

Journal of Nanophotonics

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Comparative study of cesium adsorption on GaN planar and nanowire photocathodes

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Abstract. Using first-principle calculations, we compare the quantum efficiency and stability of Cs-GaN planar model and Cs-GaN nanowire model. The results show that the work function of GaN nanowire photocathodes decreases continuously with the increase of θ_{Cs} , the “Cs-kill” phenomenon disappears, resulting in a lower work function (1.76 eV) than the conventional GaN planar photocathodes (1.82 eV). However, we find that the nanowire GaN photocathodes had a lower stability by calculating the adsorption energy. In addition, the surface atomic structures of both kinds of photocathodes are almost identical, which account for the similarity of their best adsorption sites. Our study is helpful to the growth of GaN nanowire materials in the future and can be used to guide the improvements of GaN-based equipment photoelectric efficiency. © 2019 Society of Photo-Optical Instrumentation Engineers (SPIE) [DOI: [10.1117/1.JNP.13.016011](https://doi.org/10.1117/1.JNP.13.016011)]

Keywords: GaN planar photocathode; GaN nanowire photocathode; adsorption energy; atomic structure.

Paper 18156 received Sep. 29, 2018; accepted for publication Feb. 26, 2019; published online Mar. 13, 2019.

1 Introduction

GaN materials have been widely used in ultraviolet detection, night vision image intensifiers, and high-electron-mobility transistor.^{1–6} GaN-based photocathodes perform many excellent properties in the photoemission field, such as wide bandgap, small dark current, high spin polarization, high breakdown voltage, and thermal conductivity.^{7,8} Negative electron affinity (NEA) state can be obtained by Cs atom adsorbed on the surface of GaN semiconductor materials.⁹ Lots of experimental researches have been done to study Cs adsorptivity and adsorption position to obtain highest photocurrent. Furthermore, theoretical and experimental results showed that the change in the work function and band structure of GaN materials, thus, the variation in the electronic and optical properties of GaN photocathodes covered with Cs can be demonstrated.^{10–13} In the last few years, the quantum efficiency (QE) of GaN photocathodes has continuously increased^{14–17} with the development of p-type doping technology, surface cleaning, surface activation, and gradient doping structure. Nevertheless, many problems still remain unsolved for conventional GaN planar photocathodes, such as the contradiction between photon absorption depth and electrons diffusion length.¹⁸

However, due to the development of nanomaterials, the GaN nanowire photocathode get much attention since it shows possibilities to overcome the conflict between the absorption depth and the diffusion length of the conventional GaN photocathodes, meanwhile exhibit excellent photoemission performance. Therefore, the GaN nanowires have attracted interests in the field of optoelectronics, such as investigation for application in light-emitting diodes.¹⁹ Previous studies on nanomaterial showed that the surface of the GaN nanowire photocathode possessed more hanging bonds, which were beneficial to the adsorption of Cs atoms and the liberation of

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photoelectrons.²⁰ Xia et al.²¹ reported that the QE of the GaN nanowire photocathode was 1.6 times higher than that of a conventional reflection-mode GaN planar photocathode based on their simulation on the basis of one-dimensional continuity equation.

Many researchers have demonstrated the cesium atoms could lower surface work function and subsequently introduce reaction models at the interface for GaN planar and nanowire photocathodes, while a few comparative researches were conducted on GaN planar and nanowire photocathodes. In this study, density functional theory (DFT) with an ultrasoft pseudopotential method based on first-principle calculation was used to illustrate the distinction of Cs adsorption on the GaN planar and nanowire photocathodes. And the surface adsorption energy, work functions, and atomic structures of two types of photocathodes were also discussed to provide theoretical references for the fabrication of GaN-based equipment.

2 Models and Methods

All calculation methods were implemented from the quantum mechanics program Cambridge Serial Total Energy Package based on DFT. The generalized gradient approximation with Perdew–Burke–Ernzerhof was used to depict the exchange and correlation interactions. The geometry optimization was expressed by Broyden–Fletcher–Goldfarb–Shanno (BFGS). For GaN planar and nanowire photocathodes, the energy tolerance, the force tolerance, the maximum displacement, the convergence tolerance of a single atomic energy, and the stress were $<2 \times 10^{-6}$ eV/atom, 1×10^{-5} eV/nm, 0.001 Å, 1×10^{-5} eV/atom, and 0.1 GPa, respectively. Before the calculation, we made a coverage test on the cutoff energy and k points with high symmetry, the results showed that the total energy could reach a convergence with a cutoff energy of 400 eV and k points of $4 \times 4 \times 1$ for GaN planar model while that were 450 eV and $1 \times 1 \times 4$ for GaN nanowire model. All calculations were carried out in reciprocal space. Ga: $3d^{10}4s^24p^1$, N: $2s^22p^3$, H: $1s$, and Cs: $5s^25p^66s^1$ were set as valence electrons.

As shown in Figs. 1(a) and 1(b), the surface slab was modeled with six Ga-N bilayers to simulate the GaN (0001) planar photocathode. The top three bilayers were relaxed freely and the bottom three bilayers were fixed to simulate a bulk environment. To avoid interactions between repeated slabs, a vacuum thickness of 1.3 nm was set. The dangling bonds on the back of bottom slab surface were saturated with pseudohydrogen atoms to avoid the transfer of surface charges. Previous studies have shown that the (001)-oriented GaN nanowire with a hexagonal section was energetically more favorable²² and the GaN nanowire models were obtained from $13 \times 13 \times 2$ wurtzite supercell by cutting the redundant atoms that were around the hexagonal nanowire. In this study, the diameter of the nanowire was 9.6 Å and the length was 10.5 Å. To avoid the interference of adjacent nanowires caused by periodicity during the calculation, a 25-Å vacuum space between adjoining nanowires was applied. The GaN nanowire photocathode has six perfectly equivalent (100) side faces, and then the dangling bonds of other five side faces were

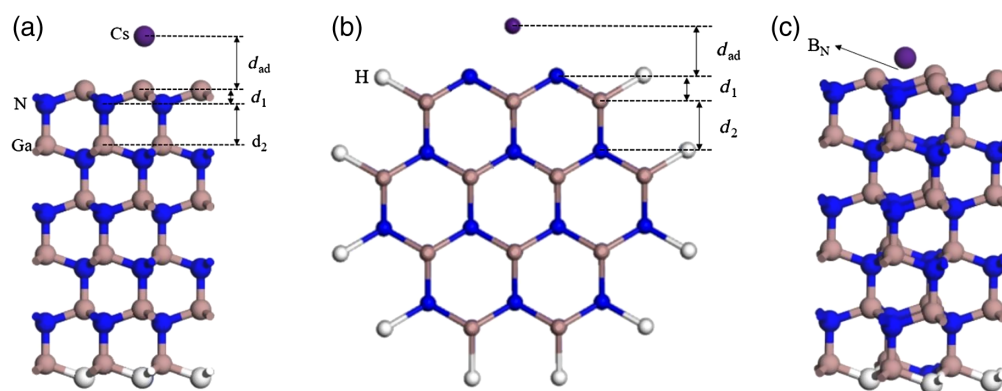


Fig. 1 (a) Side view of Cs adsorption on GaN (0001) planar surface, (b) side view of Cs adsorption on nanowire (001) crystal plane, (c) and schematic diagram of Cs adatom adsorption on B_N site.

saturated with H atoms to prevent the charge transfer of the surfaces, which can reduce surface activity and remove surface states efficiently.

3 Results and Discussions

3.1 Adsorption Energy

High-symmetry sites were chosen as GaN planar and nanowire photocathodes surface adsorption positions. There were five high-symmetry sites for Cs adsorption on the GaN planar photocathode surface, denoted by T_{Ga} (Ga top), B_{N} (N bridge), H (hollow site), B_{Ga} (Ga bridge), and T_{N} (N top). Figure 2(a) shows these five different adsorption sites on the surface of the GaN planar photocathode. And there were six highly symmetrical sites in the repeat unit of the GaN nanowire photocathode, denoted by T'_{Ga} (Ga top), B'_{N} (N bridge), $B'_{\text{Ga-N}}$ (Ga-N bridge), H' , B'_{Ga} (Ga bridge), and T'_{N} (N top). The schematic diagram of Cs adsorption on the surface of the GaN nanowire photocathode is shown in Fig. 2(b). In consideration of adsorbed atoms for each model, the adsorption energy could be calculated by the following equation:

$$E_{\text{adsorption}} = \frac{E_{\text{total}} - E_{\text{initial}} - n\mu_{\text{Cs}}}{n}, \quad (1)$$

where E_{total} , E_{initial} , n , and μ_{Cs} represent the calculated total energy of the Cs adsorption system, the initial GaN photocathode energy of the clean surface, the number of adatoms, and the chemical potential of Cs atom, respectively. When $E_{\text{adsorption}}$ is negative, it means the adsorption process is exothermic and the adsorption model is stable. While the adsorption process is an endothermic chemical process and the corresponding model is unstable if $E_{\text{adsorption}}$ is positive. The adsorption energy with only one Cs atom at different sites is shown in Table 1. As can be seen, all the adsorption energy of different sites were negative, illustrating all Cs adsorption models were stable. For the GaN planar photocathode, $E_{\text{adsorption}}$ was the smallest at B_{N} site and the largest at T_{Ga} site, which suggested the B_{N} site was the most stable adsorption sites. The Cs atom adsorption on the GaN planar photocathode followed the order: $T_{\text{Ga}} \rightarrow T_{\text{N}} \rightarrow B_{\text{Ga}} \rightarrow H \rightarrow B_{\text{N}}$. For the GaN nanowire photocathode, it could be found that the most stable site was B'_{N} and the most unstable site was T'_{Ga} , which was similar to the GaN planar photocathode.

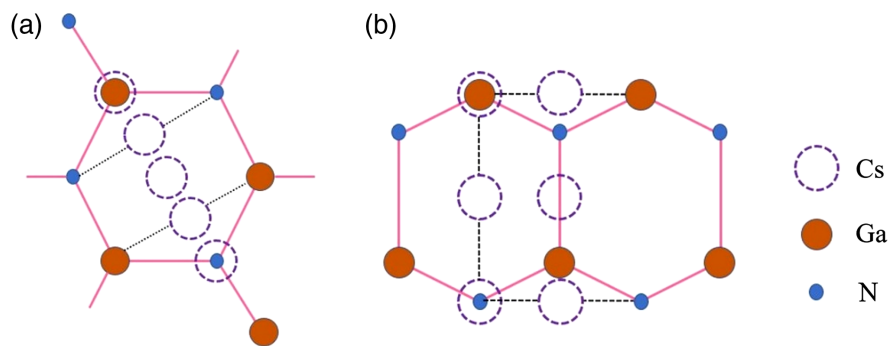


Fig. 2 (a) Top view of Cs adsorption on GaN planar photocathode surface and (b) top view of Cs adsorption on GaN nanowire photocathode surface.

Table 1 Adsorption energy of Cs adsorption on the surface of GaN planar and nanowire photocathodes.

	Planar photocathode					Nanowire photocathode						
Cs site	T_{Ga}	B_{N}	H	B_{Ga}	T_{N}	T'_{Ga}	B'_{N}	$B'_{\text{Ga-N}}$	H'	B'_{Ga}	T'_{N}	
$E_{\text{adsorption}}$	-1.89	-2.04	-2.02	-1.98	-1.96	-1.50	-1.60	-1.54	-1.53	-1.51	-1.55	

The Cs atom adsorption on the GaN nanowire surface followed the order as: $T'_{\text{Ga}} \rightarrow B'_{\text{Ga}} \rightarrow H' \rightarrow B'_{\text{Ga-N}} \rightarrow T'_{\text{N}} \rightarrow B'_{\text{N}}$. In summary, the $E_{\text{adsorption}}$ of the GaN nanowire adsorption system was higher than the GaN planar adsorption system, indicating that Cs atom adsorption on the GaN planar surface was more stable than that on the GaN nanowire surface. To simplify the calculation, the following discussions were all on B_{N} site for planar models and with B'_{N} site for nanowire models.

3.2 Work Function and Dipole Moment

The photoemission of NEA photocathodes followed a “three-step-model” proposed by Spicer and Herrera-Gomez,²³ including photon adsorption, electrons heating, and escape into vacuum. The QE of photocathodes was closely related to the escape probability of photoelectrons, and the work function was the minimum energy required for electrons to escape into vacuum. Therefore, lower work function was necessary for GaN photocathodes. The work function could be expressed as²⁴

$$\Phi = E_{\text{vac}} - E_F, \quad (2)$$

where E_{vac} and E_F represent the vacuum level and the surface Fermi level, respectively. Figure 3 shows the work function values of both types of photocathodes with different θ_{Cs} . The results indicated that the GaN planar photocathode surface performed the lowest work function (1.82 eV) when the θ_{Cs} was 0.5 ML, but with the increase of θ_{Cs} , the work function would increase slightly. This “Cs-kill” phenomenon was mainly because the adjacent Cs atoms shared electrons more easily than transfer them to the surface when too many Cs adatoms were adsorbed on the GaN planar surface. However, the work function of the GaN nanowire became smaller with the increase of θ_{Cs} and obtained the lowest work function (1.76 eV) when the θ_{Cs} was 1 ML. The Cs-kill phenomenon for the GaN nanowire photocathode disappeared mainly because the nanowire had a large surface-to-volume ratio and the surface of the nanowire photocathode had enough empty hanging bonds for Cs atoms to adsorb.

As shown in Table 2, the work function of GaN planar photocathode was decreased to 2.15 to 2.58 eV and that decreased to 2.29 to 2.39 eV of the nanowire photocathode. The work function of both types of photocathodes was decreased significantly after Cs adsorption mainly due to the existence of (Cs-GaN planar/nanowire) dipole moments and the schematic diagram is shown in Fig. 4. The electronegativity of Ga and Cs was 1.81 and 0.79, respectively.²⁵ As a result, Cs atoms losing electrons showed positive while Ga atoms obtaining these electrons became negative, then the GaN photocathode showed n-type property and the Fermi level closed to conduction band. Cs-induced dipole moments would lower the surface barrier for electrons to escape to vacuum and vary the work function, which was a benefit to improve the photoemission

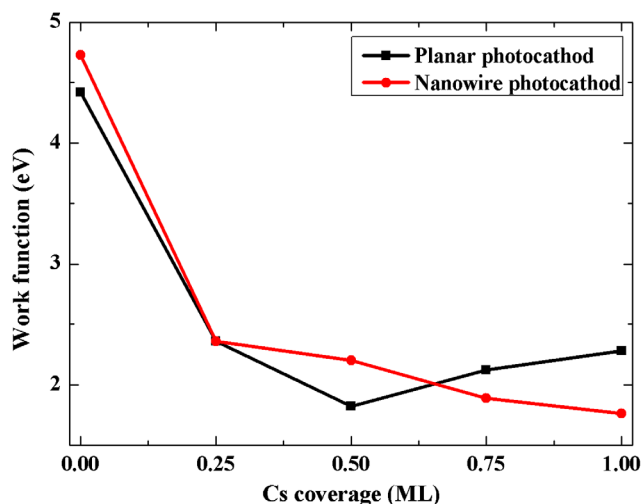
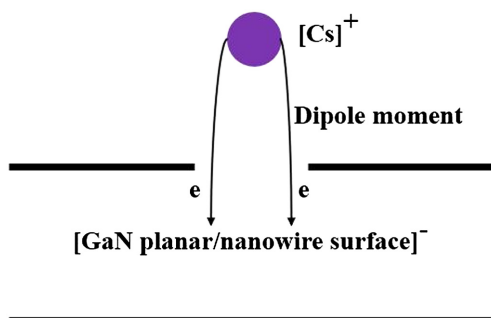


Fig. 3 The work function of GaN planar and nanowire photocathodes with different θ_{Cs} .

Table 2 The work function of GaN planar and nanowire photocathodes at different sites when θ_{Cs} was 0.25 ML.

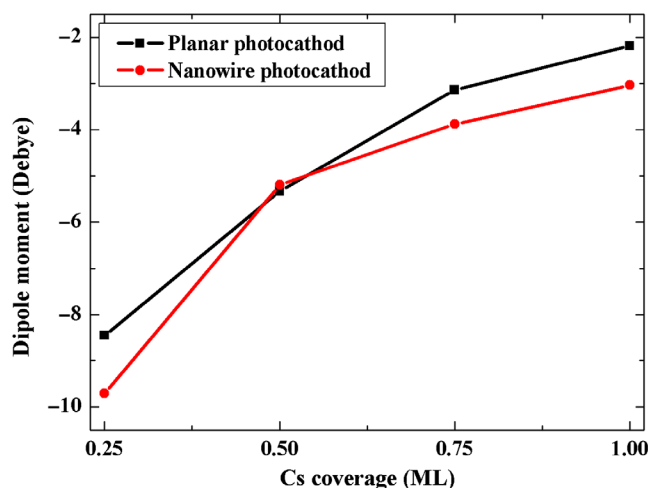
Cs site	Planar photocathode						Nanowire photocathode						
	Clean	T _{Ga}	B _N	H	B _{Ga}	T _N	Clean	T' _{Ga}	B' _N	B' _{Ga-N}	H'	B' _{Ga}	T' _N
Φ (eV)	4.42	2.58	2.35	2.15	2.34	2.37	4.73	2.38	2.29	2.36	2.35	2.33	2.39

**Fig. 4** The schematic diagram of (Cs-GaN planar/nanowire) dipole moment.

efficiency of the GaN photocathode. The dipole moments perpendicular to the surface will occur when electrons transfer from Cs atoms to the GaN planar or nanowire surface, which could be described by Helmholtz equation as²⁶

$$\mu = \frac{(12\pi)^{-1} A \Delta\varphi}{\theta}, \quad (3)$$

where A , $\Delta\varphi$, and θ represent the surface area, the work function variation, and the Cs coverage, respectively. The dipole moments μ for Cs atom adsorption on the GaN planar and nanowire surface with θ_{Cs} of 0.25, 0.5, 0.75, and 1 ML are shown in Fig. 5. Results suggested that the surface dipole moments of both kinds of photocathodes decreased as θ was increased. The change was mainly because the interaction between Cs atoms and the GaN planar and nanowire surface was affected with the increase of θ_{Cs} , the ionization of Cs atoms was decreased, and part of electrons transferred back to Cs atoms. Furthermore, the changes of dipole moments were the main reason accounting for the surface reconstruction of GaN planar and nanowire photocathodes.

**Fig. 5** The values of (Cs-GaN planar/nanowire) dipole moments with different θ_{Cs} .

3.3 Atomic Structure

After Cs atom was adsorbed on the surface of GaN planar and nanowire photocathodes, the result of geometry optimization through BFGS showed a slight change in the atomic structure of their surface. In this study, the change was explained by the E-Mulliken charge distribution of Cs adatoms. The calculated E-Mulliken atom charge distribution before and after Cs adsorption on the GaN planar and nanowire surface were shown in Table 3. It could be found that the surface Ga atoms decreased by 0.10 $|e|$ and the surface N atoms had no change for the GaN planar photocathode. For the GaN nanowire, the surface Ga atoms decreased by 0.29 $|e|$ and the surface N atoms had a negligible increase. So it was obvious to speculate that almost all of the electrons in Cs atoms were transferred to the surface Ga atoms. The interaction between Cs atoms and the surface Ga atoms became stronger and the distance between them became smaller. To obtain the changes in the electronic structure brought by the adsorption of Cs atoms to the surface of GaN planar and nanowire photocathodes, the d_{ads} (the distance from the Cs adatom to a atom in the outermost layer), d_1 (the thickness of the surface first bilayer), and d_2 (the distance between the first and second bilayers) with different θ_{Cs} were calculated and shown in Table 4. Here, d_1 showed clear decrease when Cs adsorption on the surface of the GaN planar photocathode, while it becomes larger when Cs adsorption on the GaN nanowire surface, which was consistent with previous analysis by the E-Mulliken charge distribution of surface atoms. With the increase of θ_{Cs} , the d_1 for the GaN planar model had a small decrease while a slight increase for nanowire model. There were mainly two reasons for this phenomenon; one was the more Cs adatoms adsorbed, the more difficult it was for electrons to transfer from Cs adatoms to Ga atoms on the surface of the two kinds of photocathodes. The other reason was that, with the increase of θ_{Cs} , the mutual repel of (Cs-GaN planar/nanowire) dipole moments increased gradually and part of the electrons transferred back to Cs adatoms. However, the d_2 of both kinds of photocathodes showed a negligible change, which meant almost all the electrons of Cs adatoms were transferred to the first bilayer and the second bilayer only got a few electrons.

Through the previous calculation of adsorption energy and work function, it could be found B_{N} and B'_{N} were the most stable adsorption positions of GaN planar and nanowire photocathodes, respectively. Then, the GaN planar photocathode was used as an example to explain why B_{N} site was the most stable position for Cs adatom by analyzing the geometric structure of the GaN surface. As shown in Fig. 1(c), the B_{N} site was a trench shape and it could provide enough

Table 3 The calculated E-Mulliken atom charge distribution of GaN surface before and after Cs adsorption.

	Clean surface		Cs adsorption on GaN surface	
	Planar surface	Nanowire surface	Planar surface	Nanowire surface
Cs	—	—	0.71	0.71
Ga	1.28	0.75	0.99	0.65
N	-1.05	-0.98	-1.09	-0.98

Table 4 The d_{ads} , d_1 , and d_2 of GaN planar and nanowire photocathodes with different θ_{Cs} adsorption systems.

	Planar photocathode					Nanowire photocathode				
	θ_{Cs}	0	0.25	0.50	0.75	1.00	0	0.25	0.50	0.75
d_{ads} (Å)	—	1.997	1.994	2.012	1.973	—	2.62	2.63	2.64	2.67
d_1 (Å)	0.898	0.645	0.639	0.632	0.629	1.03	1.14	1.15	1.17	1.18
d_2 (Å)	2.013	1.987	1.998	2.030	2.032	2.08	2.06	2.07	2.09	2.08

lattice space for Cs adatom to adsorb. Furthermore, N atom on each side of B_N site had strong electronegativity, which could attract Cs adatom effectively. More lattice space and electronegativity of N atoms made B_N site the most stable position for Cs adatom. According to this analysis method, B'_N site was proved as the best adsorption position for the GaN nanowire photocathode because of their similar surface morphology.

4 Conclusion

In this study, the adsorption energy, work function, dipole moment, atomic structure of GaN planar and nanowire photocathodes were calculated using first principles with DFT. After calculation and comparison, the GaN nanowire structure would get a lower work function and perform better photoemission properties than planar structure, because it possessed a larger surface-to-volume ratio. However, the system of Cs adsorption on the GaN nanowire photocathode was less stable than the planar one. By comparing the surface atomic structures of the two kinds of photocathodes, the results suggested that the nanowire structure had larger d_1 and d_2 , which was inconsistent with our previous analysis (GaN nanowire photocathode was less stable than planar photocathode). In addition, the reasons why B_N and B'_N were the optimal adsorption sites for Cs were discussed through analyzing the surface geometric structure of GaN planar and nanowire photocathodes. Through our analysis of two kinds of photocathodes, GaN nanowire photocathodes showed better photoelectric properties and application prospect. Meanwhile, further research needs to be conducted to find a more stable nanowire structure. This research is helpful to the application of GaN photocathodes in devices.

Acknowledgments

This work was supported by the National Natural Science Foundation of China under Grant Nos. 61775203, 61308089, and 6144005 and the National Key Research and Development Program of China under Grant No. 2017YFF0210800. The work was also supported in part by the National Science Foundation of the United States under Grant No. ECCS-1254902. We particularly appreciated Meishan Wang of the School of Information and Electrical Engineering, Ludong University for first-principle calculations.

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