



A first principle research on optical properties of GaN nanowire surface adsorbed with Cs/NF₃

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ABSTRACT

In order to study optical properties of GaN nanowire photocathode surface adsorbed with Cs/NF₃, GaN nanowire surface models of adsorbing Cs/NF₃, 2Cs/NF₃, 3Cs/NF₃ and 4Cs/NF₃ were built respectively. And their band structure, dielectric function, complex refractive index, absorption coefficient, reflectivity and loss function were calculated based on first principle. The results show that band gap value of GaN nanowire surface adsorbed with 4Cs/NF₃ is lower than that of nanowire surface adsorbed with Cs/NF₃, 2Cs/NF₃ and 3Cs/NF₃. And with the number of adsorbing Cs atoms increases, conduction band and valence band both shift to low energy range. Absorption coefficient curves of GaN nanowire surface adsorbed with 3Cs/NF₃ and 4Cs/NF₃ appear new peaks, while maximum value of the absorption coefficient decreases. Moreover, in view of similarities and differences of GaN nanowire photocathodes and GaN thin film photocathodes after Cs/NF₃ activation, we researched optical properties of Cs/NF₃ adsorbed on GaN nanowire surface and GaN thin film surface. This work can further guide experiment of Cs/NF₃ adsorption on GaN nanowire surface, and it is of great significance to improve photoemission performance of GaN nanowire devices.

1. Introduction

GaN based III group nitride has been recognized as the best materials for developing high-temperature and high-power electronic devices due to its wide direct band gap (1.9–6.2eV), excellent physical and chemical stability, high saturated electron drift velocity, high breakdown field strength and high thermal conductivity [1]. It is also a new negative electron affinity semiconductor material that many researchers and engineers have been pursuing [2]. With gradual maturity and improvement of nanomaterial and nanotechnology, GaN nanowire materials are emerging, which shows a better photoemission performance than traditional GaN film materials [3]. For thin film materials, lattice mismatch could result in a high dislocation density, while GaN nanowire releases stress easily due to the small contact area [4,5], which greatly reduces internal defect density of nanowire and makes efficient and life of optoelectronic devices be higher and longer [6]. And GaN nanowire photocathode can solve contradiction about thickness of emission layer between photon absorption and electron transport in the photocathode of thin film materials. Adsorption of Cs/O on nanowire surface can lead to a decline in work function and be used as a useful technique for production of NEA photocathode [7]. Therefore, activation process plays an important role in improving the performance of GaN nanowire photocathode. The idea of replacing O with NF₃ is proposed during activation process because F has a strong electronegativity and photocathode activated with Cs/NF₃ are more stable and easier to obtain [8,9]. However, researches of GaN nanowire photocathode activated by Cs/NF₃ are still

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in the initial stage of exploration at present. Theoretical studies of electrical and optical properties of Cs/NF₃ activated on GaN thin film photocathodes have been conducted [10], but researches on GaN nanowire photocathodes activated by Cs/NF₃ only have electrical properties [11], there is no enough research data on optical properties of nanowires activated by Cs/NF₃. Therefore, it is very important for guiding the activation process of NEA GaN nanowire photocathode to research optical properties of [001]-oriented GaN nanowire surface adsorbed with Cs/NF₃ based on first principle calculations.

In this paper, optical properties of Cs/NF₃ adsorption system on [001]-oriented GaN nanowires surface are calculated, other three adsorption models of 2Cs/NF₃, 3Cs/NF₃ and 4Cs/NF₃ are also built. And effects of different Cs/NF₃ adsorption ratios on optical properties of nanowires are discussed, dielectric function, complex refractive index, absorption coefficient, reflectivity and loss function are analyzed. Meanwhile, in view of similarities and differences of GaN nanowire photocathodes and GaN thin film photocathodes after Cs/NF₃ activation, we researched optical properties of Cs/NF₃ adsorbed on GaN nanowire surface and GaN thin film surface.

2. Approach

The main existing form of the bulk GaN is wurtzite structure, which is interpenetrated by hexagonal close packing lattice of Ga and hexagonal close packed lattice of N each other. It belongs to the $P6_3mc$ (186)space group; symmetry is $C6v-4$, lattice constant is $a = b = 3.189 \text{ \AA}$, $c = 5.185 \text{ \AA}$ [11], and $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$. After optimization, the lattice parameters of GaN crystal are $a = b = 3.208 \text{ \AA}$, $c = 5.227 \text{ \AA}$ [12], set as lattice constant of GaN nanowire. In addition there are different growth directions during the preparation of GaN nanowire, in which [001]-oriented nanowire with hexagonal cross section is energetically more favorable than [100]- and [110]-oriented nanowire [13]. Therefore, GaN nanowire models with a hexagonal section and [001]-oriented growth direction are built. The models are obtained from $13 \times 13 \times 1$ wurtzite supercell by cutting the redundant atoms surrounding the nanowire, the diameter of the nanowire is $9.6 \text{ \AA}$. In order to avoid the influence of adjoining nanowires caused by periodicity during the calculation, $15 \text{ \AA}$ vacuum layer is set between adjoining nanowires, and to reduce complexity of the calculation, only Cs/NF₃ adsorption process on one side surface is discussed. There are six different adsorption sites on nanowire surface named as B_N(N bridge), B_{Ga}(Ga bridge), B_{Ga-N}(Ga-N bridge), T_N(N top), T_{Ga}(Ga top) and H (hollow) respectively and there are also three different NF₃ adsorption orientations on nanowire surface named NF₃-upward, NF₃-down and NF₃-transverse. The theory shows that adsorption energy is most stable when NF₃ is adsorbed on the B_{Ga-N} site of nanowire and orientation of NF₃ molecule inclines to upward, meanwhile NF₃ molecule should be adsorbed between Cs atoms and nanowire surfaces [10]. The models of GaN nanowire surface

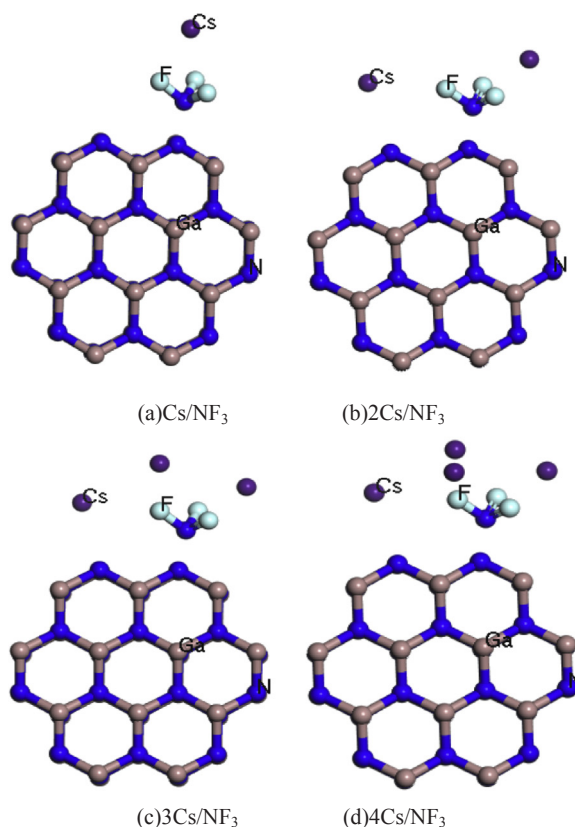


Fig. 1. GaN nanowire surface models (a)Cs/NF₃ adsorption model (b)2Cs/NF₃ adsorption model (c)3Cs/NF₃ adsorption model (d)4Cs/NF₃ adsorption model.

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