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There are many promising applications based on GaN and AlGaN-based material system. Among these, our laboratory has been targeting the realization of highly efficient Al_xGa_{1-x}N-based deep ultraviolet light-emitting diode (DUV-LED) and terahertz quantum cascade laser (THz QCL) as some portion of goals. Here, DUV-LEDs have been expected for the use of sterilization, purification and medical treatment. However, low light extraction efficiency has been preventing the attainment of high external quantum efficiency (EQE) of AlGaN-based DUV-LEDs. Our last year's usage of RIKEN's supercomputer had focused on the design and optimization of PhC which can reduce the light absorption from thick metallic layer on p-AlGaN. To conduct this investigation, very high computational power was demanded due to the very thin practical thickness of 1nm Ni in our structures. Fig 1 shows the 3D schematic and an unit cell of it.

By utilizing finite-difference time-domain (FDTD) method and HOKUSAI system, we have conducted the investigation and optimization of the PhC structure. During last vear. we used 2,529,145.4/2,927,232.0 hours (86.4%) of allocated cpu time of BigWaterfall (bwmpc) system to conduct this project. Figure 2 shows an example of calculated reflectance map for the unit cell of Figure 1. By utilizing the abundant resource, it was possible to theoretically optimize the dimension of PhC on metallic layer (Ni/Al) near 280 nm wavelength of AlGaN-based DUV-LED. As a result, an incremental increase of 8% in average reflectance for the TM mode light was obtained.

Our next step is to design a practical LED structure which guarantees the high LEE over 70%. Our strategy is to adopt optimized PhCs at both top-side on p-contact metallic layer and bottom-side on

AlGaN or AlN layer of LED structure. Our optimized PhC based on guided resonance can be used for the top-side one. In the case of bottom-side, our developed another concept of PhC which shows perfect transmittance before critical angle at the interface between AlGaN and air will be optimized simultaneously. By utilizing RIKEN's supercomputer, LEE of practical LED structures adopting both type of PhCs can be directly calculated. To perform this, existing FDTD software will be upgraded soon. Also, we have developed one more software based on non-equilibrium Green's function (NEGF) method to investigate quantum transport in QCL and LED structures. Since this NEGF methodology requires very large computational resources, using RIKEN's supercomputer will be essential again.



Figure 1. A 3D schematic of laterally periodic structure adopting photonic crystal (PhC) on metal layer and an unit cell of it.



Figure 2. An example of the reflectance mapping as functions of light incidence angle and wavelength.

Usage Report for Fiscal Year 2018 Fiscal Year 2018 List of Publications Resulting from the Use of the supercomputer

[Paper published by a journal]

 Joosun Yun, Yukio Kashima, and Hideki Hirayama, "Reflectance of a reflective photonic crystal p-contact layer for improving the light-extraction efficiency of AlGaN-based deep-ultraviolet light-emitting diodes", AIP Advances 8, 125126 (2018)

[Oral presentation]

- 1. Joosun Yun, Yukio Kashima, and Hideki Hirayama, "Reflectance of Reflective Photonic Crystal on P-contact Layer of AlGaN Deep-UV LED", JSAP Autumn meeting, Nagoya Congress Center, 19p-146-10, September 18-21, 2018
- 2. Joosun Yun and Hideki Hirayama, "Investigation of perfect reflection by 2D Photonic Crystal on the AlGaN Surface used for increasing light-extraction efficiency of deep-UV LED", 第65回応用物理学会春季学術講演会, JSAP Spring meeting, 2018

[Poster presentation]

 Joosun Yun, Yukio Kashima, and Hideki Hirayama, "Highly-reflective photonic crystal (HR-PhC) design for increasing light-extraction efficiency (LEE) of AlGaN deep-UV LEDs", International Workshop on Nitride Semiconductors (IWN) 2018, Kanazawa, Japan, MoP-OD-6, Nov. 11 – 16, 2018