

# AlGaN multi-quantum barriers for electron blocking in group III-nitride devices

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**Abstract**—In this paper we investigate the enhancement of electron blocking in AlGaN multi-quantum barriers (MQBs). Simulations of effective barrier height of  $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}/\text{GaN}$ -MQBs were performed in order to find optimal layer design. By using a strict optimization procedure the optimized MQB exhibits an increase of the effective barrier height of over 120 meV compared to a bulk electron blocking layer (EBL). This value was achieved for nearly all combinations of material parameters found in literature and for up to  $\pm 10\%$  layer thickness fluctuations. Based on the optimized design a sample series for experimental determination of effective barrier heights in AlGaN-MQB is proposed.

**Keywords**—Multi-quantum barriers, MQB, electron blocking, nitrides, light emitting diodes

## I. INTRODUCTION

AlGaN-based light emitting diodes (LEDs) with emission wavelengths in deep ultraviolet (DUV) spectral range are being investigated intensely due to strong demand for various applications. The most prominent examples are water purification, sensing and phototherapy. Nevertheless, the low output power and efficiency of these devices still hinders broad industrial application. One of the major loss mechanisms for DUV-AlGaN-LEDs has been found to be electron leakage from the active region into the p-side region, which can not be sufficiently suppressed by conventional electron blocking layers (EBLs) [1]. In order to overcome this deficiency multi-quantum barriers can be introduced. MQBs are short period superlattice heterostructures which are expected to exhibit an additional effective barrier for electrons above their conduction band edge due to electron interference analogue to photon reflection by distributed Bragg reflectors. In the last few years several groups have demonstrated improved performance of AlGaN-LEDs by replacing EBLs with MQBs [2,3]. However, the existence of additional effective barriers in current AlGaN-devices are still not proven. Other viable reasons for the performance improvements in AlGaN-devices with MQBs are improved hole injection [4] and favourable band bending [5]. Nevertheless, most of the published MQB configurations are optimized for maximum effective barrier height although the effect and dependence on the structural parameters was not yet unambiguously proven. For this reason a better understanding of the formation of effective barriers in AlGaN-heterostructures

and their role for the operation of MQBs is crucial for the MQB design.

In the present work we investigate the additional effective barriers and electron transport of MQBs in unipolar n-i-n-diodes ( $\text{GaN}/\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}/\text{GaN}$ ) using numerical simulations.

## II. SIMULATION OF AlGaN-MQB

### A. MQB concept

To realize an efficient blocking  $\text{GaN}/\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$  MQB a  $\text{GaN}/\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$  superlattice has to be combined with a thick first  $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$  barrier. The superlattice rejects higher energy electrons by so-called mini-bands even beyond the conduction band edge. The mini-bands are formed by constructive and destructive interferences and are as shown in Fig. 1 reflective or transmittive for charge carriers of certain energies. However, as the bound states in the superlattice act as transmission channels at lower energies these needs to be closed by a thick first barrier. Thus the first barrier and the superlattice are adjusted to each other in order to maximize the effective barrier height for the electrons and hence to minimize current leakage through the structure. However, in (0001) oriented AlGaN heterostructures the design optimization becomes more complicated due to the large spontaneous and piezoelectric polarisation fields at heterointerfaces causing not only an ambiguity in the barrier height of EBLs but can also lead to an electric field over the entire heterostructure. Nevertheless, an adjustment of the blocking bands can be achieved by altering composition and thickness of individual layers.

### B. Numerical model

The electron transmission and reflection probabilities are calculated by employing the transfer matrix method. A self-consistent Schrödinger-Poisson-Solver is used to calculate the band profiles serving as input for the transfer matrix calculations under consideration of internal polarisation fields and donor ionization outside the intrinsic MQB. Based on the reflection spectra the position of single mini-bands and the additional barrier height is determined. For the estimation of current leakage through the structure Esaki-Tsui formula is applied [6].

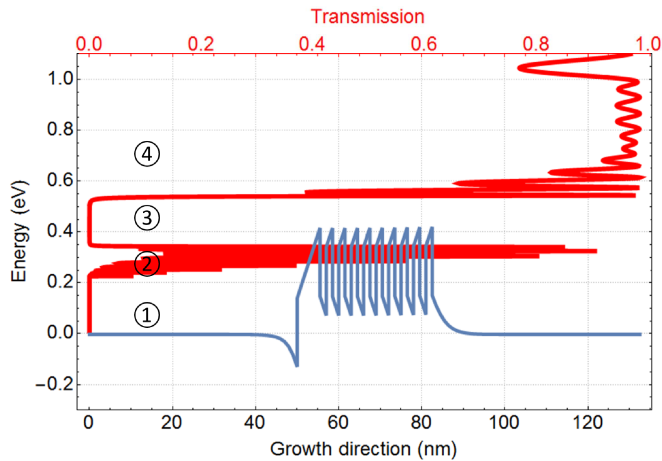


Fig. 1 Conduction band profile (blue) and the corresponding transmission characteristics (red) for an n-i-n-diode with intrinsic MQB. The electron blocking energy range of the first barrier is marked with ①, the transmittive mini-bands of the superlattice with ② and ④ and the reflective mini-band with ③.

### C. Optimization procedure and results

The simulations show that by varying individual layers of an  $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}/\text{GaN}$ -MQB an increase of the effective barrier height of up to 66% compared to an  $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$ -EBL of the same thickness can be achieved. Nevertheless, the choice of slightly different initial material parameters affects the position of mini-bands and can result in electron transmission channels, reduction or even a collapse of this additional effective barrier. In order to reduce this uncertainty, the considered  $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}/\text{GaN}$ -MQB was optimized for a wide range of still not well known AlGaIn material parameters: effective masses, band offset and the strength of the internal polarization fields. In the first step the effects of the deviation of each material parameter on the width and position of mini-bands and the conduction band profile was comprehensively studied. Based on these results an optimization was performed with respect to the period number in the superlattice, which should be high enough to allow the formation of distinct mini-bands, but not exceed the coherence length of the electrons and the horizontal alignment of the quantum wells, which is important for the well-defined interference. The calculations show that already 8 periods are sufficient for the formation of sharp mini-bands and that the horizontal alignment can be achieved by adapting the first and the last well thicknesses. Finally, an  $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}/\text{GaN}$  MQB design with a thickness of 8 nm for the first  $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$  barrier, 5 nm for the first GaN well, 2 nm for the  $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$  barriers and 1.3 nm for the GaN wells of the 8 period superlattice and 3.5 nm for the last barrier was found by independently varying the well and barrier thicknesses of the superlattice and adjusting the thickness of the first barrier. The optimized structure exhibits an additional effective barrier of over 120 meV for 95% of the assumed material parameters.

As the experimental implementation can exhibit a deviation of layer thicknesses the MQB performance of this configuration was investigated in terms of layer thickness fluctuations. It was found that the additional effective barrier of the optimized MQB configuration stays stable for deviations of the layer thickness up to  $\pm 10\%$ .

Based on these findings we propose a sample series for the experimental quantification of the additional effective barrier heights. Due to internal polarization fields changing

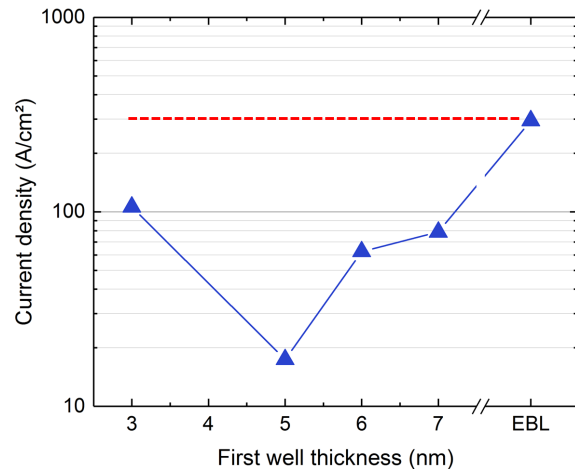


Fig. 2 Simulated current densities in the sample series with varying additional effective barrier height for a constant voltage of 0.1 V. The dashed red line marks the simulated current density for a bulk EBL without the superlattice.

the thickness of the first well in the optimized MQB-structure shifts the mini-band positions and leads to different leakage current for a constant voltage, as shown in Fig. 2. The calculated currents in the simulated series depend strongly on the structure and should provide clear results on the existence and the height of the additional effective barriers in AlGaIn-MQB.

In summary, theoretical analysis of AlGaIn-MQB for the formation of additional effective barriers was performed. Based on these results a MQB configuration was found, which exhibits a high effective barrier that is robust to the material parameter uncertainty and layer thickness variations. Additionally, an n-i-n-diode sample series with optimized MQB configurations and shifted mini-band positions is proposed for experimental quantification of additional effective barriers in AlGaIn-MQB.

### REFERENCES

- [1] M. Kim, M. F. Schubert, Q. Dai, J. K. Kim, F. Schubert, J. Piprek, and Y. Park, "Origin of efficiency droop in GaN-based light-emitting diodes," *Applied Physics Letters*, vol. 91, pp. 183507-1–183507-3, October 2007.
- [2] H. Hirayama, N. Maeda, S. Fujikawa, S. Toyoda, and N. Kamata, "Recent progress and future prospects of AlGaIn-based high-efficiency deep-ultraviolet light-emitting diodes," *Japanese Journal of Applied Physics*, vol. 53, pp. 100209-1–100209-10, September 2014.
- [3] S. Lee, S. Y. Cho, H. Y. Ryu, J. K. Son, H. S. Paek, T. Sakong, T. Jang, K. K. Choi, K. H. Ha, M. H. Yang, O. H. Nam, Y. Park, and E. Yoon, "High-power GaN-based blue-violet laser diodes with AlGaIn/GaN multiquantum barriers," *Applied Physics Letters*, vol. 88, pp. 111101-1–111101-3, March 2006.
- [4] J. Piprek and Z. M. S. Li, "Origin of InGaIn light-emitting diode efficiency improvements using chirped AlGaIn multi-quantum barriers," *Applied Physics Letters*, vol. 102, pp. 023510-1–023510-4, January 2013.
- [5] C. S. Xia, Z. M. S. Li, Z. Q. Li, and Y. Sheng, "Effect of multiquantum barriers in performance enhancement of GaN-based light-emitting diodes," *Applied Physics Letters*, vol. 14, pp. 013507-1–013507-4, January 2013.
- [6] L. Esaki and R. Tsu, "Superlattice and Negative Differential Conductivity in Semiconductors," *IBM Journal of Research and Development*, vol. 14, pp. 61–65, January 1970.