Doping and Defect Control in AlGaN-Based Deep Ultraviolet LEDs: Strategies for Enhanced Performance

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Abstract. AlGaN-based deep ultraviolet (DUV) light-emitting diodes (LEDs) are widely regarded for their potential in critical applications such as sterilization, water purification, and photolithography, operating in the 200-280 nm wavelength range. However, their performance remains limited by high defect densities, inefficient p-type doping, and low light extraction efficiency, which collectively reduce the external quantum efficiency (EQE). This paper provides a comprehensive review of current doping strategies, with an emphasis on optimizing both n-type and p-type conductivity, particularly in high-aluminum-content AlGaN. Moreover, the impact of threading dislocations and point defects on material properties is analyzed, alongside recent advancements in epitaxial growth methods like metal-organic chemical vapor deposition (MOCVD) aimed at reducing defect densities. Although significant progress has been made in defect management and doping efficiency, challenges remain, particularly in enhancing p-type doping activation. The paper concludes by suggesting future directions, including co-doping strategies and stress compensation layers, to further improve DUV LED performance and enable more efficient, commercially viable devices.

Keywords: AlGaN, DUV LEDs, Doping, Defect Control.

1. Introduction

Deep ultraviolet light-emitting diodes (DUV LEDs), characterized by their emission in the 200-280 nm wavelength range, have garnered significant attention for their applications in high-precision lithography, water and air filtration, and sterilizing. AlGaN, a ternary alloy with a tunable bandgap, serves as the foundational material for DUV LEDs, enabling the emission of ultraviolet light at desired wavelengths. Despite the potential of AlGaN-based DUV LEDs, their widespread implementation is hindered by persistent material-level challenges, notably high defect densities, the inefficiency of p-type doping, and limited light extraction capabilities. These factors critically impair the external quantum efficiency (EQE) and overall performance of DUV LED devices [1].

Recent efforts to address these issues have focused on improving the development of AlGaN materials, especially by means of metal-organic chemical vapor deposition (MOCVD) methods. Defect densities, which are frequently brought on by lattice mismatches and thermal stress during the epitaxial growth process, have significantly decreased as a result of this. Improved carrier injection efficiency and a decrease in non-radiative recombination losses are other goals of the development of innovative doping techniques, which include improvements in n-type doping with silicon and advancements in p-type doping with magnesium. Nonetheless, achieving effective p-type doping in AlGaN layers with a high aluminum content is still a difficult task, mainly because of the high activation energies of Mg acceptors and the self-compensation effects that restrict hole injection.

This paper systematically examines the current state of doping techniques and defect control strategies in AlGaN-based DUV LEDs, highlighting the most promising approaches to overcoming the material limitations that impede performance[2]. Special attention is given to co-doping strategies, quantum well design, and the integration of stress management layers as methods to enhance both electrical and optical properties. By addressing these critical material and structural issues, this work provides a roadmap for future research aimed at achieving higher efficiency and reliability in DUV LED technology.

2. Theoretical basis analysis

2.1. Deep UV LED/ Definition/Structure/Principle of operation

Deep Ultraviolet LEDs (DUV LEDs) are semiconductor light sources that emit wavelengths in the 200-280 nm range, with applications including water and air disinfection, sterilization of medical instruments, and high-precision photolithography processes. The core of DUV LEDs lies in their AlGaN-based quantum well structures. By controlling the aluminum (Al) mole fraction x, the bandgap can be adjusted to emit ultraviolet light at specific wavelengths. The typical structure of a DUV LED includes an n-type AlGaN layer, a quantum well active region, a p-type AlGaN layer, and electrode contacts. Typical structure of a DUV LED shown in figure 1.

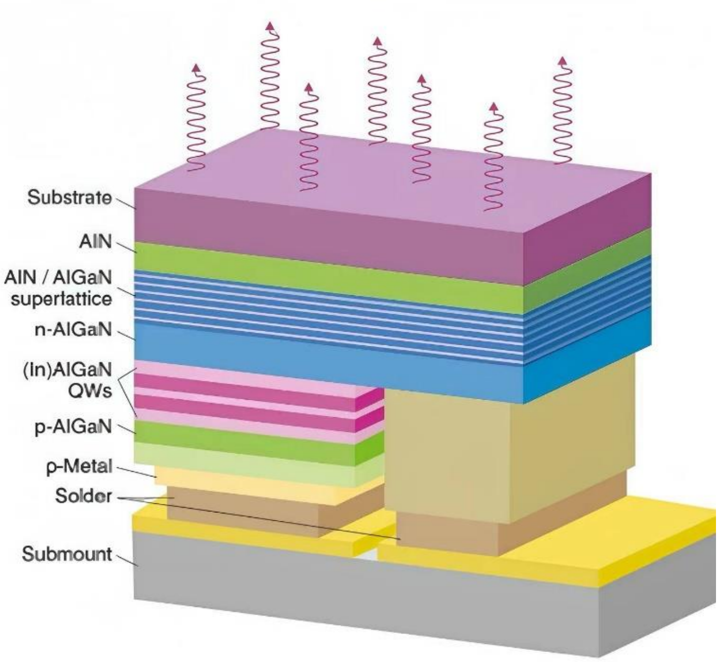

Figure 1. UV LEDs based on semiconductors nitride group III

The design of the quantum wells plays a crucial role in improving light extraction efficiency and reducing photon reabsorption. Current research indicates that optimizing the number and thickness of quantum wells can significantly enhance the light output power. For instance, Hirayama et al. demonstrated in their study that by introducing a multi-quantum well structure, DUV LEDs' external quantum efficiency (EQE) was raised to about 10% [1, 2].

However, DUV LEDs still face challenges in practical applications, such as low light extraction efficiency, poor heat dissipation, and device reliability issues. To address these challenges, researchers are working on developing novel packaging technologies and improving the doping efficiency of p-type AlGaN to enhance overall device performance [3].

2.2. Fundamental theory of AlGaN materials

2.2.1. Definition and properties of AlGaN materials

AlGaN, as a ternary alloy semiconductor, has a tunable bandgap width, with its chemical formula represented as $Al_xGa_{1-x}N$. By adjusting the value of x, the bandgap of AlGaN can be expanded from 3.4 eV for GaN to 6.2 eV for AlN, thereby covering the ultraviolet to deep ultraviolet range. The wide bandgap of this material provides unique advantages for deep ultraviolet LEDs, particularly in terms of stability under high-temperature and high-power conditions [2].

However, the fabrication process of AlGaN materials is often accompanied by a high defect density, primarily due to the increased likelihood of lattice mismatch introduced by the incorporation of aluminum. For example, the study by Li et al. pointed out that an increase in aluminum content leads to a rise in dislocation density, which negatively impacts the material's luminescence efficiency [4]. Therefore, reducing defect density is one of the key factors in enhancing the performance of DUV LEDs.

2.2.2. Doping strategies in AlGaN materials

Doping in AlGaN materials is a critical technique for achieving n-type and p-type conductivity. Typically, silicon (Si) is used for n-type doping, while magnesium (Mg) is employed for p-type doping. However, the wide bandgap of AlGaN poses significant challenges for p-type doping, especially at high aluminum content, where the efficiency of Mg doping is significantly reduced. To enhance p-type conductivity, researchers have introduced co-doping strategies, such as incorporating oxidizers or other acceptors alongside Mg to improve Mg activation efficiency [5].

Moreover, the doping process must balance the concentration of carriers with the defect density in the material. For instance, in a study by Kneissl et al., it was found that excessively high Si doping concentrations can induce a self-compensation effect, leading to a decrease in the material's conductivity [6]. Therefore, optimizing the doping concentration is crucial for improving the electrical performance of AlGaN materials.

2.2.3. Defects in AlGaN materials and their effects

Defects are critical factors that affect the optoelectronic performance of AlGaN materials. The primary defects in AlGaN materials include dislocations, vacancies, and impurity atoms. These defects can form non-radiative recombination centers, leading to a reduction in quantum efficiency. Research by Chen et al. has shown that there is a negative correlation between dislocation density and the external quantum efficiency (EQE) of the material; for every order of magnitude increase in dislocation density, the EQE decreases by approximately 10% [7].

Moreover, defects can also impact the electrical properties of the material, resulting in increased leakage current and decreased thermal stability of the device. To reduce defect density, researchers have employed various growth techniques, such as low-temperature buffer layers and surface passivation of epitaxial wafers, to improve the crystalline quality of the material and enhance device performance [8].

2.3. Shortcomings and challenges of existing research

2.3.1. Limitations of deep ultraviolet LED materials and processes

Current deep ultraviolet (DUV) LED technological advancements are encountering considerable hurdles related to both their constituent materials and fabrication methodologies [9]. Materials such as AlGaN with elevated aluminum concentrations are prone to substantial defect concentrations, which drastically curtail the external quantum efficiency (EQE) achievable in DUV LEDs [10]. Furthermore, the self-compensation phenomenon results in a negligible doping efficacy for p-type AlGaN, thereby complicating efforts to enhance the electrical characteristics of these devices.

Research indicates that in terms of process optimization, introducing low-temperature buffer layers and stress compensation layers can significantly reduce defect density. For example, Djurisic et al. demonstrated that by optimizing the epitaxial growth process, dislocation density could be reduced from 10^10 cm^-2 to 10^8 cm^-2, which substantially enhanced the light output power of DUV LEDs [11].

2.3.2. Challenges of existing doping and defect control technologies

Despite the development of various doping and defect control techniques, p-type doping in AlGaN materials with high aluminum content remains a significant challenge. Due to the wide bandgap of AlGaN, traditional p-type dopants, such as Mg, are difficult to effectively activate, resulting in high contact resistance and low carrier concentration. Researchers have introduced new doping strategies, such as co-doping or the use of superlattice structures, to enhance the effectiveness of p-type doping [12]. However, these methods have not yet achieved the desired results and still require further research and optimization.

2.3.3. The key bottleneck of deep UV LED performance improvement

The performance enhancement of current deep ultraviolet (DUV) LED technology faces multiple bottlenecks, including photon reabsorption, high p-type contact resistance, challenging thermal management, and low device reliability. For instance, photon reabsorption significantly affects the light output power of DUV LEDs, and this issue primarily stems from the self-absorption effect of AlGaN materials. Studies have shown that using novel packaging materials or nanostructure designs can effectively mitigate this issue, thereby improving light extraction efficiency [1].

Additionally, thermal management is a crucial factor influencing the lifespan of DUV LEDs. Under high-power operating conditions, heat is difficult to dissipate effectively, leading to increased device temperature and accelerated aging. To address this challenge, researchers have developed high thermal conductivity substrate materials and novel heat dissipation structures to optimize thermal management performance [13].

3. Optimization direction and analysis of research results

3.1. Material preparation and growth technology

During the production and cultivation stages of DUV LEDs, two prevalent methodologies employed are Metal-Organic Chemical Vapor Deposition (MOCVD) and Molecular Beam Epitaxy (MBE). Fine-tuning parameters like temperature, pressure, and the flow of gases during the growth phase can drastically cut down the imperfection rate within AlGaN substrates. Take, for instance, the work of Kashima and colleagues, who crafted high-reflectivity photonic crystals (HR-PhCs) with minimal damage and a lattice spacing of about 250 nm, achieved through nanoimprint lithography followed by a dry etching process. They then applied a Ni/Mg p-type electrode with high reflectivity to the HR-PhC layer by employing an angled evaporation technique. The integration of HR-PhCs and the Ni/Mg reflective electrode led to a notable enhancement in the external quantum efficiency (EQE) of standard DUV LEDs emitting at approximately 283 nm, elevating it from 4.8% to an impressive 10% [14].

Meanwhile, MBE technology allows for the precise control of material composition and growth rate, enabling the growth of highly uniform AlGaN layers. This precise control not only reduces the defect density in the material but also improves its optical and electrical properties. Additionally, researchers have explored the introduction of stress compensation layers and quantum barrier materials to further enhance the performance of DUV LEDs.

3.2. Optimization of doping conditions

3.2.1. Effect of doping concentration on properties of AlGaN materials

The doping concentration has a significant impact on the electrical and optical properties of AlGaN materials. Although a high Si doping concentration can enhance n-type conductivity, it can also increase the defect density in the material, leading to self-compensation effects that negatively impact conductivity [15]. In terms of p-type doping, the concentration of Mg must be precisely controlled; excessively high Mg concentrations can lead to increased resistivity and the formation of additional non-radiative recombination centers, thereby reducing the material's luminescence efficiency.

To address these issues, researchers have optimized material performance by precisely controlling the dopant concentration and introducing co-doping techniques. For example, Allerman et al. successfully enhanced the carrier concentration in AlGaN materials by optimizing the doping concentrations of Si and Al, while also significantly reducing the defect density in the material [16].

3.2.2. Relationship between defect density and DUV LED performance

Defect density is closely related to the light output power and efficiency of DUV LEDs. Studies have shown that high defect density leads to an increase in non-radiative recombination centers, thereby reducing the external quantum efficiency (EQE).

For instance, Zhanhong Ma et al. found through research that In contrast to threading dislocations, the major nonradiative recombination center for AlGaN epilayers is mostly associated with point defects [17]. According to Chichibu et al., point defects (PDs) are an essential component of AlxGa1−xN-based LEDs. In AlxGa1−xN, point defects (VAl, VN, or complexes) would be created during operation or stress and would spread across or near the active area [18]. These point defects have the potential to lower the optical power of the LEDs by increasing Shockley-Read-Hall (SRH) recombination and acting as non-radiative recombination sites in the active layers.

To reduce defect density, researchers have developed various epitaxial growth techniques, such as low-temperature buffer layers, stress compensation layers, and quantum barrier structures [19]. These techniques effectively reduce the formation of dislocations and vacancies, thereby improving the crystalline quality and optical performance of the material [20].

3.2.3. Synergistic effect of doping and defect

The synergistic effect between doping and defects plays a crucial role in optimizing the performance of DUV LEDs. For example, Mg doping in p-type doping not only affects the carrier concentration but can also introduce new defects, impacting the material's luminescence efficiency. Therefore, when optimizing doping conditions, defect control must also be considered.

Kneissl et al. found that the radiation efficiency is not only affected by the material defect density, another challenge is the relatively high operating voltage of AlGaN based UV leds, which is due to the poor conductivity of the AlGaN layer doped with Si and Mg, as well as the difficulty in forming low-resistance ohmic n and p contacts [3]. Especially if the aluminum molar fraction is high [21].

3.2.4. Results Comparison and analysis

In multiple experiments, researchers systematically compared the performance of DUV LEDs using different doping strategies and defect control techniques. The results showed that the optimized DUV LEDs not only achieved significant improvements in external quantum efficiency but also exhibited better thermal stability and device longevity. For example, The study of Mei Z et al. showed that in the doping behavior, dopants introducing photocatalysts can regulate photogenerated carriers and effectively regulate charge distribution by trapping holes [22]. Defect engineering can not only effectively separate charge by capturing electrons, but also optimize the photoelectric performance of photocatalysts (adjusting band gap, phase transition, exposing more active sites, enhancing charge transfer and separation, etc.) and regulate the adsorption energy of molecules [23, 24].

3.3. Defect control technique

3.3.1. Formation mechanism and control method of deep ultraviolet LED defect

The formation mechanisms of defects in AlGaN materials largely depend on the growth conditions and epitaxial processes. Studies have shown that dislocations in AlGaN materials primarily originate from lattice mismatch and thermal stress, while vacancies and impurities arise from incomplete reactions and impurity incorporation during the growth process. Research by Anderson et al. demonstrates that using hydride vapor phase epitaxy (HVPE) to achieve high-quality free-standing GaN with low extended defect density can reduce screw dislocation densities by six orders of magnitude compared to traditional GaN HEMT technology based on heteroepitaxy [25]. This significant reduction in dislocation density leads to improved crystalline quality of the material.

To further reduce defect density, researchers have developed various techniques, including low-temperature buffer layers, stress compensation layers, and surface passivation. These techniques help reduce the introduction of dislocations and impurities, thereby enhancing the optoelectronic performance of DUV LEDs and extending the device's lifespan.

3.3.2. Application effect analysis of defect control technology in material properties

Defect control techniques play a crucial role in enhancing the performance of DUV LEDs. For example, Han et al. successfully reduced the defect density of DUV LEDs by approximately an order of magnitude through the introduction of surface passivation techniques and low-temperature buffer layers, while also significantly improving light output power and device reliability [26]. Additionally, research by Ramit Kumar Mondal et al. has demonstrated that replacing UV-absorbing p-GaN with UV-transparent p-AlGaN significantly improves the external quantum efficiency of DUV LEDs [27].

These results indicate that defect control techniques can not only improve the light output efficiency of DUV LEDs but also effectively extend the lifespan of the devices, showing great potential for widespread application.

3.4. Characterization and testing methods

3.4.1. X-ray diffraction (XRD) analysis

X-ray diffraction (XRD) analysis is a technique used to characterize the crystal quality of AlGaN materials. Through XRD analysis, key information such as lattice constants, stress states, and dislocation density can be obtained. Chierchia et al., through XRD analysis, revealed the impact of crystal orientation in AlGaN materials on dislocation density and provided important insights for optimizing epitaxial growth processes [28].

Additionally, XRD analysis can also be used to evaluate the effectiveness of stress compensation layers and buffer layers, thereby assisting in the optimization of growth conditions and further improving the crystalline quality of the material.

3.4.2. Photoluminescence (PL) spectral analysis

Photoluminescence (PL) spectroscopy is a technique used to study the optical properties of AlGaN materials. Through PL spectroscopy, it is possible to measure the bandgap width, defect state distribution, and luminescence efficiency of the material. Research by Reshchikov et al. demonstrated that PL spectroscopy can identify non-radiative recombination centers within the material, which is crucial for understanding defect state distribution and optimizing doping conditions [29].

Additionally, PL spectroscopy can be used to evaluate the luminescence efficiency of quantum well structures, thereby aiding in the design of more efficient DUV LED structures.

3.4.3. Electrical characteristics test

An essential part of assessing the conductivity and carrier mobility of AlGaN materials is electrical characterization, which includes I-V curve measurement and Hall effect testing. These experiments offer important new information on how flaws and doping affect the electrical characteristics of the materials. By examining the I-V characteristics of AlGaN-based deep ultraviolet LEDs, Liu et al. carried out a thorough investigation of the electrical properties of the devices, providing important details on carrier injection efficiency and quantum barriers [30]. In particular, their I-V curve analysis revealed that in the first sample, the potential barrier height between the p-type layer and the final quantum barrier was 568 meV, but in the second sample, it was 699 meV. This suggests that the ability of the second sample to inhibit electron overflow more successfully will improve

Hall effect testing is used in addition to I-V measurements to evaluate carrier mobility and concentration, which are important factors in figuring out how successful doping methods are. Meng et al.'s research showed that the interface roughness and edge dislocation density can have a substantial impact on the electron mobility in GaN/AlGaN films [31]. The average mobility in the SH and DH GaN/AlGaN epitaxial layers was 1508 $cm^2V^{-1}s^{-1}$ and 1815 $cm^2V^{-1}s^{-1}$, respectively, for carrier concentrations between 10^{14} and 10^{20} cm^{-3}. The present study highlights the significance of edge dislocations. Specifically, the inclusion of the AlGaN interlayer in DH GaN/AlGaN epitaxial layers leads in a lower edge dislocation density than in SH GaN/AlGaN epitaxial layers, which in turn causes a reduction in overall stress and a contraction of the GaN bandgap. Poblenz et al. also showed that maximizing

4. Conclusion

This work has brought to light a number of significant developments as well as continuing difficulties in the creation of deep ultraviolet light-emitting diodes (DUV LEDs) based on AlGaN.

Important conclusions include the necessity of precisely controlling defect densities and doping schemes in order to optimize the characteristics of the AlGaN material. By creating non-radiative recombination centers, high defect densities—mainly due to lattice mismatch and stress—have a substantial effect on the external quantum efficiency (EQE) of DUV LEDs. It has been demonstrated that reducing these flaws and improving device performance may be achieved by improvements in epitaxial growth methods, such as the use of metal-organic chemical vapor deposition (MOCVD) with optimal growth conditions. Furthermore, the difficulties related to p-type doping, particularly in AlGaN with a high aluminum content, have been resolved by sophisticated doping methods and material advancements, which are essential for enhancing electrical conductivity and overall device efficiency.

Despite these advancements, several limitations remain. The high activation energy of Mg acceptors in AlGaN materials continues to hinder effective p-type doping, leading to high resistivity and suboptimal hole injection. Furthermore, while growth techniques have improved, achieving uniform and high-quality AlGaN layers with minimal defects across large substrates is still a significant challenge, affecting the scalability and cost-effectiveness of DUV LED production. Moreover, the light extraction efficiency remains a bottleneck due to internal optical losses, which are not fully addressed by current packaging and device design strategies.

Future research should focus on developing novel materials and doping approaches that further reduce defect densities and enhance p-type doping efficiency, such as exploring alternative acceptor impurities or co-doping strategies to mitigate the self-compensation effects observed in AlGaN.Additionally, advancements in epitaxial growth technologies, including the use of stress management layers and nanostructured substrates, could offer pathways to achieving higher crystalline quality and uniformity. Investigating new device architectures and light extraction techniques, such as photonic crystals or plasmonic enhancements, may also play a pivotal role in overcoming current efficiency limitations. Continued interdisciplinary efforts integrating material science, physics, and engineering will be essential to propel DUV LED technology towards broader commercial applications and higher performance standards.

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