scanning electron microscopy (Emcrafts-Cube, Series C). The current voltage characteristics of synthesized heterojunction device were carried out using semiconductor parameter analyzer (Keithley SMU-4200) to evaluate the electrical performance of thin-film heterojunction. Capacitance-voltage characteristics were determined to inspect the built-in potential. Optical characteristics of each hetero-partner thin film were examined through UV-Vis absorption spectroscopy (Lambda 25, Perkin Elmer). Photoluminescence (PL) was performed using a typical laser of excitation wavelength of ~ 532 nm to investigate the optical emission spectra of prepared films. Furthermore, photovoltaic parameters of the fabricated thin-film heterostructure solar cell were extracted from J-V measurements performed under 1-sun illumination with an incident power density of 100 mWcm^{-2} .

3 Result and discussion

3.1 XRD analysis

Figure 2 represents the XRD analysis of the NiO and ZTO oxide-films, synthesized on quartz glass. XRD-spectrum of ZTO thin film indicate the formation of a highly crystalline zinc stannate (Zn_2SnO_4) phase at optimal annealing of 500 °C [28]. The diffraction peaks were observed at $2\theta = 34.5^\circ$ and 36.1° , 41.9° , and 60.8° correspond to the (311), (222), (400), and (440) crystallographic planes respectively, well matched with standard JCPDS card no. 73-1725. The formation of distinct crystal structure of Zn_2SnO_4 ternary alloy can be attributed to its inverse-spinel configuration, where Sn^{4+} ions preferentially occupy octahedral sites, while Zn^{2+} cations reside on octahedral sites

of crystal lattice [29]. Previous studies have frequently reported the detection of residual metallic traces in post-annealed Zn_2SnO_4 thin films, indicating partial or incomplete oxidation of metallic precursors during the annealing process [25, 28, 30]. In contrast, the present study demonstrates the formation of stoichiometric ZTO films without any metal-content, providing a strong evidence of complete oxidation under optimal annealing conditions. Herein, an additional diffraction peak is observed at $2\theta = 31.7^\circ$ along (100) plane of the hexagonal wurtzite ZnO structure, indicating the formation of a secondary phase towards lower diffraction angle, attributed to thermal activation and re-crystallization of strain-relaxed grains of ternary Zn-Sn-O alloy under heat treatment. In contrast, the XRD spectra of p-type counterpart, NiO thin film duly confirmed the phase-singularity with higher order of crystallinity, as presented in Fig. 2(a). The diffraction peaks observed at $2\theta = 38.2^\circ, 43.5^\circ, 44.6^\circ$, and 63.8° were indexed to the (012), (200), (104), and (018) crystallographic planes, respectively. The diffraction spectra is completely matched with the standard JCPDS card No. 85-1977. Figure 2(b,c) presents the estimated value of full width at half maximum (FWHM) for each of hetero-partner thin film through Gauss fitting. Major diffraction peak of Zn_2SnO_4 (appeared at $\sim 34.5^\circ$) and for NiO (detected at $\sim 38.2^\circ$) exhibited an approximate value of FWHM of $\sim 0.38^\circ$ and 0.29° , respectively [7, 31]. Summary of structural parameters obtained from XRD-analysis of both NiO and ZTO oxide-films are given in Table 1.

Table 1
Summary of XRD-parameters for each of the oxide-film deposited on glass substrate.

Thin Film	2θ (Degree)	Miller Indices (hkl)	FWHM (λ) (Degree)	Crystallite Size (D) (nm)	Inter-Planner Spacing (d) (nm)	Micro Strain ($\times 10^{-3}$) (ϵ)	Dislocation density ($\times 10^{-3}$) (δ) (nm^{-2})
ZTO	34.4°	(311)	0.38°	22.33	0.022	1.58	2.00
NiO	38.2°	(012)	0.29°	29.60	0.025	1.19	1.14

3.2 UV-Vis-NIR and PL spectroscopic analysis

The optical properties of both hetero-partner ZTO and NiO thin films were investigated using UV-VIS-NIR absorption and photoluminescence (PL) spectroscopy. Figure 3 (a,b) presents the absorbance spectra of thermally oxidized ZTO and NiO films, respectively recorded across the spectral range of 250–1000 nm. Both films exhibit strong optical absorption in UV-region, highlighting their potential for UV-sensitive optoelectronic applications [35, 36]. The optical transmittance spectra of both the constituent oxide hetero-partner thin films are highlighted in the insets of Fig. 3 (a) and (b), respectively. Both constituent oxide-films demonstrated a relatively high and consistent optical transmittance (of $\sim 80\%$) throughout the visible region, consistent with prior studies [17, 37]. Such a combination of strong UV-absorption with high optical transparency in visible region is highly desirable for photovoltaic devices, regarding efficient photo-generation of charge carriers across the hetero-interface. Photoluminescence (PL) spectra of each oxide-film (ZTO and NiO) are presented in Fig. 3 (c,d), respectively. ZTO-film exhibited a strong UV-emission at a wavelength of ~ 335 nm, corresponding to a photon energy of ~ 3.7 eV. This emission can be assigned to the near-band-edge (NBE) transition, arising predominantly from the radiative recombination of photo-generated charge carriers near the conduction band minimum (CBM) and valence band maximum (VBM). Notably, the extracted value of this fundamental band-edge emission energy is closely matched with the direct optical band gap (~ 3.8 eV) determined from the UV-Vis-NIR absorption spectroscopy using Tauc’s method, as shown in the inset of Fig. 3(c).

Moreover, a relatively broad emission band is also observed at λ 489 (i.e, 2.53 eV) which probably be associated with deep-level-emission (DLE), arising from defect-related localized states and secondary phases under heat treatment, as evidenced in XRD-analysis. Similar defect-related luminescence has been reported in Zn₂SnO₄ nanowires has been reported where an additional broad emission band was attributed to deep-level defect states [38, 39]. Figure 3(d) presents the PL spectrum of NiO thin film, exhibiting a distinct emission band centered at $\sim$ 339 nm, corresponding to a photon energy of $\sim$ 3.65 eV that is in good agreement with values reported in the literature [40, 41]. The observed band-edge radiative emission energy is consistent with the direct optical band gap of NiO (i.e., $E_g \sim$ 3.61 eV) extracted from Tauc's plot, shown in the inset of Fig. 3d. The suggested band-edge transition validates the reliability of the optical band gap derived for p-type NiO counterpart.

3.3 SEM analysis

Figure 4(a-d) demonstrate the structural and morphological analysis of oxide-films and heterojunction at a scan size of 10 μ m, deposited on glass substrate. Figure 4a highlights the SEM-micrograph of ZTO-film signifying a granular morphology comprising of spherical-shaped nanoparticles that are uniformly distributed across the entire surface of film with an average particle size of $\sim$ 500 nm. Moreover, pronounced cluster formation, accompanied by considerable surface debris indicating a rough surface of ZTO-film. In contrast, the NiO film exhibits a comparatively smooth and homogeneous surface, as shown in Fig. 4b. The surface displays a blended-morphology comprising closely-packed fine grains, indicating a compact film structure. However, small pits and crater-like features are also observed, which may be attributed to localized structural defects generated during the heat-treatment process [33]. Figure 4c displays the SEM micrograph of ZTO/NiO thin-film heterojunction, exhibiting a relatively dense and compact morphology, with fine grains distributed across the film surface. In addition, the presence of small voids and localized agglomeration results in island-formation, suggesting enhanced surface roughness. The cross-sectional SEM image of heterojunction is highlighted in Fig. 4d, confirming the formation of a well-defined bilayer ZTO/NiO structure on ITO substrate. The SEM micrograph reveals a ZTO and NiO layer of a thickness of $\sim$ 400 nm, $\sim$ 100 nm, respectively.

3.4 Electrical properties of heterostructure device

Figure 5 (a-c) illustrates the current-voltage characteristics of the p-NiO/n-ZTO heterojunction grown over ITO substrate at room temperature. J-V measurements of the fabricated p-n heterojunction diode exhibited a rectification ratio of $\sim$ 2.6 at $\pm$ 2 V. Under forward biasing, the heterojunction device displayed a turn on (i.e., knee) voltage of $\sim$ 1.44V, as exposed in Fig. 5(a). The schematic configuration of the fabricated ITO/ZTO/NiO/Al p-n heterojunction device was demonstrated in Fig. 5(a) inset. The electron-affinity model was utilized to evaluate the fundamental diodic-parameters while incorporating the effects of interfacial defects in the vicinity of metallurgical junction as described by the given relation [32]:

$$I_{total} = I_o \left[\exp \left(\frac{qV}{nkT} \right) - 1 \right] \text{-----} (I)$$

where I_{total} and I_o denote the total forward current and dark current, respectively. The ideality factor was extracted from the slope of the linear region of the semilogarithmic plot of non-negative current density ($|J|$) as a function of forward-bias voltage, yielding an average value of $\sim$ 2.58 $\pm$ 0.05, as shown in Fig. 5(b) [33]. The obtained ideality factor ($n > 2$) suggests that charge transport across the heterojunction is predominantly governed by recombination processes rather than diffusion. According to the Shockley ideal diode model, the ideality factor is generally expected to lie within the range of 1–2. The observed deviation from the ideal value is attributed to interface

recombination, which promotes defect-assisted carrier transport across the heterojunction due to unfavorable band discontinuities at the NiO/Zn₂SnO₄ hetero-interface [33]. The inset of Fig. 5(b) shows the plot of current density as a function of the applied voltage over the entire voltage range, including both forward- and reverse-bias regions, on a semilogarithmic scale. Another important diode parameter, the series resistance (R_s), was determined using the Cheung-Cheung method by evaluating the slope of $\partial V / \partial \ln(I)$ through linear fitting. The extracted value of series resistance was approximately $2.8 \Omega \pm 0.05$, as shown in Fig. 5c, indicating a relatively low resistive losses at metal-semiconductor junction. The inset of Fig. 5c illustrates the schematic geometry of the Al/NiO contact together with its linear J-V characteristics. The formation of Al/NiO Ohmic contact promotes efficient carrier extraction, thereby improving the overall electrical performance of the fabricated heterojunction device [34].

To assess the interface quality and gain deeper insight into the band alignment of the NiO/ZTO p-n heterojunction, capacitance-voltage (C-V) measurements were performed at room temperature to determine the built-in potential (V_{bi}) as shown in Fig. 5(d). The built-in potential (V_{bi}) was calculated from Mott-Schottky analysis under reverse bias conditions, by plotting $1/C^2$ as a function of the applied voltage (V). The linear region of the curve was extrapolated to the voltage axis where $1/C^2 = 0$, yielding a built-in voltage of $\sim 0.54V$, as revealed in the inset of Fig. 5(d). The relatively higher value of V_{bi} compared with previously reported values suggests improved interfacial band alignment [24, 26]. It indicates the formation of a strong internal electric field across the NiO/ZTO hetero-interface which facilitates efficient charge separation and suppresses carrier recombination at the junction interface.

3.5 UV-Vis-NIR and PL spectroscopic analysis

To investigate the carrier dynamics across p-n junction, the band diagram was constructed using Anderson's electron-affinity model. At electrical neutrality, the band structure of NiO/ZTO p-n heterojunction was predicted based on known fundamental parameters such as optical band gap (E_g), electron affinity (χ), and work function (Φ) of each hetero-partner [42–44] presented in Fig. 6a. However, at electrical equilibrium when the Fermi-levels are aligned, the resulting band bending is schematically illustrated in Fig. 6b. In order to elucidate the band alignment engineering, band offsets were also calculated. The conduction band offset ($\Delta E_c = \chi_n - \chi_p$) was estimated ~ 2.70 eV, while the valence band offset $\Delta E_v = (E_g + \chi)_n - (E_g + \chi)_p$ was found ~ 2.96 eV. Notably, a non-negative conduction band offset signifies the spike-formation at band edges across NiO/ZTO heterojunction. Moreover, the condition $\Delta E_c < \Delta E_v$ indicates a relatively weaker potential barrier for electrons compared with holes, resulting in more pronounced hole confinement at the p-NiO/n-ZTO interface [33, 34]. In addition, the lower value of effective energy gap (i.e., $E_{g,eff} \sim 0.9$ eV) compared with the bandgap energy of each hetero-partner may reduce the energy barrier for interfacial carrier transport across p-n heterojunction and thereby facilitate the tunneling induced dipole effect that is consistent with the carrier-transfer characteristics, generally witnessed in Type-II band alignment [32, 45].

3.6 Photovoltaic performance of heterostructure solar cell

The photovoltaic performance of proposed heterostructure solar cell was characterized under standard 1-sun illumination at an incident power density of 100 mWcm^{-2} . The corresponding current-voltage measurements revealed an open circuit voltage (V_{oc}) of ~ 0.62 V, and a short circuit current density (J_{sc}) of $\sim 15.4 \text{ mAcm}^{-2}$. The heterojunction device exhibited a fill factor (FF) of $\sim 31\%$, resulting in a power conversion efficiency (PCE) of $\sim 2.96\%$, as presented in Fig. 7. Notably, the heterostructure device demonstrates a substantial improvement in photovoltaic performance compared with previously reported all-oxide ZTO-based heterojunction devices, highlighting the effectiveness of the proposed device architecture [24, 46].

A comparative analysis of fundamental diode and photovoltaic parameters extracted from J-V measurements for the proposed NiO/ZTO p-n heterojunction device is presented in Table 2.

Table 2

Summary of diode and solar cell parameters of heterojunction device Al/p-NiO/n-ZTO/ITO, acquired from current-voltage measurements.

Thin-film p-n Heterojunction	Band alignment	Diode Parameters					Solar Cell Parameters				
Al/NiO/ZTO/ITO	Staggered gap (Type-II)	$I_{\text{for}}/I_{\text{rev}}$	$V_{\text{turn on}}$	n	R_s	ΔE_v	ΔE_c	V_{oc}	J_{sc}	FF	PCE
		at $\pm 2\text{V}$	(V)		(Ω)	(eV)	(eV)	(V)	(mAcm^{-2})	(%)	(%)
		2.6	1.44	2.58	2.8	2.96	2.7	0.54	15.4	31	2.95

It is believed that the device performance can be further tuned by regulating band discontinuities achieve favorable band alignment, particularly for a type-II heterojunction [44]. To assess reproducibility, multiple devices were fabricated following the same recipe, exhibiting consistent rectifying and photovoltaic characteristics. Additionally, aging-tests conducted over approximately four months revealed no substantial degradation in device performance, highlighting good short-term stability under ambient conditions. The improved performance of p-NiO/n-ZTO/ITO heterojunction solar cell demonstrates the potential of ZTO-based all-oxide thin-film heterostructures for next-generation photovoltaic applications.

4 Conclusion

A highly transparent NiO/Zn₂SnO₄ p-n heterojunction was fabricated using a simple combinatorial approach involving thermal evaporation followed by optimized heat treatment. The structural, morphological, and optical properties of each thin film were systematically analyzed to evaluate their suitability for heterojunction device applications. The prepared n-NiO and n-ZTO oxide-heteropartner thin films exhibited optical band gap of ~ 3.61 eV and ~ 3.80 eV, respectively. The proposed thin-film p-n heterojunction Al/NiO/ZTO/ITO displayed a pronounced rectifying behavior with a turn-on voltage of ~ 1.44 V, parasitic resistance of ~ 2.8 Ω , and ideality factor of ~ 2.58. C-V measurements revealed a built-in-potential of ~ 0.54 V across the hetero-interface. The photovoltaic parameters were extracted from the same device under 1-sun illumination, yielding a V_{oc} of ~ 0.62 V, J_{sc} of ~ 15.4 mAcm^{-2} , and FF of ~ 31%, resulting in a power conversion efficiency (η) of ~ 2.95%. The E-k diagram of NiO/ZTO heterojunction suggests a type-II band alignment that is highly desirable for suppressing interfacial recombination and promoting efficient charge transport, thereby enhancing the photovoltaic performance.

Declarations

Declaration of Competing Interest

I, Dr. Kashif Javaid, the corresponding author, hereby declare on behalf of all co-authors that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Ethical approval

This manuscript has no human and animal studies.

Author Contribution

Rimsha Anjum: Investigation, data acquisition and analysis, methodology, and original manuscript preparation. Kashif Javaid: Conceptualization, supervision, interpretation of results, critical revision of the manuscript, and project administration. Both authors approved the final version of the manuscript and agreed to be accountable for all aspects of the work, including the accuracy and integrity of the research.

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Data availability

No datasets were generated or analysed during the current study.

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Figures



Figure 1

Schematic depiction of the experimental procedure employed for the fabrication of thin-film heterojunction device.

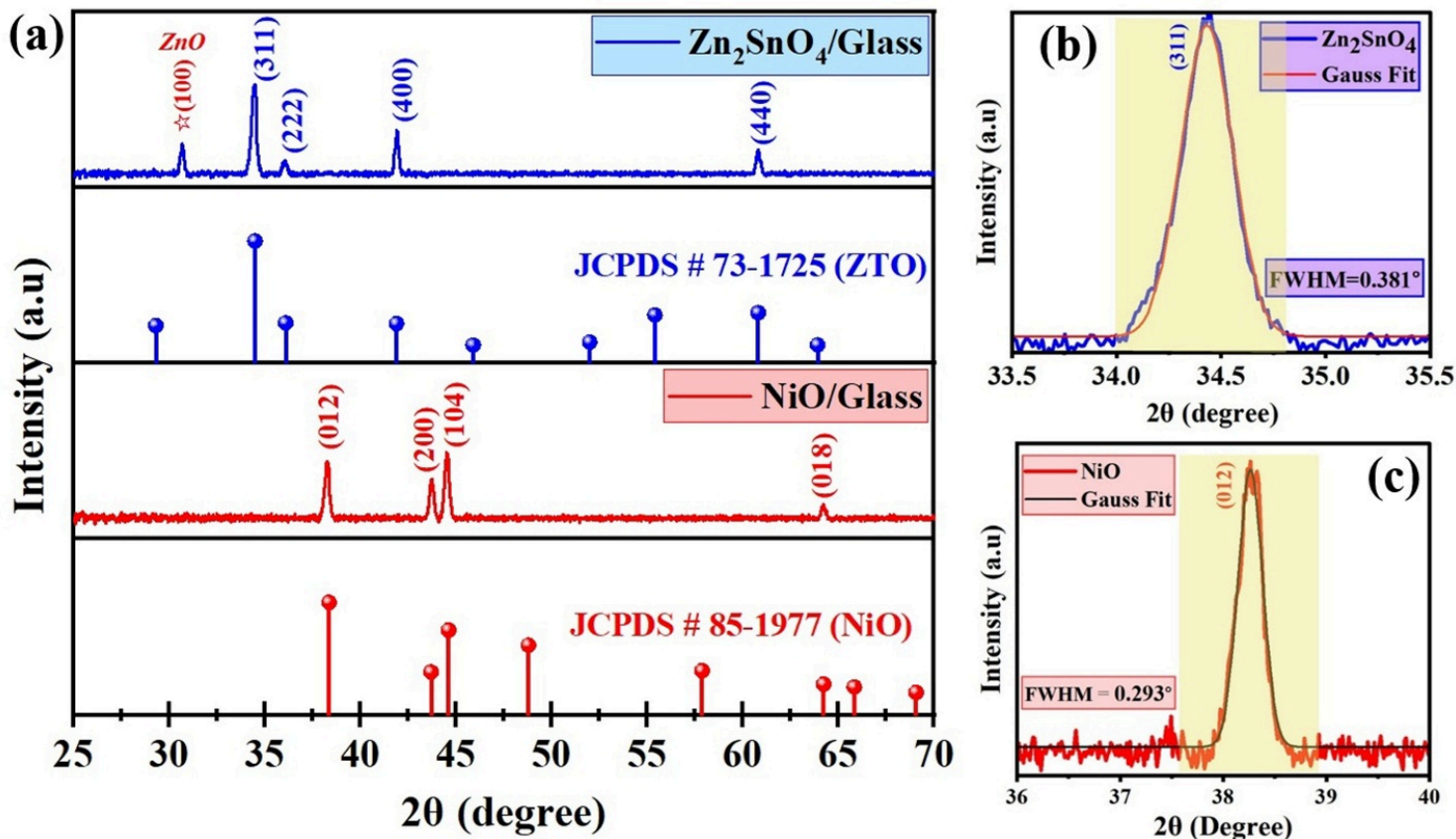


Figure 2

(a)- X-ray diffraction (XRD) patterns of thermally oxidized ZTO and NiO thin films annealed at 500 °C, (b, c)- Magnified view of major characteristic diffraction peak for detecting the approximate value of FWHM of ZTO and NiO thin films, respectively.

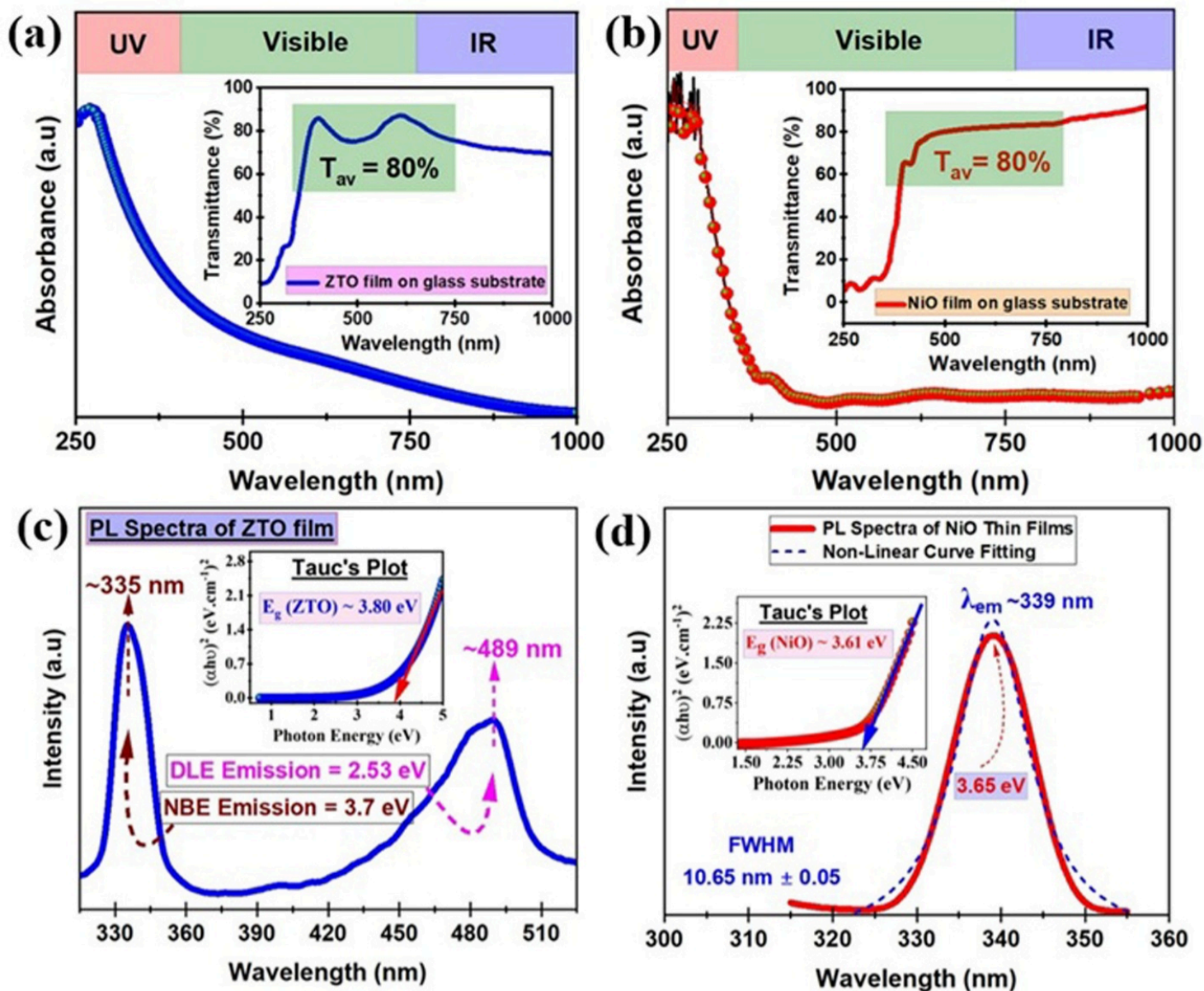


Figure 3

Optical properties of thermally oxidized ZTO and NiO thin films: (a,b)- UV-Vis-NIR absorbance spectrum of the ZTO and NiO thin films with the corresponding optical transmittance spectra, highlighted in the insets, respectively (c,d)- Photoluminescence (PL) spectra of the ZTO and NiO thin films coupled with respective Tauc's plot for the estimation of band gap shown in the insets, accordingly.

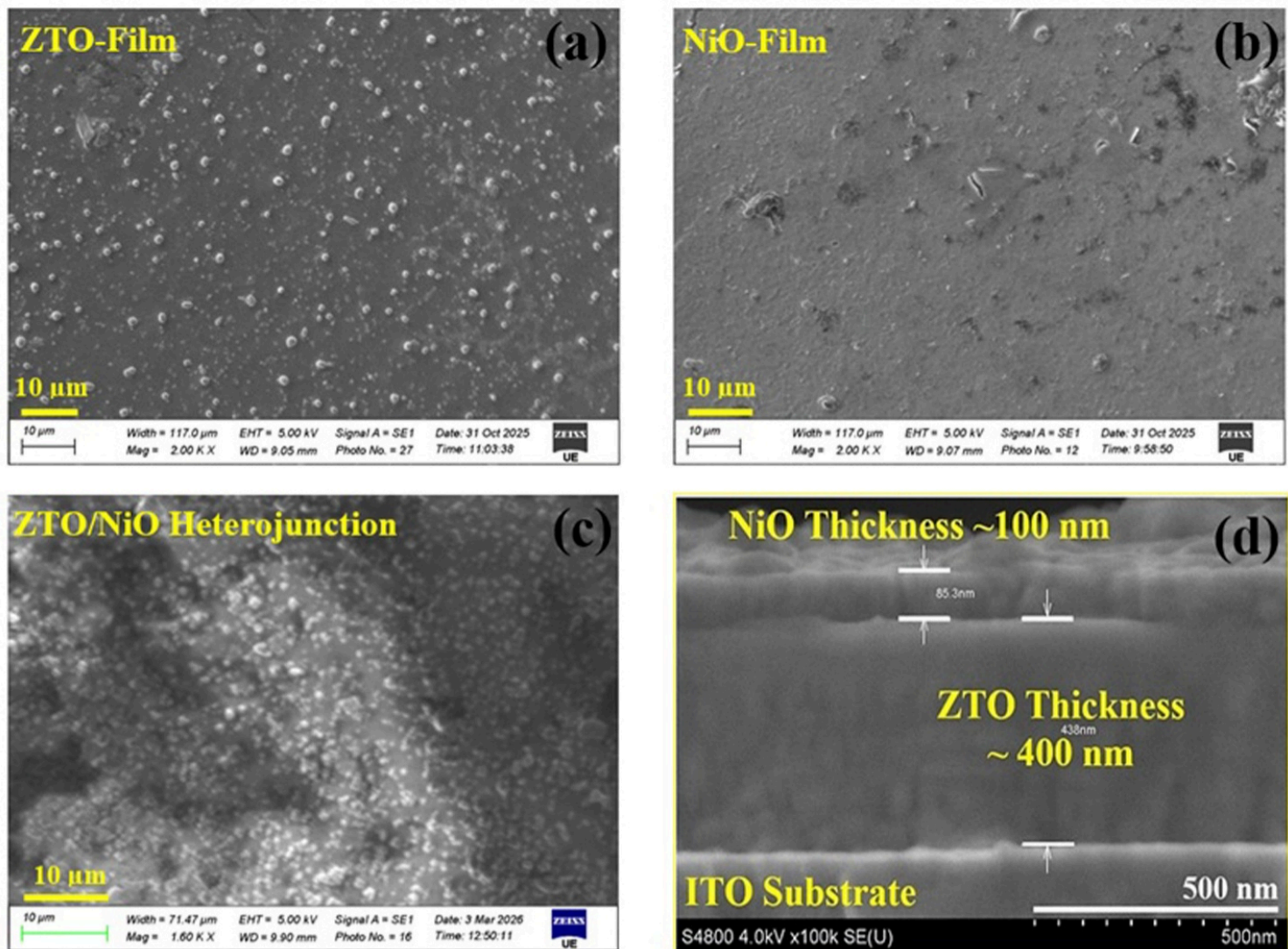


Figure 4

(a,b)- SEM micrographs of the constituent ZTO and NiO layers of the heterojunction, **(c)**- Surface morphology of NiO/ZTO heterojunction on glass slides,, **(d)**- Cross-sectional SEM analysis of NiO/ZTO heterojunction for thickness estimation.

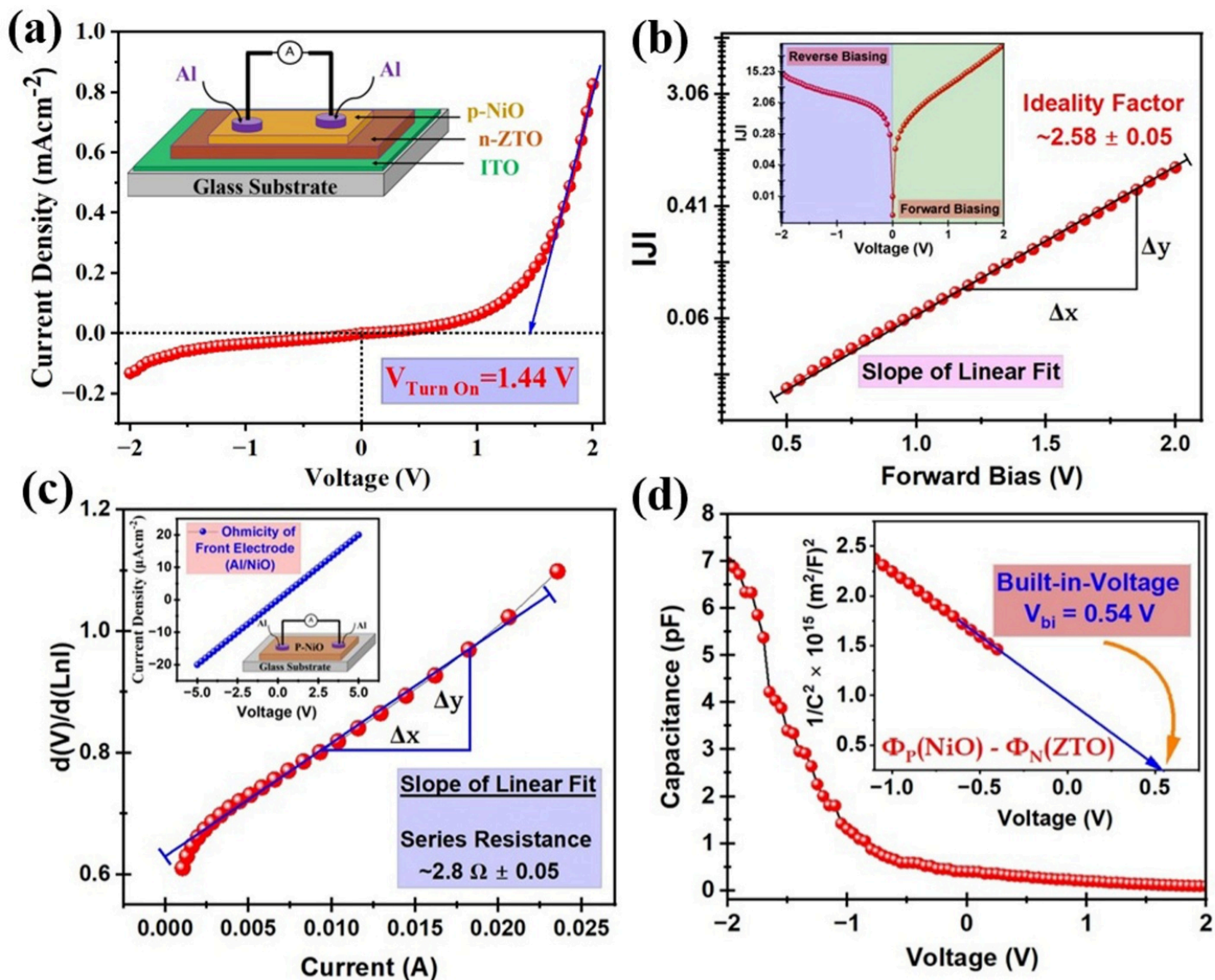


Figure 5

Electrical properties of the fabricated Al/p-NiO/n-ZTO/ITO heterojunction diode: **(a)**- Current-voltage measurements of thin-film heterojunction demonstrating its rectifying behavior, while the inset shows the schematic structure of fabricated device, **(b)**- Estimation of ideality factor, **(c)**- Assessment of series resistance using the Cheung-Cheung method, whereas inset shows the Ohmic electrode with contact geometry, and **(d)**-Determination of the built in potential from Mott-Schottky plot.

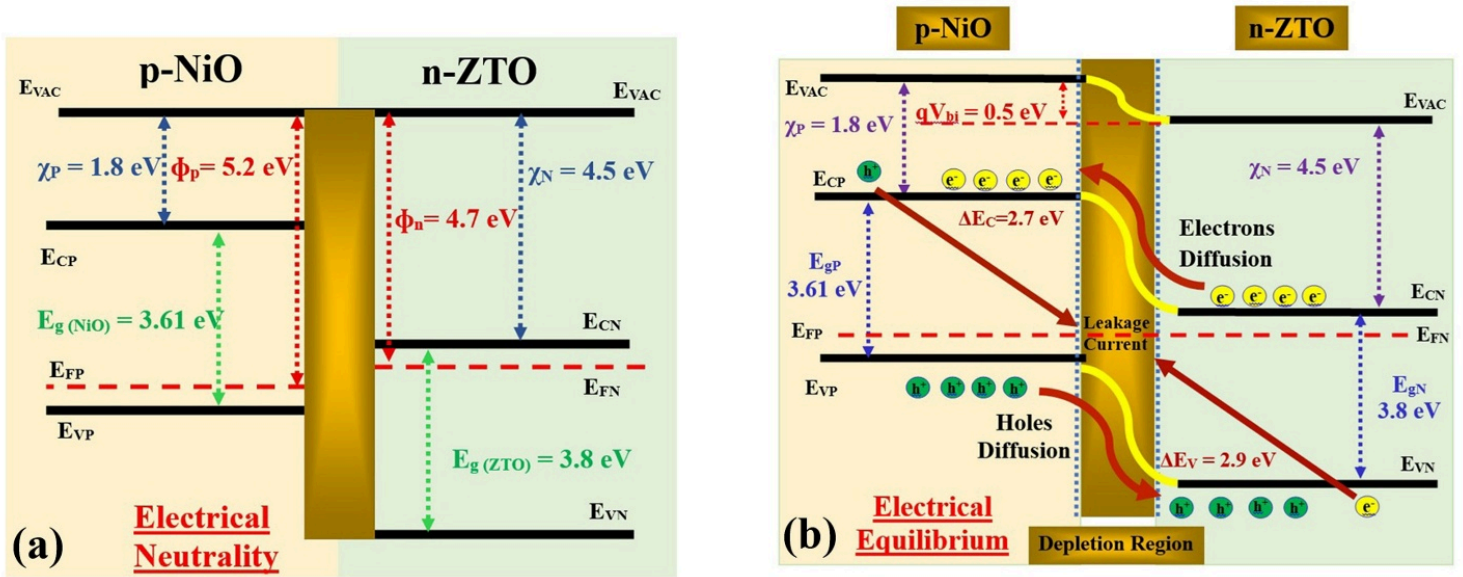


Figure 6

Band alignment of NiO/ZTO p-n heterojunction, (a)-Electrical neutrality, (b)- Electrodynamic equilibrium when the Fermi-levels are aligned.

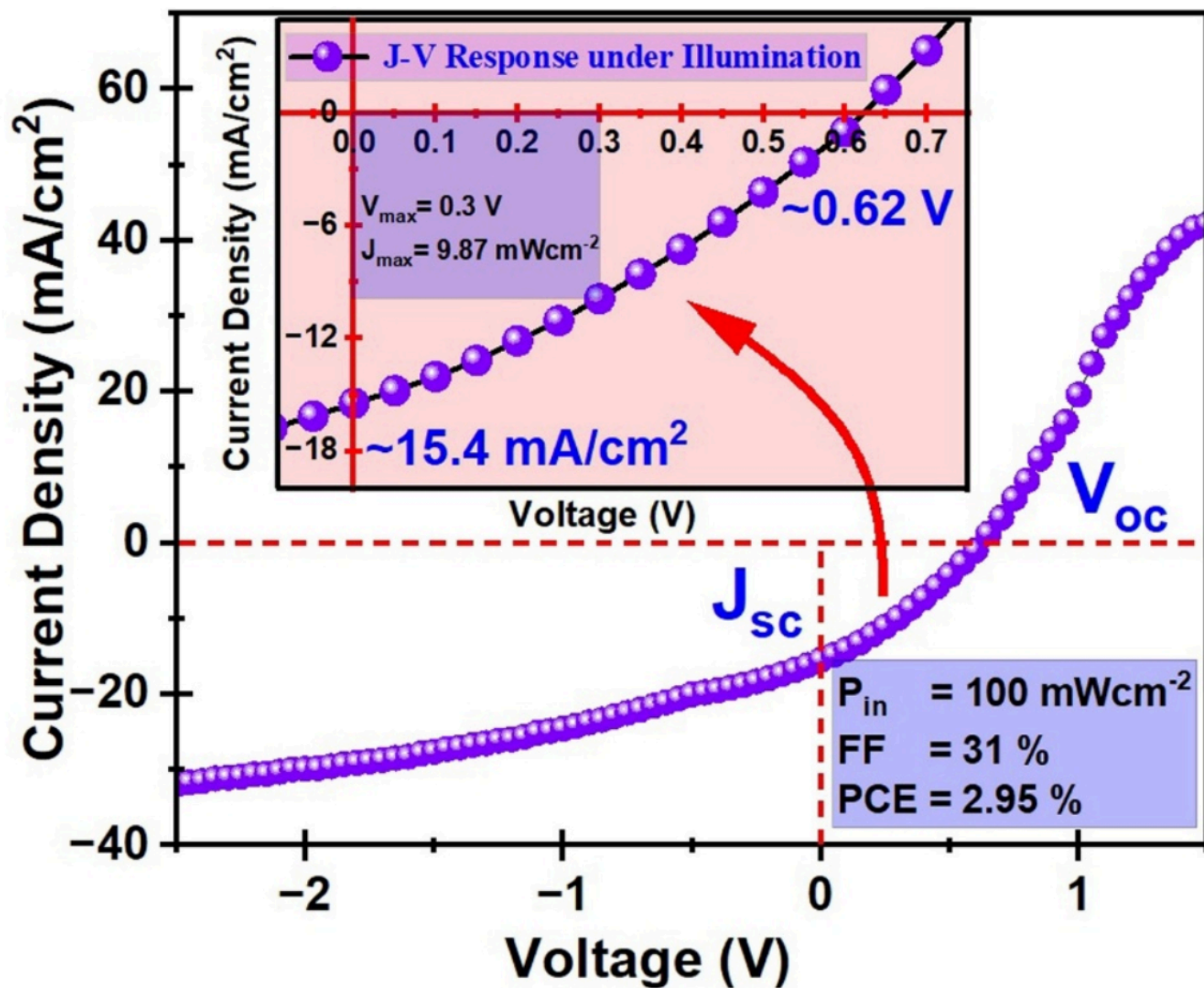


Figure 7

Photovoltaic J-V characteristics of NiO/ZTO thin-film heterojunction solar cell under AM 1.5G illumination.