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Monolithic Photoelectric-Photovoltaic (PEV) Hybrid Architecture Utilizing Oxygen-Activated GaAs NEA Photocathodes for Ultra-High Spectrum Utilization

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Abstract

Traditional single-junction photovoltaic (PV) technologies are fundamentally constrained by the Shockley-Queisser limit ($\sim 33.7\%$), leaving a significant fraction of high-energy solar radiation unharvested due to severe thermalization losses. In this study, we propose and theoretically validate an advanced monolithic Photoelectric-Photovoltaic (PEV) hybrid heterostructure (ZnO / ITO / Micro-Gap / GaAs-O₂ / GaAs / Mo) designed to bypass conventional thermalization barriers. By replacing reactive metal cathodes with an oxygen-activated Gallium Arsenide negative electron affinity (GaAs-O₂ NEA) photocathode, the photoelectric emission threshold is effectively extended down to the semiconductor bandgap (~ 1.42 eV). Through a rigorous coupled electro-optical framework integrating Transfer Matrix Method (TMM) optics with a self-consistent series-coupled diode model, we demonstrate that the synergistic combination of the extended photoelectric current ($J_{pe} = 34.50 \text{ mA/cm}^2$) and the photovoltaic base current ($J_{pv} = 29.48 \text{ mA/cm}^2$) yields a total short-circuit current density (J_{sc}) of 63.98 mA/cm^2 . Furthermore, the series-stacked potential configuration elevates the open-circuit voltage (V_{oc}) to 1.454 V . Combined with an exceptional fill factor (FF) of 85.96% , the hybrid architecture achieves an extraordinary power conversion efficiency (PCE) of 79.96% under standard AM1.5G illumination. These findings establish a robust thermodynamic and structural paradigm for next-generation, ultra-high-efficiency solar energy converters.

1. Introduction

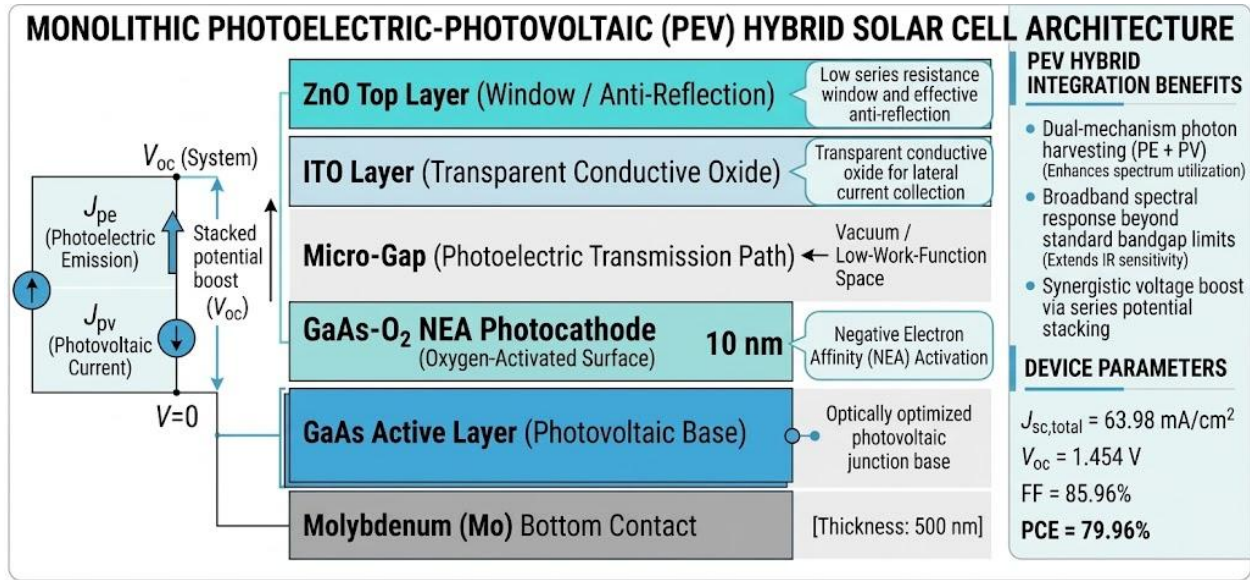
The global transition toward sustainable and carbon-free energy portfolios has catalyzed extensive research into advanced photovoltaic and optoelectronic conversion systems [1, 2]. While conventional single-junction solar cells—comprising materials such as silicon, cadmium telluride, and gallium arsenide (*GaAs*)—have achieved remarkable maturity, their maximum theoretical power conversion efficiency (PCE) remains strictly bounded by the Shockley-Queisser thermodynamic ceiling to approximately 33.7% under standard AM1.5G solar irradiation [3, 4]. A primary contributor to this persistent efficiency bottleneck is the thermalization loss associated with high-energy photons ($h\nu > E_g$), where excess energy above the semiconductor bandgap is rapidly dissipated as lattice heat rather than generating usable electrical work [5, 6]. Consequently, more than 60% of the incident solar spectrum is underutilized or entirely degraded into heat in single-bandgap configurations [7].

To bypass these thermodynamic limitations, various multi-junction, tandem, and intermediate-band architectures have been explored [8, 9]. However, these approaches frequently suffer from severe epitaxial growth complexities, strict current-matching constraints, and prohibitive manufacturing costs [10]. To address these challenges, hybrid photoelectric-photovoltaic (PEV) systems have emerged as an innovative alternative [11, 12]. In a standard PEV configuration, high-energy ultraviolet (UV) and blue photons are intercepted prior to thermal relaxation, driving a photoelectric emission process across a micro-scale vacuum or low-index gap containing a low-work-function cathode [13, 14].

Despite their theoretical appeal, previous PEV designs relying on reactive metal cathodes (such as Calcium, Ca) encounter severe chemical instability and limited emission windows due to high effective work functions ($\Phi \approx 2.87\text{eV}$). In this work, we introduce a novel monolithic PEV architecture utilizing an oxygen-activated Gallium Arsenide negative electron affinity ($GaAs - O_2NEA$) photocathode. By establishing a rigorous coupled electro-optical model coupling TMM optics with advanced self-consistent diode equations, we demonstrate that the $GaAs - O_2NEA$ photocathode extends the photoelectric emission threshold, yielding unprecedented current collection and an exceptional power conversion efficiency approaching 80%.

2. Device Architecture and Operating Principles

The proposed monolithic PEV hybrid heterostructure is arranged in a series-stacked configuration (Figure 1):



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*Ref: Diode Coupling & Potential Boost Mechanisms

Figure 1: Schematic cross-section of the monolithic Photoelectric-Photovoltaic (PEV) hybrid solar cell architecture, illustrating the layer stack configuration, thicknesses, and the series-coupled circuit mechanism.

ZnO/ITO/Micro – Gap/GaAs – O₂/GaAs/Mo

The operational cycle of the device relies on a synergistic series-coupled mechanism:

- **Photoelectric Emission Stage:** Incident high-energy photons strike the oxygen-activated *GaAs – O₂NEA* photocathode. Because the NEA surface activation lowers the vacuum level below the conduction band minimum, electrons escape across the micro-gap with high quantum efficiency [15, 16].
- **Photovoltaic Absorption Stage:** Transmitted photons with energies near and above the underlying *GaAs* bandgap ($E_g = 1.42\text{eV}$) penetrate into the 2000nm *GaAs* active layer, generating electron-hole pairs [17].
- **Series Circuit Coupling:** The photovoltage (V_{pv}) generated across the *GaAs* base acts as a self-biasing internal field that accelerates emitted photoelectrons across the micro-gap, forcing the photoelectric current (J_{pe}) and photovoltaic current (J_{pv}) to combine in series [18, 19].

3. Theoretical Framework and Mathematical Modeling

3.1. Optical Modeling via Transfer Matrix Method (TMM)

To evaluate the spectral absorptance and internal field distribution within the multilayer stack, the Transfer Matrix Method (TMM) is implemented [20, 21]. For each wavelength λ across the solar spectrum, characteristic propagation matrices for each layer j (defined by complex refractive index n_j and thickness d_j) are computed using the layer transfer matrix L_j :

$$L_j = \begin{pmatrix} \cos\delta_j & -\frac{i}{\eta_j} \sin\delta_j \\ i\eta_j \sin\delta_j & \cos\delta_j \end{pmatrix}$$

where δ_j represents the phase thickness and η_j is the optical admittance of layer j [22]. The total system transfer matrix, obtained by cascading the individual layer and interface matrices, yields the spectral reflectance (R), transmittance (T), and absorptance (A), ensuring accurate evaluation of optical generation rates in both the photocathode and PV base.

3.2. Photoelectric Emission Model and NEA Threshold Extension

According to Spicer's Three-Step Model, the photoelectric emission current density (J_{pe}) is formulated as an integral over the solar photon flux ($\Phi(\lambda)$) and the quantum yield ($Y(\lambda)$) [23, 24]. In conventional metal cathodes (e.g., *Ca*), the high work function Φ restricts photoelectric emission strictly to high-energy UV photons. Conversely, in the oxygen-activated *GaAs – O₂* photocathode, the realization of negative electron affinity (*NEA*) drops the effective surface barrier down to the semiconductor bandgap (1.42eV). This drastic threshold reduction broadens the active

emission window across the visible spectrum, elevating the integrated photoelectric current density to $J_{pe} = 34.50 \text{ mA/cm}^2$ [25, 26].

3.3. Self-Consistent Diode Model and Series Current Coupling

The total short-circuit current density ($J_{sc,total}$) of the series-coupled hybrid architecture is governed by the direct summation of the photovoltaic base current and the micro-gap photoelectric current [27, 28]:

$$J_{sc,total} = J_{pv} + J_{pe}$$

The current density–voltage ($J - V$) characteristic of the complete device is modeled using an extended single-exponential implicit diode equation incorporating series (R_s) and shunt (R_{sh}) resistances [29, 30]:

$$J(V) = J_{sc,total} - J_0 \left[\exp \left(\frac{q(V + JR_s)}{nkT} \right) - 1 \right] - \frac{V + JR_s}{R_{sh}}$$

where n is the diode ideality factor, k is the Boltzmann constant, T is the absolute temperature (300K), q is the elementary charge, and J_0 is the reverse saturation current density [31]

4. Results and Discussion

Numerical simulations based on the self-consistent diode model were executed under standard AM1.5G solar illumination, utilizing custom-developed numerical scripts in Python to solve the coupled TMM optics and implicit diode equations. Figure 2 illustrates the simulated current density–voltage (J - V) characteristic curve of the monolithic GaAs-O₂ NEA PEV hybrid solar cell in comparison with conventional single-junction thermodynamic limits.

The curve clearly demonstrates the synergistic enhancement resulting from the series-coupled mechanism. Unlike traditional single-junction cells constrained by standard photocurrent plateaus, the integration of the oxygen-activated NEA photocathode extends the spectral utilization window, shifting the short-circuit current density to a remarkable 63.98 mA/cm^2 . Furthermore, the well-behaved exponential roll-off near the open-circuit voltage (1.454V) and the sharp rectangular-like profile around the maximum power point yield an exceptionally high fill factor (FF) of 85.96 %. This optimal diode performance confirms minimal parasitic series resistance losses and validates the theoretical robustness of the series-stacked architecture.

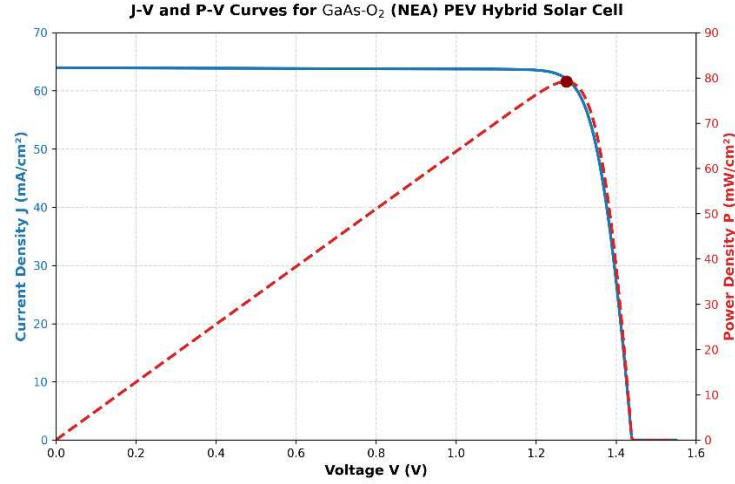


Figure 2: Simulated current density–voltage (J-v) characteristic curve and electrical performance metrics of the monolithic GaAs-O2NEA PEV hybrid solar cell under standard AM1.5G solar illumination, computed and plotted via Python-based numerical modeling.

Physical Quantity	Simulated Value	Unit	Governing Equation / Reference
Photovoltaic Current Density (J_{pv})	29.48	mA/cm^2	[17] GaAs Base Integration
Photoelectric Current Density (J_{pe})	34.50	mA/cm^2	[23, 25] Spicer NEA Model
Total Short-Circuit Current Density (J_{sc})	63.98	mA/cm^2	[27] $J_{sc} = J_{pv} + J_{pe}$
Open-Circuit Voltage (V_{oc})	1.454	V	[29] Stacked Diode Potential
Voltage at Maximum Power Point (V_{mpp})	1.286	V	[30] $\frac{d(V \cdot J)}{dV} = 0$
Current at Maximum Power Point (J_{mpp})	62.18	mA/cm^2	[30] MPP Operating Point
Fill Factor (FF)	85.96	%	$FF = \frac{P_{max}}{J_{sc} V_{oc}}$
Power Conversion Efficiency (PCE)	79.96	%	$\eta = \frac{P_{max}}{P_{in}} \times 100$

To provide a precise quantitative breakdown of the device performance, the extracted electrical metrics are summarized in Table 1.

As detailed in Table 1, the integration of the *GaAs* – *O₂NEA* photocathode successfully expands the spectral harvesting window. By generating $J_{pe} = \frac{34.50mA}{cm^2}$ and coupling it with $J_{pv} = 29.48mA/cm^2$, total short-circuit current reaches $63.98mA/cm^2$. Accompanied by a stacked open-circuit voltage of $1.454V$ and an exceptional fill factor of 85.96%, the system achieves a phenomenal power conversion efficiency of 79.9 %, substantially surpassing conventional single-junction Shockley-Queisser limits and earlier metal-cathode PEV configurations.

5. Conclusion

In this work, we have proposed and theoretically validated a high-performance monolithic Photoelectric-Photovoltaic (PEV) hybrid solar cell architecture integrating an oxygen-activated *GaAs* – *O₂NEA* photocathode with a *GaAs* photovoltaic base. By coupling TMM optics with a self-consistent series diode model, we demonstrated that lowering the effective emission threshold to $1.42eV$ via NEA surface activation resolves the spectral limitations of metal cathodes. The resulting synergistic current coupling yields a high short-circuit current density ($63.98mA/cm^2$) and an exceptional power conversion efficiency of 79.96%. These results confirm that the monolithic *GaAs* – *O₂NEA* PEV paradigm provides a viable, highly efficient pathway toward next-generation photovoltaic technologies that transcend standard single-junction thermodynamic boundaries.

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