

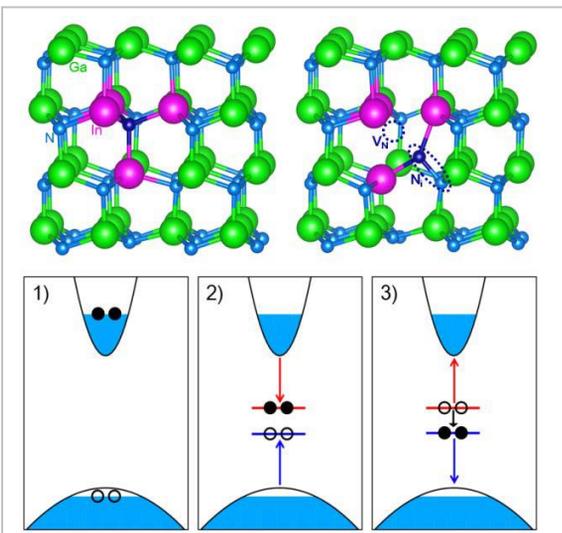
## 청. 백색 LED 발광 효율 저하에 대한 새로운 원인 규명으로 발광 효율 및 성능 향상 길 열려

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- Scientific Reports / 2016. 4.

### 연구내용

일상생활에서 사용되는 LED의 발광효율을 저하시키는 새로운 원인을 규명함에 따라, 향후 LED 성능 향상을 위한 새로운 연구기반이 마련됨.

LED가 작동하기 위해 주입된 전류에 의해 질화갈륨(GaN) 반도체 내에서 지속적으로 결함의 생성-소멸 과정을 일으킬 수 있으며, 이 과정에서 비발광 재결합을 일으켜 효율이 저하 될 수 있음을 밝혀낸 것, 정상적인 상태에서 인듐(In)과 결합되어 있던 질소(N)가, 주입된 전자의 영향으로 인듐과의 결합을 끊으며 결함을 생성시키고, 전자와 정공은 새로 생성된 결함을 매개로 비발광 재결합을 일으켜 에너지 손실이 발생할 수 있음을 밝힘. 그동안 효율 저하 원인으로 알려진 SHR 재결합, 오제(Auger) 재결합, 전자 넘침(carrier overflow) 등을 줄이기 위하여 질화갈륨(GaN) 반도체 막질 특성을 향상시키거나 소자 설계를 수정하는 방향으로 연구가 진행되어 왔으며, 이번 연구로 질화갈륨(GaN) 반도체 LED 소자 성능 향상을 위한 새로운 가능성이 열리게 됨.



[그림 1] 주입된 전자에 의해 GaN 반도체 내에 생성되는 결함의 구조 (위)와 이 결함이 생성되고 소멸되는 동안에 발생하는 전자의 비발광 재결합 과정

### 기대효과

새로 발견된 비발광 재결합 과정은 다른 물질에서도 발생할 수 있는 일반적인 현상으로 앞으로 다른 광전소자 물질 내 비발광 재결합 과정에 대한 추가 연구를 통해 광전소자의 성능을 향상시킬 수 있을 것으로 기대됨.

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# SCIENTIFIC REPORTS

OPEN **Carrier-induced transient defect mechanism for non-radiative recombination in InGaN light-emitting devices**

Received: 26 February 2016  
Accepted: 11 March 2016  
Published: 14 April 2016

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**Non-radiative recombination (NRR) of excited carriers poses a serious challenge to optoelectronic device efficiency. Understanding the mechanism is thus crucial to defect physics and technological applications. Here, by using first-principles calculations, we propose a new NRR mechanism, where excited carriers recombine via a Frenkel-pair (FP) defect formation. While in the ground state the FP is high in energy and is unlikely to form, in the electronic excited states its formation is enabled by a strong electron-phonon coupling of the excited carriers. This NRR mechanism is expected to be general for wide-gap semiconductors, rather than being limited to InGaN-based light emitting devices.**

Nonradiative recombination (NRR) refers to physical processes in semiconductors under electrical or optical excitations, where electrons and holes recombine without emitting photons. NRR is currently the most important factor limiting the efficiency of optoelectronic and photovoltaic devices in energy applications<sup>1–3</sup>. A good example is the efficiency loss in white light-emitting diodes (LEDs) based on GaN and its alloys<sup>4–6</sup>. The wide LEDs hold great promises to revolutionize current lighting technology<sup>7–11</sup>. Their efficiencies, however, are still not enough to penetrate the general lighting market, which is currently dominated by cheap compact fluorescent lamps. Revealing the physics of NRR in such devices is therefore critical to fostering new technology breakthroughs.

The field of NRR study is dominated by the widely-accepted Shockley-Read-Hall (SRH)<sup>12,13</sup> model and the Auger recombination (AR)<sup>14,15</sup>. In the SRH model, defect with deep levels inside the band gap assist carrier recombination such that the energy of the excited carriers is dissipated through lattice vibration or phonon emission. In recent years, other defect-specific NRR processes have also been proposed<sup>16–19</sup>. In the AR process, in contrast, the carrier recombination is mediated by carrier-carrier scattering and, the energy is transferred by generating higher energy carriers inside bulk energy continuum, which is then dissipated through phonon emission. The two models can be characterized as a defect-centric model and a defect-free model, which has been the paradigm for NRR study over decades.

In this work, we show that the formation of defects, especially the Frenkel-pair (FP) defects, due to the presence of excited carriers creates a new type of NRR centers. The energy of the carriers is dissipated through a transient defect generation and annihilation process. In other words, it starts and ends with no deep level inside the band gap as opposed to the SRH mechanism, but the involvement of the transient defects makes it fundamentally different from the AR. Using first-principles calculations we found that in InGaN, the carrier-induced transient FP formation and associated NRR process can readily take place and complete effectively with radiative recombination. The transient nature of the NRR defects may have made them escape experimental detection, which is largely framed by the current thinking and lack of sub-ns-to-ns time resolutions.

To be more specific, first let us discuss the concept behind the carrier-induced transient-defect NRR. In a typical binary semiconductor, such as GaN, the top part of the valence band (VB) mainly consists of anion-derived bonding states, while the bottom part of the conduction band (CB) mainly consists of cation-derived anti-bonding states<sup>20</sup>. Figure 1(a) shows the initial occupations of the electronic states under carrier injection, e.g., in the active region of a working LED, where electrons and holes establish their respective quasi-equilibria at the VB and CB. When an anion is displaced from its original lattice site to an interstitial site, a Frenkel pair (FP) defect (i.e.

SCIENTIFIC REPORTS | 6:2440 | DOI: 10.1038/srep24404

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