

## SIMULATION OF PHYSICAL PROCESSES

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### Numerical investigation of influence GaP nanowire geometry to light extraction efficiency of red light-emitting diode

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**Abstract.** Currently, micro-LEDs are promising optoelectronic devices. Numerical investigation was carried out to study the influence of the GaP nanowires geometric parameters on the light extraction efficiency to improve micro-LEDs efficiency. The nanowires diameter has been shown to significantly alter the light extraction efficiency. The optimal nanowire diameter for a wavelength of 650 nm is close to 200 nm.

**Keywords:** Red LEDs, GaP, NWs, molecular beam epitaxy, light extraction efficiency

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Материалы конференции

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### Численное исследование влияния геометрии нитевидных нанокристаллов GaP на эффективность экстракции света в красном светодиоде

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**Аннотация.** В работе проведено численное исследование влияния геометрических параметров нитевидных нанокристаллов GaP на эффективность экстракции света. Было показано, что диаметр нитевидных нанокристаллов значительно изменяет эффективность экстракции света. Оптимальное значение диаметра НК для длины волны 650 нм находится вблизи 200 нм.

**Ключевые слова:** красные светодиоды, фосфид галлия, нитевидные нанокристаллы, молекулярно-пучковая эпитаксия, эффективность экстракции света

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**Ссылка при цитировании:** Новикова К.Н., Фунтикова А.С., Можаров А.М., Мухин И.С. Численное исследование влияния геометрии нитевидных нанокристаллов GaP на эффективность экстракции света в красном светодиоде // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2024. Т. 3.2 № .17. С. 84–87. DOI: <https://doi.org/10.18721/JPM.173.215>

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## Introduction

Currently, micro-LEDs are promising optoelectronic devices [1, 2]. Gallium phosphide is advanced material for creating micro-LEDs due to its waveguide properties and the ability to form a direct-gap solid solution with the addition of As and N. In addition, the crystal lattice period proximity of GaP and silicon makes it possible to create optoelectronic devices based on established silicon technologies on cheap substrates. LED efficiency is a combination of internal quantum efficiency and light extraction efficiency (LEE). Unfortunately, when creating micro-LEDs using the standard «top-down» method, during microdevices etching, upon reaching a certain minimum size, the internal quantum efficiency decreases down to 1% [1]. The radiation generated in a planar micro-LED spreads in all directions and increases optical loss, so the light extraction efficiency in a planar micro-LED also needs to be optimized [3]. As an alternative to planar structures, nanowires (NWs) can be used to increase the micro-LEDs efficiency. NWs are synthesized using «bottom-up» technology without material etching stages. This approach ensures high crystalline perfection and when the active region is integrated inside the LED, for example, in the form of a quantum dot [4], the active region is completely isolated from the external environment and the internal quantum efficiency increases. In addition, the NWs geometric dimensions commensurability and the radiation wavelength makes it possible to control the LEE, which distinguishes the NWs from planar LEDs in which all radiation directions are equivalent even when micro-LED size is 10  $\mu\text{m}$  in diameter.

Unfortunately, the extraction efficiency of NW-based LEDs in the GaP/GaPNAs material system has received insufficient attention to date, so this work aims to investigate LEE by optimizing the geometric parameters of NWs.

## Materials and Methods

Full-wave optical modeling of light propagation was carried out using the COMSOL Multiphysics package to select the optimal geometric parameters of the LED. The system under study consisted of a GaP NW on a silicon substrate in an air environment. An optical point dipole was used as a radiation source, the orientation and position of which varied during the calculation. The system schematic cross-sectional representation is presented in Fig. 1, *a*.

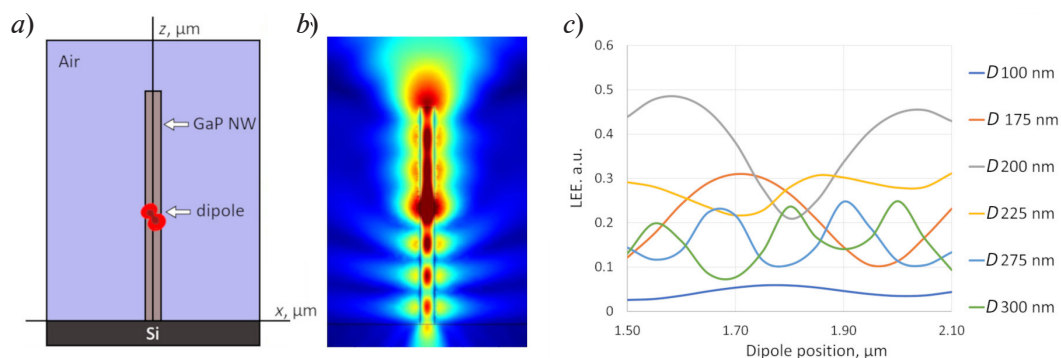


Fig. 1. System under study in cross section (*a*), typical distribution of normalized electric field in the system under study (*b*) and LEE depending graphs on dipole position on NW axis (*c*)

The length of the GaP NWs was fixed at a distance of 3  $\mu\text{m}$ , and the diameter ranged from 50 to 500 nm. Material properties of Si and GaP are taken from [5, 6]. The calculation was carried out for a wavelength of 650 nm, which corresponds to the expected band gap for the GaPNAs solid solution [7].

### Results and Discussion

As a result of full-wave optical light distribution modeling, the LEE dependences on the NW geometric parameters, as well as the normalized electric field distribution in the system under study, were obtained. As part of the calculation, for each geometric configuration, the dipole polarization angle was varied and the power fraction of the electromagnetic wave emitted by the dipole that went into the upper plane of the system under study was determined. A typical electric field distribution for a fixed dipole configuration is shown in Fig. 1, *b*. As a result of numerical modeling, the LEE in the vertical direction from the position of the emitting center along the NW axis was calculated for diameters from 50 to 500 nm. Fig. 1, *c* shows the LEE dependences for diameters from 100 to 300 nm. It has been established that the movement of the emission center on wavelength scales significantly affects the extraction efficiency. This is due to the fact that the NW is a resonator with a certain mode composition. Therefore, for effective radiation extraction, it is necessary to fulfill the condition of constructive interference for the output radiation, which will lead to modulation of the light extraction efficiency.

The LEE values were averaged over one LEE modulation period and a summary of the average light extraction efficiency as a function of NW diameter is presented in Fig. 2, *a*. A monotonous increase in the average LEE value is shown with an increase in the NW diameter to 200 nm and a further decrease. The maximum LEE value was almost 40% for random polarization and dipole position along the NW axis.

As part of the mode analysis, NWs with diameters equal to 100, 200 and 300 nm were studied (Fig. 2, *b*, *c*, *d*). At small NW diameters (Fig. 2, *b*), the electromagnetic wave goes upward, but diverges greatly. As the diameter increases, the NW begins to function as a resonator and the wave has greater directivity, as can be seen in Fig. 1, *b*. This is also noticeable from Fig. 2, *c* because the wave spreads throughout the NW. A further increase in the diameter (Fig. 2, *d*) leads to the dominance of higher-order modes, which are shifted from the NW axis and the point dipole does not emit in them.

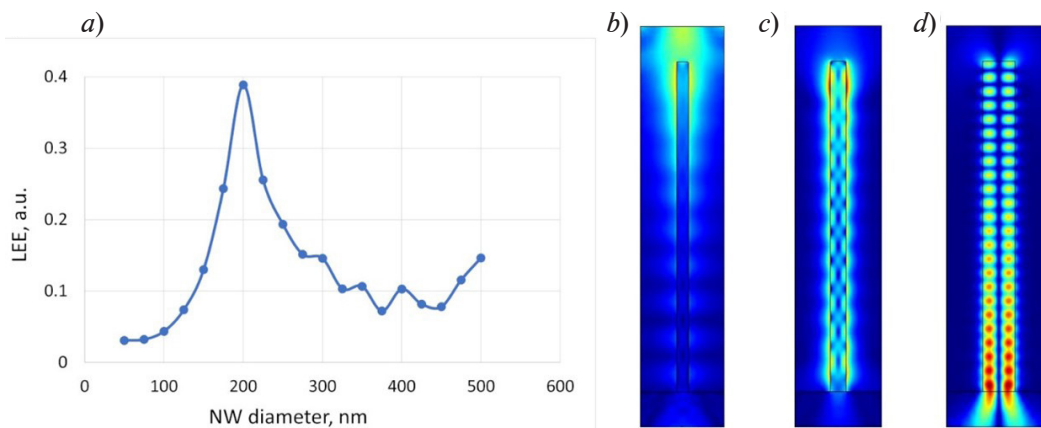


Fig. 2 Dependence of average LEE value on NW diameter (*a*) and eigenmodes for NW diameters equal to 100 nm (*b*), 200 nm (*c*) and 300 nm (*d*)

### Conclusion

We demonstrated a numerical study of GaP NWs with a point-emitting center in various geometric configurations. The NWs diameter has been shown to significantly modify the light extraction efficiency. The optimal value of the NW diameter for a wavelength of 650 nm is close to 200 nm. The results of this simulation can be used to synthesize NWs with specified optimal geometric parameters and create highly efficient red micro-LEDs based on them.

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**REFERENCES**

1. **Pandey A., Malhotra Y., Wang P., et al.**, N-polar InGaN/GaN nanowires: overcoming the efficiency cliff of red-emitting micro-LEDs, *Photonics Res.* 4 (10) (2022) 1107.
2. **Belyaev V.**, Solid state and organic micro-LEDs – technology, market, prospects, *ELECTRONICS: Science, Technology, Business.* (8) (2018) 102–112.
3. **Hu R., Cao B., Zou Y., et al.**, Modeling the Light Extraction Efficiency of Bi-Layer Phosphors in White LEDs, *IEEE Photonics Technology Letters.* 12 (25) (2013) 1141–1144.
4. **Barettin D., Shtrom I.V., Reznik R.R., Cirilin G.E.**, Model of a GaAs Quantum Dot in a Direct Band Gap AlGaAs Wurtzite Nanowire, *Nanomaterials.* 11 (13) (2023) 1737.
5. **Green M.A.**, Self-consistent optical parameters of intrinsic silicon at 300K including temperature coefficients, *Solar Energy Materials and Solar Cells.* 11 (92) (2008) 1305–1310.
6. **Adachi S.**, Optical dispersion relations for GaP, GaAs, GaSb, InP, InAs, InSb,  $\text{Al}_x\text{Ga}_{1-x}\text{As}$ , and  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$ , *J Appl Phys.* 12 (66) (1989) 6030–6040.
7. **Mozharov A.M., Kudryashov D.A., Bolshakov A.D., et al.**, Numerical simulation of the properties of solar cells based on GaPNAs/Si heterostructures and GaN nanowires, *Semiconductors.* 11 (50) (2016) 1521–1525.

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