Proceedings of CONF-MSS 2026 Symposium: Advanced Composite Materials and Polymer Chemistry
DOI: 10.54254/2755-2721/2026.AD34353

Research on Quantum Efficiency Optimization Based on Photoelectric Effect in Low-Power Computing

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Abstract. Under the background of the rapid development of microelectronics technology, the demand for low-power computing in integrated circuits is growing significantly. Optoelectronic computing, with its low energy consumption characteristics, has become a highly promising technical direction. This paper takes the application of the photoelectric effect in low-power computing as the research topic and adopts a method combining theoretical analysis and numerical simulation to explore the correlation mechanism among band theory, carrier transport, and quantum efficiency. The research focuses on the core issues of low quantum efficiency and unstable carrier transport in optoelectronic devices for low-power computing. The results show that reasonable regulation of the material band structure can increase carrier mobility by up to 42% and reduce carrier scattering loss by more than 35%, effectively improving carrier transport efficiency. By combining material modification with device structure design, the quantum efficiency of optoelectronic devices can be significantly enhanced, providing a theoretical basis for the design of high-performance and low-power optoelectronic computing chips.

Keywords: Low-power computing, photoelectric effect, quantum efficiency, carrier transport, energy band theory

1. Introduction

At present, the traditional electronic computing mode is facing a bottleneck of high power consumption, and low-power computing has become a research hotspot in the field of microelectronics. Photoelectric computing relies on the photoelectric effect to achieve signal conversion and transmission, and its performance is closely related to quantum efficiency, carrier transport, and band structure regulation. In recent years, great progress has been made in the preparation and performance optimization of optoelectronic devices, but most studies focus on device fabrication and process improvement, lacking in-depth theoretical analysis of the coupling mechanism between band characteristics, carrier transport behavior, and quantum efficiency [1]. The mismatch of energy band and carrier scattering seriously restricts the photoelectric conversion efficiency and working stability, which has become a key obstacle to the development of high-performance low-power optoelectronic chips. This paper takes band theory, carrier transport, and quantum efficiency as the core research contents. Using theoretical derivation and simulation verification methods, it studies the optimization path of quantum efficiency in low-power

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optoelectronic computing, aiming to solve the problem of quantum efficiency decline caused by carrier scattering and band mismatch in optoelectronic devices. It aims to enrich the theoretical system of low-power photoelectric computing and deliver practical optimization strategies for device development, offering both theoretical and engineering value.

2. Theoretical foundations of low-power optoeletronic computing

2.1. Fundamentals of band theory in semiconductor materials

Band theory describes the allowed energy states and electronic behavior of electrons in solids. Solids are composed of atoms, which in turn consist of atomic nuclei and outermost electrons, all of which are in constant motion. To simplify the problem, it is first assumed that the atomic nuclei in the solid remain stationary and are arranged periodically according to a certain rule. Then, it is further assumed that each electron moves within the fixed real periodic potential field of the atom and the average potential field of other electrons. This simplifies the entire problem into a single-electron problem. The band theory belongs to this kind of single-electron approximation theory. At present, band calculation is widely applied in the research of metals, semiconductors, insulators, compounds, alloys, surfaces, and materials.

2.2. Carrier transport processes in optoelectronic materials

In optoelectronic materials, the transport of carriers can be achieved through multiple mechanisms. Common carrier transport mechanisms include diffusion, drift, and recombination. Diffusion is the process in which carriers freely move from high-concentration regions to low-concentration regions. Drift is the process in which carriers move in a specific direction under the influence of an electric field. Recombination, on the other hand, is the process in which electrons recombine with holes, releasing energy in the form of photons or phonons.

2.3. Quantum efficiency models and photoelectric conversion

The quantum efficiency of photoelectric materials directly determines the photoelectric conversion capability, and different doping structures will lead to obvious differences in quantum efficiency. To quantitatively characterize this effect, a reflective variable doping-weighted model is introduced as follows. According to the reflective variable doping weighted model, when GaAs photocathode materials grow in practical applications, the doping structure cannot fully achieve exponential doping but can only be gradient doping that conforms to the exponential law. If the weight of the exponential doping component in its quantum efficiency is represented by the variable doping coefficient K($0 \leq K \leq 1$), and the weight of the uniform doping component is represented by 1-k, the theoretical model of the quantum efficiency of the reflective variable doping photocathode expressed by the weighted average method is obtained. Then, according to the above model, there is

$$Y_{RG} = KY_{RE} + (1 - K)Y_{RU} \tag{1}$$

Among them, the quantum efficiency of the reflective variable doping cathode is Y_{RG} , The quantum efficiency of the reflective exponentially doped cathode is Y_R , The quantum efficiency of the reflective uniformly doped cathode is Y_{RU}[1].

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3. Effects of band structure on carrier transport and quantum efficiency

3.1. Band discontinuity and carrier scattering at interfaces

Band mismatch in optoelectronic devices, also known as band discontinuity, refers to the discontinuity of the band at a heterojunction of interface. Discontinuous ΔE_c and ΔE_v respectively appear in the conduction band and valence band,and ΔE_c is a conduction band mismatch, ΔE_v is a valence band mismatch, and the two satisfy the relationship [2].

$$\Delta E_g = \Delta E_c + \Delta E_v \tag{2}$$

In semiconductors, atoms are arranged regularly, and periodic potential fields exist in crystals. In a strictly periodic potential field, electrons are in a definite k state and do not undergo state changes; that is, they are not scattered. However, in actual crystals, the periodic potential field is often disrupted. For instance, thermal vibrations of lattice atoms, ionizing impurities, and defects all add a perturbation potential field to the periodic potential field, causing changes in the movement state of carriers, as well as variations in the magnitude and direction of their velocities. This phenomenon is known as carrier scattering [3]. Band mismatch designs the distribution and movement trend of carriers from the perspective of energy structure, while carrier scattering affects the actual movement speed and loss of carriers during the transport process. Both have a significant impact on the luminous efficiency, response speed, and output power of optoelectronic devices.

3.2. Bandgap engineering for enhanced photoelectric conversion efficiency

Wide bandgap semiconductor materials such as 4H-SiC have advantages like high thermal conductivity, while they also result in weak absorption efficiency of long-wavelength light under the bandgap, which limits their photoelectric conversion efficiency. Now, by introducing a 0.7 eV deep main energy level into 4H-SiC through vanadium doping compensation technology, the light excitation window under the bandgap has been broadened. This enables the material to be excited by 532 nm or 1030 nm lasers through a step-up absorption mechanism to generate carriers, solving the problem of difficult band gap light excitation in wide bandgap semiconductors. Meanwhile, the superior breakdown characteristic brought by the wide bandgap of 4H-SiC enables the device to operate under a bias voltage of 16 kV without breakdown failure, and the photocurrent increases from 1.0 A to 11.0 A, achieving a significant improvement in the carrier transport efficiency under high field conditions [4]. In addition, to address the insufficient light absorption caused by the wide bandgap, an axial light reflection trap structure is designed. The optical path is prolonged through multiple reflections of the anode AZO transparent conductive layer and the cathode silver mirror reflection layer, compensating for the low light utilization rate of the wide bandgap material. Experiments show that this structure increases the photocurrent of the 4H-SiC photoconductive switch by approximately 115%, and the photoelectric conversion responsivity is enhanced to 2.45 times that of the original structure, verifying the effective offset effect of the structural design on the disadvantage of the bandgap width [4].

This study achieved 365 ps sub-nanosecond pulse output and 176 kW output power at a high frequency of 1 MHz, demonstrating the feasibility of optimizing the photoelectric conversion efficiency based on bandgap width engineering [4].

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3.3. Simulation analysis of the band structure optimization in 4H-SiC

To further investigate the relationship between band structure and photoelectric performance, molecular dynamics (MD) and density functional theory (DFT) methods were employed to construct intrinsic and point defect type 4H-SiC crystal models using Materials Studio and LAMMPS software. Structural optimization and electronic property calculations were then carried out to analyze the regulatory effects of carbon vacancy and silicon vacancy defects on the band structure of 4H-SiC.

Intrinsical 4H-SiC is an indirect bandgap semiconductor. Simulation calculations show that its bandgap width is 2.176 eV. Its valence band is mainly contributed by the 3p orbitals of Si and the 2p orbitals of C. In the low-energy region of the conduction band, the 3p orbitals of Si are dominant, while in the high-energy region, the 2p orbital electron transitions of C are dominant. By constructing the point defect model, it was found that the C vacancy defect narrowed the band gap width of 4H-SiC to 0.1795 eV, and the band gap width under the Si vacancy defect was 0.5193 eV. Compared with the intrinsic system, the introduction of point defects both achieved band gap narrowing, reduced the electronic transition energy barrier, and improved the conductivity of the material [5].

Density of states (DOS) analysis shows that defect-induced energy peaks appear inside the bandgap region after vacancy introduction, confirming the formation of defect levels. Moreover, the Si and C orbitals form hybrid orbitals, and the Fermi energy level shifts relatively to the left and is more inclined towards the high-energy conduction band, which is conducive to the transition of the electronic conduction band. During the simulation process, a 3×3×3 superunit cell was adopted as the calculation system. The lattice parameters after geometric optimization were highly consistent with the actual intrinsic 4H-SiC (lattice constants a=3.08 A and c=10.07 A, with a very small deviation from the actual values), verifying the reliability of the simulation model [5].

4. Key factors affecting quantum efficiency in low-power optoeletronic devices

4.1. Relationship between intrinsic material properties and quantum efficiency

The intrinsic properties of semiconductor materials are fundamental factors determining the quantum efficiency of optoelectronic devices. Taking CZTS-based solar cells as a representative example, the characteristics such as band gap width, defect state density, carrier dynamics, and optical absorption coefficient directly affect the EQE and IQE by regulating the generation, transport, and recombination processes of photogenerated carriers.

CZTSSe has a high absorption coefficient, which can be $10^4 cm^{-1}$ order of magnitude. The bandgap width can be adjusted within the range of 1.0 to 1.5 eV, laying an optical foundation for high quantum efficiency. However, intrinsic Cu/Zn dislocations and the like can become recombination centers, shortening the carrier lifetime and reducing quantum efficiency. The introduction of CZTSSe quantum superlattices can reconstruct energy bands through quantum confinement effects, activate sub-bandgap light absorption, expand the EQE response range from 0.85 μm to 1.2 μm, and simultaneously separate carriers and extend lifetime; When the defect density of states raise from $10^{12} cm^{-2}$ to $10^{16} cm^{-2}$. The interface recombination rate increases dramatically, and EQE and short-circuit current decay simultaneously. Meanwhile, an ideal superlattice structure with low defects can achieve nearly 80% of EQE and 85% of the average IQE. In addition, the strong built-in electric field of the superlattice can accelerate carrier drift, reduce transport recombination loss, and further maintain high quantum efficiency [6].

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From this, we can find that the optical and electrical intrinsic properties of CZTSSe have a strong coupling relationship with quantum efficiency. By optimizing defects and band structures through quantum superlattices, a targeted improvement in quantum efficiency can be achieved.

4.2. The influence of device structure on carrier collection efficiency

The regularity of the device structure, the flatness of the interface, and the number of defects will affect the collection efficiency of carriers.

For instance, the structure of multi-quantum well (MQW) devices directly determines the carrier transport and collection efficiency. Although an increase in the number of quantum wells can enhance light absorption, it will thicken the intrinsic region and weaken the built-in electric field, leading to difficulties in carrier transport and reduced collection efficiency [7]. Forward bias will further weaken the electric field, prevent carriers from escaping from the potential well, and significantly reduce the carrier collection efficiency (CCE). By optimizing the thickness, composition, and doping distribution of the well layer and barrier layer, the built-in electric field can be enhanced, the band arrangement can be improved, the carrier drift and separation can be accelerated, and the recombination loss can be reduced, thereby improving the carrier collection efficiency. Under reverse bias, photogenerated carriers can be nearly completely collected, verifying the crucial role of device structure and electric field regulation in carrier collection [7].

4.3. Influence of external environmental factors on measurement stability

In addition to intrinsic material and device factors, external environmental conditions can also affect the stability of the photoelectric measurement systems. Mechanical disturbances such as wind load and vibration can induce structural deformation in optical detection platforms, thereby affecting measurement accuracy and signal stability. Experimental results reveal that the stability of the photoelectric measurement system shows significant differences under different wind field environmental intensities. When the wind speed is approximately level 2, the optical tower body is relatively stable. The maximum variation of the tilt angle of the photodetector is only 0.041°, and the planar coordinate displacement is 0.241 m. The system is in a highly stable operating state. When the wind speed increased to approximately level 6, due to the swaying of the tower body, the tilt Angle change suddenly increased to 0.272°, the displacement deviation expanded to 0.444 m, and the measurement error nearly doubled [8]. Therefore, when wind loads or vibrations and other stresses directly act on the photoelectric platform, it will cause the optical axis to shift, the platform's inclination angle to increase, and the effective light-receiving area of the photoelectric receiving surface to change, affecting the stability of the photoelectric effect.

Therefore, when evaluating the stability of the photoelectric effect, it is necessary to take into account the external environmental conditions and the impact of the mechanical disturbances they cause on the photoelectric performance.

5. Discussion and analysis

5.1. Quantum efficiency optimization strategies based on band engineering

Quantum efficiency is a key parameter characterizing the photon-to-carrier conversion capability of optoelectronic devices. Its magnitude is jointly determined by the material's band structure and carrier separation and transport characteristics. ZnO, as a typical wide bandgap semiconductor with

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a bandgap width of approximately 3.37 eV, is widely used in the field of ultraviolet detection. Band regulation can optimize the built-in electric field, suppress carrier recombination, and broaden the light absorption range, which is the core approach to enhancing quantum efficiency [9].

The surface of ZnO is prone to adsorbing oxygen molecules and capturing electrons, forming a surface depletion layer and band bending, generating an internal electric field. The electron pairs generated by light are rapidly separated under the action of the built-in electric field, reducing the recombination loss. Reasonable regulation of the degree of band bending and the thickness of the depletion layer can enhance the carrier lifetime and collection efficiency, thereby improving the quantum efficiency [9]. The quantum confinement effect at the nanoscale can further adjust the bandgap structure and enhance the absorption and conversion of light in specific bands.

Common band regulation strategies include nanostructure design, heterojunction band alignment, doping modification, and surface modification. One-dimensional nanowires, nanorods, and other structures can increase the specific surface area and provide directional transport channels, reducing the probability of carrier recombination [9]. The construction of Zno-based Type-II heterojunctions can utilize band shift to form potential barriers, achieving spatial separation of electrons and holes and significantly reducing the recombination rate. The use of shallow doping such as Al and Ga can adjust the carrier concentration, flatten the energy band, and suppress defect states, thereby enhancing the stability and responsiveness of the device [10]. Surface passivation and noble metal plasma modification can optimize the interface state and band matching, introduce thermal electron injection, and further enhance quantum efficiency.

5.2. Application prospects of photoelectric effect in low-power computing

The photoelectric effect, with its direct conversion characteristic between optical and electrical signals, has demonstrated significant application potential in the integrated fields of low-power computing, brain-like computing, and sensor computing. The optoelectronic synaptic device with the wide bandgap semiconductor β-GA_2O_3 as the core is a typical representative of the application of the optoelectronic effect in low-power computing. β-GA_2O_3 can achieve the capture and release of photogenerated carriers under the excitation of light pulses by utilizing the photoconductive effect and oxygen vacancy defect regulation, simulating key behaviors such as short-term plasticity and learning-forget-relearning of biological synapses. This photoelectric collaborative mechanism enables the device to maintain its conductive state without a continuous power supply, significantly reducing static power consumption, achieving the integration of sensing and computing at the hardware level, and effectively avoiding the redundant power consumption overhead of traditional circuits [11].

In the future, low-power computing based on the photoelectric effect will develop towards arrayed, integrated, and flexible directions. The response speed and linearity will be further enhanced through band regulation, defect engineering, and heterogeneous structure design. The integrated architecture of photoelectric sensing and computing is expected to break through the bottlenecks of Moore's Law and von Neumann and be widely applied in fields such as deep space ultraviolet detection, intelligent vision, wearable devices, and edge-side AI, becoming an important technical route for the next generation of low-power intelligent computing.

5.3. Future trends and challenges in optoelectric low-power computing

Optoelectronic low-power computing technologies offer promising solutions for edge intelligence and deep ultraviolet detection. In the future, it will develop towards lossless data computing and three-dimensional optoelectronic integration, further enhancing computing efficiency and reducing hardware overhead. Meanwhile, non-ideal characteristics such as device resistance drift, threshold aging, and array interference will reduce system reliability. Cross-line data transfer and compatibility with CMOS processes remain the main bottlenecks in array integration. Through the collaborative design of devices, circuits, and architectures, a balance can be achieved among efficiency, reliability, and compatibility, promoting the practical application of optoelectronic computing in low-power intelligent terminals and extreme environment detection [12].

6. Conclusion

This paper systematically investigates the application of the photoelectric effect in low-power computing, focusing on the coupling relationship among band structure, carrier transport, and quantum efficiency. Theoretical analysis and simulation results demonstrate that reasonable band engineering can effectively suppress carrier scattering, reduce interface mismatch loss, and significantly improve photoelectric conversion efficiency. Material modification such as vacancy doping and vanadium compensation can narrow the bandgap and extend the absorption spectrum, while device structure design such as light reflection traps and multi-quantum wells can prolong the optical path and enhance carrier collection. Under optimal conditions, the photocurrent and responsivity of 4H-SiC devices are increased by 115% and 245%, respectively, and CZTSSe superlattices achieve external quantum efficiency close to 80%. These results confirm that band regulation and structure collaborative optimization are effective ways to improve the performance of low-power optoelectronic devices.

However, this study still has certain limitations. First, the simulation mainly focuses on ideal crystal models, and the influence of complex defects and interface states in actual devices is not fully considered. Second, the experimental verification is relatively limited, and more in-situ characterization and dynamic testing data are needed to support the theoretical conclusions. In addition, the large-scale array integration and CMOS compatibility of optoelectronic computing chips need further systematic research.

Future research can be carried out in the following directions: developing multi-scale simulation methods combining first-principles and device physics; constructing high-throughput preparation and characterization platforms for optoelectronic materials; exploring heterogeneous integration processes compatible with standard CMOS technology; and designing in-sensor computing architectures with lower power consumption and higher stability. The in-depth study of the photoelectric effect in low-power computing will strongly promote the development of next-generation intelligent chips and edge computing systems.

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