The effect of geometry parameters on light harvesting performance of GaN nanostructure arrays—a numerical investigation and simulation

Xingyue Zhangyang, Lei Liu, Zhisheng Lv, Feifei Lu and Jian Tian
Department of optoelectronic technology, School of Electronic and Optical Engineering, Nanjing University of Science and Technology, Nanjing 210094, People’s Republic of China
E-mail: liu1133.cn@sina.com.cn

Keywords: GaN nanostructure, photocathode, FEM, COMSOL multiphysics, light harvesting

Abstract

In this paper, COMSOL Multiphysics Commercial Package software is used to simulate the models of two kinds of GaN nanostructure arrays, and to study how the geometric structure and periodicity of arrays affect the optical properties of GaN nanostructures. By analyzing the schematic diagram of electric field distribution and absorption curves of GaN nanostructure arrays, we concluded that the absorptivity is a decreasing function of periodicity in non-homogenous shaped nanostructures. In addition, a gentle change in geometric structure or having a lower effective refraction index on the incident side of the light are more conducive to enhancing the light absorption ability of GaN nanostructure arrays. Simulation experiments on GaN nanostructures will provide some references for the structural design of photocathodes, which will help UV detectors to achieve efficient light absorption.

Nomenclature

| Short forms | Full name                   |
|-------------|----------------------------|
| GaN         | gallium nitride            |
| CVD         | chemical vapor deposition method |
| ZnO         | zinc oxide                 |
| AR          | anti-reflection            |
| FEM         | Finite Element Method      |
| 3D          | three-dimensional          |
| MG          | Maxwell-Garnett            |
| TM          | transverse magnetic polarizations |
| PML         | perfect matching layer     |
| UV          | Ultraviolet (200 nm–400 nm) |
| UVC         | Ultraviolet C (200 nm–280 nm) |

1. Introduction

As a semiconductor material with superior optical and electrical properties, gallium nitride (GaN) has been widely used as photocathode material. GaN semiconductor material has good photoemission performance, low electron affinity, and stable physical and chemical properties. Therefore, GaN nanostructures are widely used in photoemission devices [1–5]. Zhen C et al have synthesized GaN nanopencils and nanotowers and single-crystalline bamboo shoot-shaped GaN nanowires and a layer-structure GaN nanowires by a chemical vapor deposition (CVD) method. In the work of Yeong Jae Kim et al they concluded that the saturation of
photocurrent in the truncated nanocones was increased by about 3 times compared to planar GaN [6–10]. Li Zeping et al. have found that GaN truncated nanocones have high absorption and photoelectrochemical efficiency compared with planar counterpart [11]. In the research of Lu Hu and Gang Chen reveals that nanowire arrays with suitable filling ratio will have smaller reflections than thin films [12]. Junshuai Li et al. studied the silicon nanowire diameter and the periodic variation of the arrays. It is found that the periodicity has a higher influence on the optical properties of the nanowire arrays [13, 14]. It is concluded by Chiu et al. that refractive index gradient and filling factor determine the design and manufacture of disordered AR nanostructures [15]. In the study of Yahia Makableh et al. optical properties of six different shapes of zinc oxide (ZnO) nanostructures were investigated, in those geometries, rods and hexagonal shapes have less reflectivity over a wide wavelength range [16]. In the papers of Zhaopeng Xu et al. the optical absorption of three nanostructures was calculated respectively within the visible solar spectrum and the results reveal that the nanocones have the highest average absorption [17]. The work of Hao Lin et al. revealed that the optical properties of nanostructures are primarily affected by geometrical factors such as structural spacing, material fill ratio, and aspect ratio [18]. As can be seen from the overview of the above article, most of the past work is aimed at anti-reflection. Therefore, it is particularly important to study the optical properties of GaN nanostructure arrays, especially the light collection properties in the ultraviolet range.

GaN is used as the material of nanostructures, the first part of the simulation is to find the suitable height and width of the nanostructures. And the unified geometry parameters are used in the subsequent simulation works. The simulated models are divided into two categories. (1) Homogenous shaped nanostructures—cube, cylinder and hexagonal cylinder; (2) Non-homogenous shaped nanostructures—cone, inverted cone, pyramid, truncated cone, motheye, inverted pencil. By using COMSOL Multiphysics Commercial Package software, the optical properties revealed by electric field distribution and absorption performance in nanostructures was studied.

2. Methods

COMSOL Multiphysics is a simulation software that implements real physical phenomena by solving partial differential equations based on the Finite Element Method (FEM). It uses mathematical methods to solve real-world physical phenomena. It has powerful meshing capabilities and supports multiple meshing. ‘Wave Optics Module’ is an add-on module to the COMSOL Multiphysics platform software. The ‘Wave Optics Module’ provides a traditional full-wave propagation method based on direct discretization of Maxwell’s equations, based on the FEM. The ‘Wave Optics, Electromagnetic Wave, Frequency Domain’ interface is used to solve the time harmonic electromagnetic field distribution. ‘Wavelength domain’ studies are used to calculate the response of a linear or linear model when excited by harmonics of one or more wavelengths. In electromagnetic wave propagation, it is used to calculate the transmittance and reflectivity of a structure as a function of wavelength. ‘Wavelength domain’ studies illustrate the effects of all feature patterns correctly resolved by the mesh and how they couple with the applied stimulus.

2.1. Structure design

The geometry of nanostructures is usually classified into two categories, according to whether the effective refractive index changes homogeneously of their transverse section in the axial [16]. And the specific classifications are homogeneous and non-homogeneous. In the simulation models, homogenous shaped 3D nanostructures include cube, cylinder and hexagonal cylinder, and non-homogenous shaped 3D nanostructures include cone, inverted cone, pyramid, truncated cone, motheye, inverted pencil. Calculating the optical properties of the simulation model requires the use of the refractive index of the material. However, the refractive index of the nanostructured materials cannot use that of thin film structure. The effective medium theory can be applied in order to obtain the effective refractive index of these 3D shaped nanostructured arrays. Materials with integral heterogeneity have refractive index that depends on the topology structure. Because incident light gets scattered by nanoscale structure. Maxwell-Garnett proposed mathematical models called MG model to calculate the effective refractive index of a homogeneous mixture under the incident light. Homogeneous mixture with volume fraction of inclusion is \( f \). MG model can be extended to give the effective refractive index as a function of \( f \). However, for non-homogenous mixtures, the MG model can also be used to give the formula containing \( f \). The effective refractive index of non-homogenous mixtures can be determined by treating the heterogeneous mixtures as homogeneous mixtures superimposed layer by layer [19, 20]. The effective refractive index for transverse magnetic (TM) polarizations is expressed as equation (1) [21]:
where $n_{\text{eff,TM}}$ is the effective refractive index for TM polarization, and $f$ is the filling factor of every layer of the nanostructures.

### 2.2. Simulation details

In this paper, COMSOL Multiphysics is used to simulate the electric field distribution and absorption performance of nanostructures with incident light. The geometric parameters of the nanostructure are realized by the 'parameter' function in 'global definition', which can easily change the parameter settings of the entire model. The parameter values that change in the geometric model are related to the cross section. In the first part of the simulation, the cube has a length of 70 nm to 130 nm, a period of 150 nm to 250 nm, and a height of 200 nm to 1000 nm. By analyzing the first part of the simulation results, some suitable parameter values were selected for the construction of the model in the following work, in which the axial height of all the nanostructures was set to 500 nm. In the homogeneous shaped nanostructures of the second part, the width of the cube is 100 nm, the diameter of the cylinder is 100 nm, and the side length of the hexagonal cylinder is 50 nm (the longest diagonal is 100 nm). In non-homogenous shaped nanostructures of the third part, the cone bottom diameter is 100 nm, parameter of the inverted cone is the same with that of the cone. The width of the bottom of the pyramid is 100 nm. The diameter of the bottom surface of the truncated cone is 100 nm, and the diameter of the top surface is 50 nm. The diameter of the bottom surface of the motheye is 100 nm as well. The structure of the inverted pencil consists of two parts, a cylinder with a height of 460 nm and a cone with a height of 40 nm, both of them have a diameter of 100 nm. The material model contains the refractive index of GaN and air. The model assumes that the real part of the refractive index of air is 1 and the imaginary part of the refractive index is 0. The complex refractive index of GaN is from the thin film structure of the material.

The simulation model in this paper solves the scattering field in 'electromagnetic wave, frequency domain'. 'The electric displacement field model' selects the 'refractive index' option, and the refractive index is derived from the material model. In order to simulate the propagation of incident light in the simulation region in a real scene, perfect matching layer (PML) with thickness of 200 nm is defined. As shown in figure 1(a), at the top and the bottom of the simulation region are the PMLs. By using the PML, it is possible to eliminate unwanted reflections in the simulation region and interference caused by reflected light. The S parameter is used to calculate the reflection and transmission of the simulation model, which is obtained by setting the two boundaries immediately adjacent to the PMLs as ‘port’. Absorption is calculated by equation (2):

$$ A(\lambda) = 1 - R(\lambda) - T(\lambda) $$

where $A(\lambda)$ is the absorption of the simulation models, $R(\lambda)$ is the reflection calculated by port S1 and $T(\lambda)$ is the reflection calculated by port S2.
The TM field source is implemented by setting the internal port boundary to the slit boundary and setting the port as a ‘periodic port’. As shown in figures 1(a) and (b), the top boundary creates ‘port wave excitation’, which means the incident light. In order to reduce the workload and computational complexity, ‘periodic boundary conditions’ are defined to obtain the arrays. As shown in figure 1(c), the two facing boundaries are set in the ‘periodic boundary condition’. The other two faces of the simulation region are also set to periodic boundary condition to achieve a nanostructure array. The periodic type selects the ‘Floquet period’, and its k vector is from the periodic port. As shown in figure 1(d) is schematic diagram of meshing, the PMLs are set to ‘sweep’ and the rest of the simulation region is set to the ‘freely split tetrahedral mesh’. For this physics interface, the maximum grid cell size is preferably less than a certain fraction of the wavelength. The incident light wavelength range of this simulation model is 200 nm to 400 nm, so the maximum cell size is 50 nm and the minimum cell size is 2 nm. All simulation models use the same grid cell size to maintain computational rigor.

3. Results and discussions

All electric field distribution pictures in this paper are calculated by COMSOL Multiphysics software. It is not easy to understand the change of absorption through the variation of electric field, because it cannot provide a clear number of increase or decrease to determine the overall absorption of nanostructure. Therefore, we analyze the overall optical properties of the nanostructure by combining the absorptivity curve and the electric field distribution, which can provide clear values.

3.1. Cube nanostructure

As shown in figure 2(a), this is the simulation result of the cube nanostructures for the cube width in the case where the array cell period changed. The average absorptivity of the structure with a width of 100 nm or more is better, but the curve of the nanostructure with a width of 100 nm which intersect with the other three lines is smoother. Therefore, the value of the cube cross-sectional width of 100 nm is selected for subsequent simulation work. As shown in figure 2(b) is the average absorptivity of cube nanostructures which their width are 100 nm and height change from 200 nm to 1000 nm. The absorptivity from 200 nm to 500 nm rises fast, but the values are low, so it is not suitable for the subsequent simulation work. Then the average value of the absorptivity between 600 nm to 1000 nm rises slower, which means the increase of height can contribute less to the absorption. To obtain a very high absorption by height will make our work meaningless. Therefore, 500 nm is selected as the appropriate height to build the nanostructures in the other simulation models.

3.2. Homogenous shaped nanostructures

As shown in figures 3(a) and (b), the electric field inside the nanostructure at the wavelength of 240 nm with a period value of 190 nm is not much different from the electric field distribution at the period of 150 nm, but the reflection above the cube is significantly weakened. However, the transmission of the cube is slightly increased, and it can be considered that the nanostructure with period of 190 nm obtains higher absorption. The electric field distribution inside the nanostructures at the period of 250 nm clearly shows the attenuation of the amplitude, that is, the absorption of the nanostructures under this period is less than that of the nanostructures with a period of 190 nm. Therefore, by the change of the absorptivity curve with wavelength, the value of the absorptivity at the wavelength of 240 nm increases with the increase of the period and then decreases. On the contrary, the electric field at the wavelength of 370 nm shows a significant decrease in reflection and a slight
decrease in transmission with the increase of the period. The electric field distribution inside the nanostructures show an increase in the absorption length, which means an increase in the optical coupling strength. So, the electric field distribution changing with the period can be explained by the increase of the absorptivity curves. It can be seen that the relationship between the light absorption and the period of the nanostructure arrays is a nonlinear curve with the change of wavelength.

As shown in figures 3(c) and (d), with the increase of the period, it can be observed from the electric field at the wavelength of 250 nm that the reflection decreased above the cylinder and the transmission increased. In addition, a significant decrease in the optical coupling strength can be seen from the electric field distribution in the cylinder. It can be confirmed that the absorptivity at 250 nm wavelength decreases gradually with the increase of the period. On the contrary, the electric field distribution at the wavelength of 340 nm shows decrease in reflection and transmission. The optical coupling strength in the cylinder is reduced but the increase in absorption length does not reduce the absorption of the nanostructures. Therefore, it is not difficult to draw a conclusion similar to that of the cube.

In the case of hexagonal cylinder, similar results and conclusions can be found. As shown in figures 3(e) and (f), the electric field distribution at the wavelength of 230 nm shows reduced optical coupling strength which means decreased absorption inside the hexagonal cylinder with the increase of period. The distribution of electric field in the wavelength of 320 nm shows different results, optical coupling strength reduced but the absorption length increased. In addition, the absorptivity curves show an increasing trend. Finally, the same conclusion can be obtained under the hexagonal cylinder nanostructure, that is, the relationship between the light absorption and the period is a nonlinear curve with the change of wavelength.

It can be clearly seen from the average absorptivity curves in figure 3 that the absorptivity in the band of 370 nm to 400 nm decreased rapidly, so the average absorptivity in the band of 200 nm to 370 nm were selected for analysis. As shown in figure 4, the maximum absorptivity of the cube nanostructure is obtained when the period is about 210 nm. The maximum absorptivity of the cylinder nanostructure is obtained when the period is about 190 nm. The maximum absorptivity of the hexagonal cylinder is obtained when the period is about 170 nm. It is not difficult to conclude that the relation between the average absorptivity and the period is a convex function, which means, the maximum absorptivity can be obtained in a certain period in the homogenous shaped nanostructure arrays.

### 3.3. Non-homogenous shaped nanostructures

As shown in figures 5(a) and (b), the electric field distribution inside the cone at the wavelength of 240 nm and 350 nm show that reduced coupling strength and shorter absorption length. In the absorptivity curves show a downward trend, which is sufficient to prove that the absorption of the cone decreases with the increase of the period. In addition, it can be noted in the electric field distribution diagram that there is a strong reflection near the tip of the cone, and the absorption in the cone is mainly concentrated in the middle and lower part. When the
period increases or the wavelength of incident light becomes longer, a lot of transmission will be caused at the bottom of the cone, thus reducing its absorptivity.

As shown in figures 5(c) and (d), in the nanostructures of inverted cone absorption curves show a downward trend with the increasing period. The performance of electric field distribution at the wavelength of 240 nm and 350 nm shows that the coupling strength is reduced and the absorption length is shortened inside the inverted cone. In the inverted cone nanostructure, absorption occurs mainly at the upper part of the inverted cone, while at the tip of the cone, there is not any contribution to absorption.

As shown in figures 5(e) and (f), the absorptivity curves of truncated cone nanostructure show a trend of decreasing with the increase of the period. By observing the electric field distribution in the truncated cone, it can be found that the coupling strength inside the truncated cone decreases as the period increases. In the electric field distribution at the wavelength of 240 nm, absorption is mainly concentrated in the upper half of the truncated cone. As the period value increases the shortening of absorption length can be seen. In the electric field distribution at the wavelength of 350 nm, absorption almost occurs in the whole nanostructure. However, with the increase of the period, the top of the truncated cone absorbs light no longer, and the absorption in the middle and bottom is weakened.

In the motheye nanostructure shown in figures 6(a) and (b), absorption curves of different period overlap with each other in the wavelength of 320 nm to 340 nm, but the absorption curves of the parts beyond that still decrease with the increase of period. In the electric field distribution with a wavelength of 240 nm, absorption is mainly concentrated in the upper part of motheye, and the coupling strength is obviously weakened. In the
electric field distribution with a wavelength of 350 nm, absorption occurs in the whole nanostructure, but with the increase of the period, the tip no longer absorbs light and the overall absorption declines. The difference between the absorptivity curves with period of 350 nm is not significant, but the change in the electric field distribution can indicate a decrease in absorption.

As shown in figures 6(c) and (d), the trend of absorptivity curves of pyramid nanostructures is similar to that of other non-homogenous nanostructures. The electric field distribution of the pyramid nanostructure is similar to that of the cone nanostructure. In the electric field distribution with a wavelength of 240 nm, absorption is mainly concentrated in the middle part of the pyramid, and the absorption gradually decreases. However, compared with the cone nanostructure, the coupling strength of the pyramid is obviously higher. In the electric field distribution with a wavelength of 350 nm, absorption is mainly concentrated in the lower half of the pyramid. The coupling strength at the tip of the pyramid is very low, and the whole nanostructure shows a decrease in absorption with the increase of the period.

In the absorptivity curves of the inverted pencil nanostructure in figures 6(e) and (f), it can be seen that the trend is similar to that of the cylinder nanostructure. In other words, the relationship between the light absorption of the inverted pencil nanostructure and the period is a non-linear curve with the change of wavelength. The electric field distribution with a wavelength of 240 nm shows a decrease in absorption which concentrated on the top of the nanostructure, a decrease in reflection and an increase in transmission. Combined with the absorptivity changing with the period at this wavelength, it can be considered that the absorption of the nanostructure decreases with the increase of the period. In the electric field distribution with a wavelength of 350 nm, the electric field distribution in the nanostructure showed a decrease in absorption. But the reflection above and below the nanostructure indicated that the overall absorption of the nanostructure was actually increasing, which was also consistent with the results shown in the absorptivity curves.

In the absorption curves of the six nanostructures, absorptivity began to decrease rapidly near the wavelength of 280 nm, so the average absorption within the wavelength band of 200 nm to 280 nm (UVC) was selected for analysis, as shown in figure 7(a). As shown in figure 7(b) is the curves of average absorptivity, the one of truncated cone is the highest, and curves of pyramid, motheye and inverted pencil intersect with each other with the period changed, while the absorptivity of cone and inverted cone is much lower. First of all, four kinds of non-homogenous nanostructures with tip structures were analyzed. It can be seen from the curve of effective refractive index that those four kinds of nanostructures have almost the same refractive index at the beginning and end-point, but the difference is their rate of change with height increasing. The inverted pencil has a cylindrical structure below the height of 460 nm and a cone at the top of it with a height of 40 nm. The structure of inverted pencil makes the electric field distribution similar to that of the cylinder nanostructure, so the average absorptivity of them is very similar in value and trend. By comparing average absorptivity curves between motheye and cone, the average absorptivity of motheye is higher than cone about 0.05. That is because on the geometric structure, at the top of motheye has a relative smooth change, and the tip of the cone changes sharp, which led to the tip of the cone is hard to make contribution on absorption but
reflection. In addition, by comparing the effective index curve, it is found that the effective index of cone is a straight line varying with height, while the effective index of motheye is a nonlinear curve approximating a quadratic curve. The electric field distribution and the average absorptivity change trend of pyramid nanostructure are similar to that of cone, but the absorptivity of pyramid is higher than that of cone. It is because that the filling factor of pyramid is larger than the one of cone at the same height. It embodies in the effective refractive index is that pyramid has a lower effective refractive index than cone, therefore, the pyramid has a relatively large absorption area to achieve a higher absorptivity.

Secondly, inverted cone nanostructure has the lowest average absorption. It is because at the tip of the cone can be approximated to be a cylinder, which makes inverted cone made some light absorption. But when the height lower, the tapered structure lost materials which can absorb light, led to more transmission under the nanostructure at the same time. The inverted cone nanostructure makes the light absorption rely mainly on the top of the inverted cone, apparently that is the reason of lowest average absorptivity.

Finally, through the effective refractive index curves of the six nanostructures changes with height found that the truncated cone has effective refractive index of 2.3 at the height of 500 nm. In the case of the removal of inverted cone, its effective refractive index is very low right from the start and then changes with height is the gentlest one. The truncated cone is a nanostructure which guide light absorption in the nanostructure more gently, and the tip of the truncated cone is not a sharp one that causes more reflection just like cone. It means that the truncated cone nanostructure has better light absorption ability than the four structures with a tip.

4. Conclusion

In this paper, COMSOL Multiphysics Commercial Package software is used to simulate GaN nanostructure arrays.

1. In the first part of chapter 3, consistent nanostructure parameter values are selected to ensure the rigor and accuracy of the simulation work. After the simulation of the cube nanostructure arrays, 100 nm is defined as the width of the cube, because the average absorptivity curve changes gently with the period and the value is not low. 500 nm is chosen as the height of the cube, because the average absorptivity of the nanostructures with a height of 500 nm is not low but there is room for improvement.

2. The homogenous nanostructures of cube, cylinder, and hexagonal cylinder. The relationship between the light absorption and the period of the nanostructure is a nonlinear curve with wavelength, and the change of the corresponding nanostructure electric field distribution can also prove this conclusion. In the next analysis of the average absorptivity, it is concluded that the relationship between the average absorptivity of the homogenous nanostructure and the period in the wavelength of 200 nm to 370 nm is a convex function. Which means that homogenous nanostructures can find an optimal period value to achieve maximum absorptivity.

3. In the third part, the non-homogenous nanostructures of cone, inverted cone, truncated cone, motheye, pyramid, and inverted pencil were simulated. The nanostructures of motheye and inverted pencil have the same conclusion with homogenous nanostructures such as cube. The other four nanostructures have different conclusions, which the absorptivity decreases with the period increases. The relationship between the average absorptivity of the non-homogenous nanostructures and the period in the wavelength of 200 nm to 280 nm is a decreasing function. By analyzing the geometry of the nanostructures, it is concluded
that the more gradual and rounded geometric changes the more conducive to improving the light absorption capacity of the nanostructures. In addition, by analyzing the curve of the effective refractive index of the non-homogenous nanostructures as a function of height, it is concluded that low effective refractive index of the nanostructures at the incident side is more favorable for enhancing the light absorption capacity of the nanostructures.

Acknowledgments

This work is supported by Qing Lan Project of Jiangsu Province-China (Grant No.2017-AD41779), the Fundamental Research Funds for the Central Universities-China (Grant No. 30916011206) and the Six Talent Peaks Project in Jiangsu Province-China (Grant No. 2015-XCL-008). Qinghua Lv of Hubei University of Technology is greatly appreciated for the help of COMSOL Multiphysics Business Package calculations.

ORCID iDs

Lei Liu https://orcid.org/0000-0002-4966-5914

References

[1] Cheng H, Li J, Wu D, Li Y, Wang Z, Wang X and Zheng X 2015 J. Nanomater. 2015 272–76
[2] Look D C, Jones R I and Sun X L 2002 J. Phys. Condens. Matter 14 13337
[3] Xia S, Liu L, Diao Y and Kong Y 2017 Mater. Res. Express 4 035034
[4] Diao Y, Liu L, Xia S and Kong Y 2017 Mater. Res. Express 4 035907
[5] Diao Y and Liu L 2018 Mater. Res. Express 5 065047
[6] Zhen C and Enling L 2018 Rare Metal Materials & Engineering 47 43–46
[7] Cui Z, Li E and Shi W 2015 Ceram. Int. 41 6074–6078
[8] Zhen C, Li M and Li E 2018 Superlattices & Microstructures 120 257–261
[9] Cui Z et al 2014 Mater. Res. Bull. 56 80–85
[10] Kim Y J and Lee G J 2019 ACS Applied Materials & Interfaces 10 28672–28678
[11] Zeping L, Dongjing L and Aixia W 2019 Nanotechnology 30 40
[12] Xu Z, Qiao H and Huangfu H 2015 Opt. Express 22 31907
[13] Han L and Zhao H 2014 Opt. Express 22 31907