IEEE Photonics Journal
An IEEE Photonics Society Publication

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Volume 8, Number 6, December 2016

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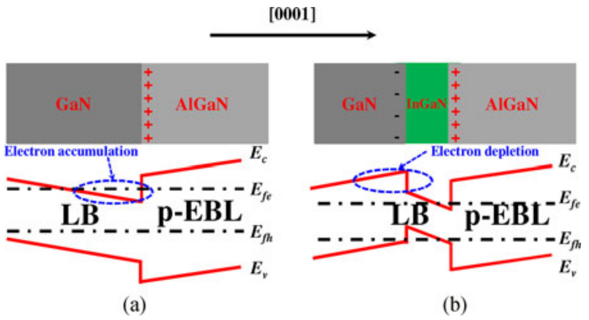

DOI: 10.1109/JPHOT.2016.2628205
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On the Importance of the Polarity for GaN/InGaN Last Quantum Barriers in III-Nitride-Based Light-Emitting Diodes

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DOI:10.1109/JPHOT.2016.2628205

Manuscript received October 26, 2016; revised November 5, 2016; accepted November 9, 2016. Date of publication November 16, 2016; date of current version November 29, 2016. This work was supported by in part by the National Natural Science Foundation of China (Project no. 51502074), in part by the Natural Science Foundation of Tianjin City (Project no. 16JCYBJC16200), in part by the Technology Foundation for Selected Overseas Chinese Scholars by Ministry of Human Resources and Social Security of the People's Republic of China (Project no. CG2016008001), and in part by the Research Grant for Top Young Scientist of Excellence of Hebei Province (Project no. 210013), and the National Key Research and Development Program of China (Program No. 2016YFB0400800, Project No. 2016YFB0400801). Corresponding authors: Z.-H. Zhang and W. Bi (e-mail: zh.zhang@hebut.edu.cn; wbi@hebut.edu.cn).

This paper has supplementary downloadable material available at http://ieeexplore.ieee.org provided by the author.

Abstract: In this paper, we investigate the electron injection efficiency in terms of different polarities and different polarization charge densities at the GaN/InGaN interface. We find that the growth orientation for the GaN/InGaN-type last quantum barrier is essentially vital, i.e., the GaN/InGaN-type last quantum barrier is not able to effectively reduce the electron leakage and will degrade the light-emitting diode (LED) performance when the GaN/InGaN interface is [000–1] polarized. However, a suppressed electron leakage and enhanced optical power can be obtained for III-nitride LEDs grown along the [0001] orientation when the GaN/InGaN interface possesses polarization-induced negative charges. We conclude that the polarization-induced negative charges at the [0001] oriented GaN/InGaN interface facilitate the surface depletion in the GaN region, i.e., the conduction band of the GaN region is bent in the way of favoring electron depletion and contributes to an enhanced conduction band barrier height for electrons.

Index Terms: Polarization inversion, electron injection efficiency, quantum efficiency, light-emitting diode (LED).

1. Introduction

Depending on different emission wavelengths, III-nitride based light-emitting diodes (LEDs) have found various applications in lighting, displays, optical sensing, medical treatment, water sterilization, polymer solidifying, etc. [1], [2]. However, an important criterion to justify the LED performance is to demonstrate the external quantum efficiency (EQE). Among those factors, the EQE is strongly impacted by the electron leakage [2]–[4], which is caused by the asymmetric mobility and concentration between electrons and holes. A direct way to suppress the electron leakage is to employ a heterostructure with different energy band gaps and electron affinity values so that a larger conduction band barrier height can be obtained. Based on this consideration, a p-type electron blocking layer (p-EBL) has been suggested [5]. However, for [0001] oriented LEDs, a strong polarization between the GaN last quantum barrier (LB) and the p-AlGaN EBL significantly bends the conduction band for the GaN LB, which then favors the electron accumulation at the polarization-mismatched $\mathrm{GaN/p-EBL}$ interface and causes substantial electron leakage [2]. To eliminate the polarization induced energy band bending for the GaN LB, a polarization matched p-AlGaInN EBL has been proposed and shown the advantage in decreasing the electron accumulation at the $\mathrm{GaN/p-EBL}$ interface and reducing the electron leakage level [6], [7]. Recently, as has been suggested by Zhang and co-workers, the polarization discontinuity between the LB and the p-EBL can be suppressed by adopting a polarization self-screened p-EBL [8], in which the polarization induced negative bulk charges in the p-EBL can partially compensate the polarization induced positive sheet charges at the LB/p-EBL interface and alleviates the electron accumulation level. Furthermore, an AlN insertion layer with an optimized thickness and Mg doping level also proves useful to increase the conduction band barrier height and reduces the electron leakage level for the sub-250 nm III-nitride LED [9]. Another alternative proposal to reduce the electron leakage is to “cool down” electrons by adopting an InGaN electron cooler [10]–[13] or a n-type AlGaN EBL [14], because the multiple quantum wells (MQWs) are able to more efficiently capture electrons once electrons lose energy via electron-phonon collision taking place in the electron cooler or via the polarization induced electric field generated in the [0001] oriented n-type AlGaN EBL. Alternatively, optimizing the active region is also effective to reduce the electron leakage and a collection of the proposed methods includes increasing the conduction band offset between the quantum well and the quantum barrier [15], adopting the polarization matched quantum well/quantum barrier architecture [16], and in the meanwhile, a [000–1] oriented quantum well/quantum barrier offers another epi-structure against the electron leakage [17]. Recently, GaN/InGaN-type LBs have shown the effectiveness in decreasing the electron leakage level and improving the EQE for both ultra violet (UV) and blue LEDs, respectively [18]–[22]. They report that the reduced electron leakage is attributed to the higher conduction band barrier height in the p-EBL. However, we have known that the effective conduction band barrier height (Φ_b) for the p-EBL can be formulated as $\Phi_b = \Delta E_C - kT \cdot \ln(n_{LB/EBL}/N_C)$, in which ΔE_C is the conduction band offset between the LB and the p-EBL, k is the Boltzmann constant, T is the carrier temperature, N_C is the effective density state of electrons, and $n_{LB/EBL}$ is the electron concentration accumulated at the interface of the LB and the p-EBL [8]. On one hand, the [0001] oriented $\mathrm{InGaN/p-AlGaN}$ EBL interface has a lager ΔE_C and can unambiguously increase the value of Φ_b and helps to suppress the electron overshooting. On the other hand, according to our findings in this work, if the GaN/InGaN interface is [000–1] polarized, a larger ΔE_C for the InGaN/p-AlGaN EBL interface does not help to reduce the electron overshooting, which is on the contrary to the common belief. In this work, we test the impact of the GaN/InGaN-type LB on the electron injection efficiency by employing a III-nitride based UV LED, and we also illustrate that the polarity at the GaN/InGaN interface is vitally important in affecting the electron leakage level, e.g., the GaN/InGaN-type LB contributes to increase the electron injection efficiency only for the [0001] oriented epi-structure, rather than the [000–1] oriented one, and the underlying reasons will be given subsequently. Meanwhile, besides modifying the p-EBL, we suggest that the LB is also very useful in reducing the electron leakage if properly designed.

Fig. 1(a) and (b) show the schematic diagrams for GaN and GaN/InGaN LBs, respectively. We also employ AlGaN as the p-EBL. The structures are designed to be along the [0001] orientation, and therefore, both the GaN/AlGaN interface and the InGaN/AlGaN interface in Fig. 1(a) and (b) possess polarization induced positive charges, while the GaN/InGaN interface in Fig. 1(b) is polarized with negative charges. The polarization induced positive charges at the GaN/AlGaN interface cause a strong electron accumulation, yielding a high local electron concentration and a reduced effective conduction band barrier height in the p-EBL, note that $\Phi_b = \Delta E_C - kT \cdot \ln(n_{LB/EBL}/N_C)$ [8]. On the other hand, an electron depletion mode can be obtained when the GaN/AlGaN interface has negative polarization induced charges, i.e., a polarization inverted p-EBL. A polarization inverted p-EBL has ever been numerically reported by Meyaard *et al.* [23]. However, the way they propose to

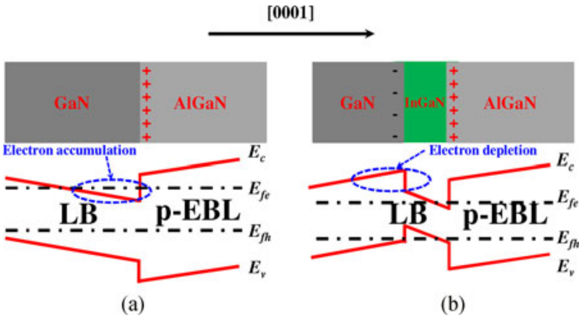


Fig. 1. Schematic drawings for [0001] oriented (a) GaN/AlGaN as the LB/p − EBL structure and (b) GaN/InGaN/AlGaN as the LB/p − EBL structure. Along with the respective schematic energy diagrams, E_c, E_v, E_{fe} and E_{fh} denote the conduction band, valance band, quasi-Fermi level for electrons, and quasi-Fermi level for holes, respectively. The symbols for the polarization induced positive charges at the GaN/AlGaN and InGaN/AlGaN interfaces and the polarization induced negative charges at the GaN/InGaN interface are denoted as + and –, respectively.

experimentally realize such a III-nitride LED with the polarization inverted p-EBL involves substrate removal by laser lift-off, wafer bonding etc., which significantly increases the fabrication cost and also induces material damages. Here, we propose using the GaN/InGaN-type last quantum barrier [see Fig. 1(b)] to make the polarization inversion come true for the [0001] oriented III-nitride LED. The polarization inverted LB will not cause electron accumulation at the GaN region, thus increasing the effective conduction band barrier height in the GaN region and improving the electron blocking effect by the LB, which simultaneously helps to reduce the electron overshooting across the p-EBL. Furthermore, such design can be easily achieved experimentally and cost effective.

2. Device Architectures

The impact of the polarization inverted LB on the electron leakage is probed by numerically calculating two sets of III-nitride based UV LEDs. The studied LEDs have a 4 μm thick n-GaN layer with a Si doping concentration of 5×10^{18} cm^{-3}, which are then followed by five In$_{0.08}$ Ga$_{0.92}$ N/GaN quantum wells with a ~395 nm peak emission wavelength, and the quantum well and the quantum barrier thickness is set to 3 and 12 nm, respectively. We also include a 20 nm thick p − Al$_{0.10}$ Ga$_{0.90}$N as the EBL and a 100 nm thick p-GaN as the hole supplying layer, for which the effective hole concentration is set to 3×10^{17} cm^{-3}. The two sets of LEDs differ only at the last quantum barrier, which uses a 15 nm GaN layer for Set I LEDs and 10 nm − GaN/5 nm-In$_{0.03}$ Ga$_{0.97}$ N for Set II LEDs. We reduce the InN composition in the GaN/InGaN LB to 3% for avoiding the UV absorption. The computations are performed by using APSYS [24], which can well manage Schrödinger equations and Poisson equations self-consistently with proper boundary conditions. Carrier drift and diffusion processes are included when modeling the carrier transport. Meanwhile, both the thermionic emission and the carrier intraband tunneling models are considered, and more importantly, the spontaneous and piezo-electric polarizations for the lattice-mismatched polar III-nitride heterostructure interfaces are reflected by setting the polarization induced sheet charges, which can be calculated by the method reported in [25]. Considering the polarization release by generating dislocations, we have assumed a 40% polarization level for the polarization-mismatched heterostructure interfaces except for the last quantum barriers [8], [13], [14], [24]. The polarization level and the polarization induced charge density at the GaN/p − EBL interface for Set I LEDs and the GaN/InGaN interface for Set II LEDs are shown in Table I.

3. Results and Discussions

First, we verify the validity of our model. According to Fig. 2, we have numerically reproduced the experimentally measured optical output power for a UV LED with GaN layer as the LB, which proves

TABLE 1

Assumed Polarization Level, Polarization Charge Density at the GaN/p-EBL Interface for Set I LEDs, and Polarization Charge Density at the GaN/InGaN Interface for Set II LEDs

Polarization level	Set I LEDs: charge density at GaN/p-EBL interface (m^{-2})	Set II LEDs: charge density at GaN/InGaN interface (m^{-2})
–100%	-0.41×10^{17}	0.24×10^{17}
–80%	-0.33×10^{17}	0.19×10^{17}
–60%	-0.24×10^{17}	0.15×10^{17}
–40%	-0.16×10^{17}	0.97×10^{16}
–20%	-0.82×10^{16}	0.48×10^{16}
0%	0	0
20%	0.82×10^{16}	-0.48×10^{16}
40%	0.16×10^{17}	-0.97×10^{16}
60%	0.24×10^{17}	-0.15×10^{17}
80%	0.33×10^{17}	-0.19×10^{17}
100%	0.41×10^{17}	-0.24×10^{17}

Here, positive and negative polarization levels represent that the GaN/p – EBL and GaN/InGaN interfaces are [0001] and [000–1] polarized, respectively.

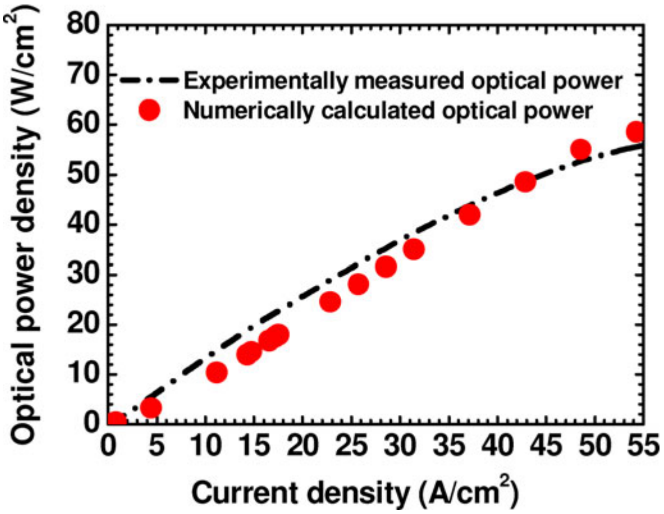
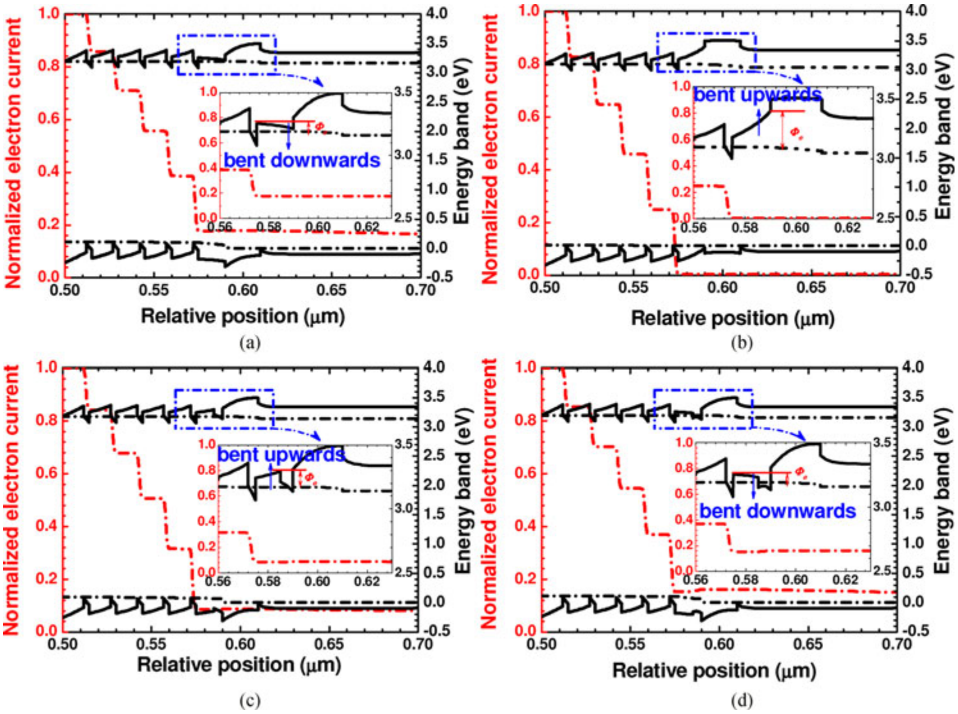


Fig. 2. Experimentally measured and numerically calculated optical powers in terms of the injection current for the LED device with GaN layer as the LB. We empirically set the polarization level to 40% here.

that the physical parameters and the models have been properly set for our numerical calculations. Note that in Fig. 2 we have set a 40% polarization level to obtain the polarization charge density at all the polarization mismatched heterostructure interfaces.

We then show the energy band diagrams and the normalized electron current levels at the current density of 30 A/cm^2 for the following LEDs: Set I LED with a 40% polarization level at the GaN/p – EBL interface [see Fig. 3(a)], Set I LED with a –40% polarization level at the GaN/p – EBL interface [see Fig. 3(b)], Set II LED with a 40% polarization level at the GaN/InGaN interface [see Fig. 3(c)], and Set II LED with a –40% polarization level at the GaN/InGaN interface [see Fig. 3(d)].



(a) (b) (c) (d)

Fig. 3. Energy band diagrams and normalized electron current levels for (a) Set I LEDs with a 40% polarization level and (b) a –40% polarization level at the GaN/p − EBL interface, (c) Set II LEDs with a 40% polarization level, and (d) a –40% polarization level at the GaN/InGaN interface. Φ_e is defined as the effective conduction band barrier height in the LB for electrons.

According to Fig. 3(a), we can see that the conduction band for the GaN LB is bent downwards because of the polarization induced positive charges at the GaN/p − EBL interface, and this leads to a smaller Φ_e of 62.3 meV. Furthermore, besides the thermionic emission, the triangular conduction band for the GaN layer decreases the effective thickness of the LB, thus inducing electron tunneling, which correspondingly causes a strong electron accumulation at the GaN/p − EBL interface. As has been reported, a high local electron concentration reduces the effective conduction barrier height for electrons and inevitably promotes the electron overshooting process (the electron leakage current is 17.81%) [8]. However, if the GaN/p − EBL interface is inversely polarized as shown in Fig. 3(b), then the conduction band for the GaN LB will be bent upwards, the advantage of which is the suppressed electron tunneling through the GaN LB and the alleviation of the electron accumulation as the result of the negative polarization induced charges at the GaN/p − EBL interface. For this reason, the effective conduction band barrier height can be increased to 304.8 meV and the electron leakage current can be negligible. However, it is challenging to obtain the polarization induced negative charges at the GaN/p − EBL interface for [0001] oriented LEDs. Fortunately, the polarization inversion can be easily realized by inserting an InGaN layer between the GaN layer and the p-EBL. In this work, we have utilized a 5 nm thick InGaN layer with the InN composition of 3% for demonstration. As shown in Fig. 3(c), the negative polarization induced charges at the GaN/InGaN interface can suppress the electron accumulation at the GaN region and align the conduction band for the GaN region upwards. As a result, compared to the case in Fig. 3(a), the Φ_e is increased to 120.8 meV. Meanwhile, the design increases the effective thickness for the electron intraband tunnel region which is helpful to reduce the electron tunneling process through the GaN layer and then enables an improved electron blocking effect by the GaN layer. Once the GaN layer can better confine electrons, the electron concentration in the InGaN layer will be correspondingly reduced, and this partially helps to suppress the leakage current level which is as low as 8.65%. It is interesting to see that when compared to the case in Fig. 3(b), the GaN/InGaN-type LB with the

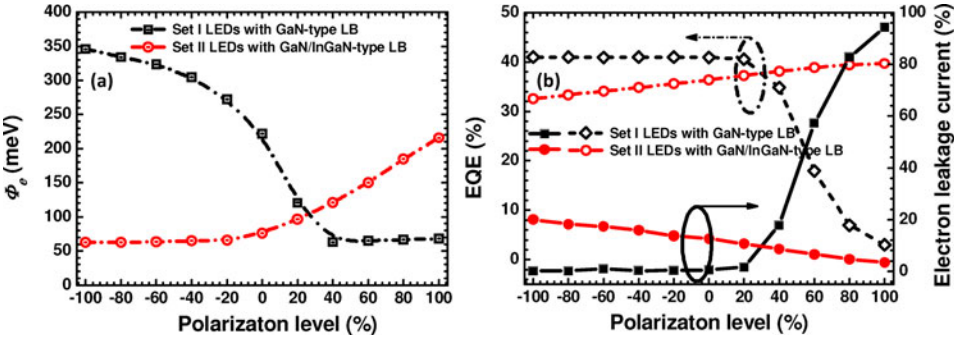


Fig. 4. (a) Effective conduction band barrier height (Φ_e) in the LB region. (b) Electron leakage current levels and EQE at different polarization levels for Set I LEDs and Set II LEDs.

positive polarization in Fig. 3(d) does not help to increase Φ_e, and the larger ΔE_C for the InGaN/p-EBL interface seems to be of less contribution in reducing the electron leakage [Φ_e and the electron leakage current are 64.9 meV and 15.9%, respectively, in Fig. 3(d)]. We attribute our observations in Fig. 3(d) to the positive charges at the GaN/InGaN interface, which bend the conduction band for the GaN layer downwards, thus decreasing Φ_e. Meanwhile, it also reduces the effective thickness for the electron intraband tunnel region. Hence, both the thermionic emission and the electron tunneling processes are serious, which then cause a high electron concentration in the InGaN layer and give rise to the electron overshooting despite an increased ΔE_C between the InGaN layer and the p-EBL. Note that the details on the respective electron current levels and the electron concentration profiles in the p-GaN layer for both Set I and Set II LEDs can be found in the supplementary material [see Figs. S1(a) and S1(b)]. In the meanwhile, the GaN/InGaN LB used in this work does not reserve holes in the InGaN region, and the corresponding discussions on the hole concentration levels in the multiple quantum well region are provided in the supplementary material [see Figs. S2(a) and S2(b)].

We only show the energy band diagrams in Fig. 3 for polarization levels of –40% and 40%, since the physical images to explain the impact of the other polarization values (e.g., –100%, –80%, –60%, –20%, 0%, 20%, 60%, 80%, and 100%) on the Φ_e and the electron leakage do not change. Next, we calculate and summarize the Φ_e, the electron leakage current level and the EQE at different polarization values (see Table I) for both Set I LEDs and Set II LEDs in Fig. 4(a) and (b), respectively. Clearly, we can see that the Φ_e for LEDs with GaN-type LBs decreases as the polarization level changes from –100% to 100% [see Fig. 4(a)], and this is associated with the different leakage current levels, such that the leakage current level increases as the polarization level varies from –100% to 100% [see Fig. 4(b)], agreeing well with the trending details for the EQE values [see Fig. 4(b)]. It shall be noted that the strongest electron leakage current and the lowest EQE take place when the $\mathrm{GaN/p-EBL}$ interface is fully positively polarized. However, it is interesting to observe that the effectiveness of the GaN/InGaN-type LB in increasing the Φ_e, suppressing the electron leakage current and improving the EQE vanishes when the GaN/InGaN interface is of [000–1] polarized, indicating that the GaN/InGaN-type LB is useful for reducing the electron overshooting and enhance the optical power only for [0001] oriented epi-structures (the electron injection efficiency can be found in Fig. S3 in the supplementary material). It is worth noting that the GaN/InGaN-type LB exhibits the largest effectiveness when the $\mathrm{LB/p-EBL}$ interface is strongly polarized, e.g., 100%.

4. Conclusions

To summarize, we have performed detailed analysis on the polarization polarity and the polarization induced charges at the GaN/InGaN interface, which are found to be vitally important to affect the electron distribution in the LB and the effective conduction band barrier height. Compared to the

GaN LB, the GaN/InGaN-type LB is effective in reducing the electron overshooting for [0001] oriented LEDs. However, it is not able to efficiently confine electrons for [000–1] oriented LEDs, and this is also further revealed by the comprehensive discussions in the supplementary material, which illustrates the impact of the GaN/InGaN LB on the electron current, the hole concentration, and the EQE for [000–1] oriented UV LEDs [see Figs. S4(a)–(d)]. It is worth suggesting that considering the uncertainty of the polarization level for various LEDs grown by different technologies, it is difficult to assess the most optimized GaN/InGaN-type LB without direct experimental measurements. However, we believe the findings in this work are very useful to further understand the device physics for optical devices and are even more important to realize high-performance III-nitride based deep ultraviolet (DUV) LEDs, i.e., DUV LED can adopt $Al_x\ Ga_{1-x}\ N/Al_y\ Ga_{1-y}$ N-type last quantum barrier with $x > y$.

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