Structural enhancement mechanism of field emission from multilayer semiconductor films

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A self-consistent quantum model is developed to investigate the structural enhancement mechanism of field emission (FE) from multilayer semiconductor films. Compared with previous two-step FE mechanism, our self-consistent model is straightforward to understanding the whole tunneling process of the FE from multilayer semiconductor films. Calculated results show that FE characteristics can be remarkably improved only by structure modulation. The distinct structure effect of the FE characteristics mainly result from two reasons: one is the energy level shift and the other is effective surface barrier reduction due to accumulation of electrons in the occupied states. The present study offered new insights in structural effects for field emitters, which opened the possibility of carrying field emission research and application from an alternative approach.

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I. INTRODUCTION

Field emission (FE) materials have important applications in vacuum microelectronic devices[1] such as FE display and microwave amplifier, and hence become one of the hottest materials. However, the materials are still far from commercial utilization in devices.[2] It is because for conventional field emitters, such as metal or Si tip, preparation procedure is technologically untoward and high-cost; while for advanced FE materials, such as wide band-gap semiconductor (WBGS) films[3] or carbon nanotubes (CNTs),[4] device characteristics is not satisfactory. Generally speaking, either the FE current density available from WBGS films is not high enough and/or the operational voltage is not low enough;[2] as for CNTs, a too high FE current is unstable and may lead to a vacuum breakdown.[5]

In previous studies on FE, people mainly focused on exploiting emission characteristics of new materials by which increased emission ability could be expected. Recently, some studies began to improve the FE properties by using special emitter structures. In 1998, Geis *et al.*[6] firstly designed a metal-diamond-vacuum trijunction FE structure with diamond layer as the cathode. Resulting from an optimized FE process, the structure exhibited some of the lowest operational voltages achieved so far when applicable current densities were obtained. In 2000, Binh *et al.*[7] constructed a solid-state field-controlled emitter (SSE) structure, consisting of a WBGS layer on a metallic surface, and stable currents were obtained at room temperature in poor vacuum environment, and with the operational fields of 2–3 orders in magnitude less than for conventional field emission. In 2004, Semet *et al.*[8] first presented experimental measurements of electron emission from multilayer SSE cold cathodes, and the threshold field was 50 V/mm, with stable FE current densities up to 3×10^{-2} A/cm^2. The results mentioned above indicate that FE current densities can be increased evidently and operational fields can be decreased remarkably when an advisable structure of FE films is adopted. It suggests the possibility to improve FE properties by modulating the structures of FE emitters. However, to our knowledge, there have no systemically experimental or theoretical studies on the structure effects yet. To explain the enhancement of the advisable structure of FE films, only qualitative but not quantitive models were presented, i.e., Geis *et al.* proposed[6] that the lowest operational voltages originated from the electrons being accelerated to energies sufficient to be ejected into vacuum, and Binh *et al.*[7–9] suggested a serial two-step mechanism including space charge redistributing, for which the excellent FE characteristic resulted from the surface potential barrier depressed greatly by a large concentration of electrons near the emission surface. Obviously, a precise model based on quantum calculation was needed to unambiguously address the realistic mechanism, and furthermore to offer hints for further improvements of emitter properties.

In this paper, by performing self-consistent quantum FE calculations, we investigated the structural enhancement mechanism of FE from multilayer semiconductor films. Calculated results show that, field emission could be greatly enhanced with a quantum well (QW) formed in the multilayer film structures which on one hand, accumulated electrons by confine energy levels and on the other hand, lowered the effective surface potential. We show that by fine tuning factors which determined the potential shape the QW, i.e. structural parameters such as thickness of each film, the electron emission ability could be enhanced dramatically. Furthermore, we also computed the FE current densities when the surface barriers were artificially modulated and gave a theoretical proof that depressing the effective surface barrier also plays an important role on increasing FE current.

II. SELF-CONSISTENT BAND BENDING MODELS

In the previous two-step mechanism for the FE from multilayer semiconductor films,[8] in order to explain the change in the surface barrier, the FE process is considered to be divided forcibly into two steps. The first step is the electron resonant tunneling into near the surface layer, and the second step is an effective lowering of the surface barrier due to accumulated electrons. Here, we integrated the two FE

processes into a single structure effect quantitatively by a self-consistent quantum model. If considering the electrons incident from only one boundary, based on Tsu-Esaki formula,[10] the FE current from a semiconductor film can be written as

$$J = \frac{4\pi q m_t k_B T}{h^3} \int T(E_x) \ln[1 + e^{-(E_x - E_F)/k_B T}] dE_x$$
$$= J_0 \int J(E_x) dE_x = J_0 J_T, \tag{1}$$

where $J_0 = 4\pi q m_t k_B T/h^3$, which results in the electron supply, J_T is defined by the tunneling factor of the FE structure, q unit charge, m_t electron transverse mass, k_B is Boltzmann's constant, $E_x = P_x^2/2m$ normal energy, T is temperature, h is Planck's constant, and E_F is Fermi energy. To compute the FE current, the transmission coefficient $T(E_x)$ is the most important parameter, which can be calculated by the quantum transfer matrix (TM) method[11,12] based on analytical solution of Schrödinger equation with a linear potential, and the solution can be expressed as a linear combination of the Airy function or other wave functions. In this method, an arbitrary potential barrier can be divided into square segments which could be treated as linear barriers. Compared with the conventional Wentzel-Kramers-Brillioun (WKB) method or the Lippmann-Schwinger (LS) self-consistent equation,[7] the TM method is based on an accurate solution of the Schrödinger equation so the results are much closer to the realistic scenery of tunneling process during field emission. To compute $T(E_x)$ by TM methods, the FE structure must be provided with the stable potential distribution. Invalidity of the previous two-step FE mechanism in multilayer semiconductor films makes it impossible to investigate the FE process by quantum TM methods. So, here upon using self-consistent band bending model and integrating the two-step FE mechanism to the structural enhancement mechanism, the potential barrier of the FE structure will be stable when an external field applied. Then it becomes simple to investigate the structure effect for the controllable field emission from multilayer semiconductor films by the quantum TM method.

To compare with experimental results directly, we select the emitter structures in Ref. 8 (with band structure as plotted in Fig. 1) in our calculations. In our previous works, we developed a band bending model to compute the distribution of space charges in the FE structure with a single WBGS layer on metal or n-Si substrate.[13] But for two WBGS layers, additional interface effect between the two layers must be considered. As shown in Fig. 1, when a high field is applied, the distribution of space charges can be described by Poisson's equation in the GaN layer,

$$\frac{d^2\phi_1(x)}{dx^2} = \frac{e}{\varepsilon_1 \varepsilon_0} \rho_1(x). \tag{2}$$

Here $\phi_1(x)$ and $\rho_1(x)$ denote, respectively, the potential energy and the total volume charge density at the place with distance x from the GaN-vacuum interface, and ε_0 and ε_1 are the vacuum permittivity and the dielectric constant of GaN,

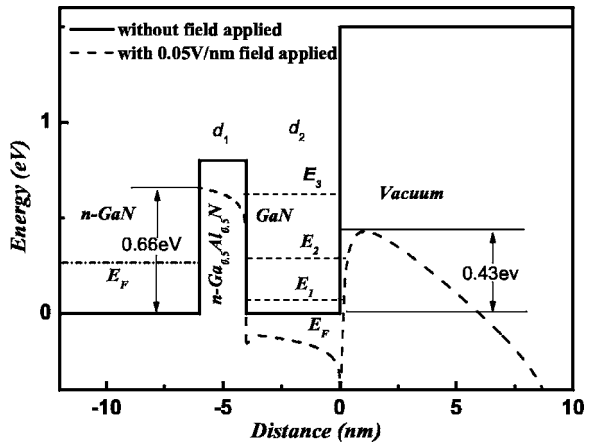

FIG. 1. Energy band diagram of the n-GaN/$Ga_{0.5}Al_{0.5}N$-GaN/vacuum FE structure, where solid curve is the case without field applied, and dash curve is the case with 0.05 V/nm field applied. Here n-GaN is substrate, $d_1 = 2$ nm and $d_2 = 4$ nm are, respectively, the layer thickness of $Ga_{0.5}Al_{0.5}N$-GaN and GaN, and the vacuum gap is 10 nm.

respectively. When a high field is applied, the distribution of space charge can also be described by Poisson's equation in the $Ga_{0.5}Al_{0.5}N$ layer

$$\frac{d^2\phi_2(x)}{dx^2} = \frac{e}{\varepsilon_2 \varepsilon_0} \rho_2(x). \tag{3}$$

Here $\phi_2(x)$ and $\rho_2(x)$ denote, respectively, the potential energy and the total volume charge density at distance x from the $Ga_{0.5}Al_{0.5}N$-GaN interface, and ε_2 is the dielectric constant of $Ga_{0.5}Al_{0.5}N$.

At the $Ga_{0.5}Al_{0.5}N$-GaN interface, the potential distribution is subject to the Gauss theorem and the following equation could be obtained

$$\varepsilon_1 \frac{d\phi_1(x)}{dx} = \varepsilon_2 \frac{d\phi_2(x)}{dx}. \tag{4}$$

In the GaN layer, one can obtain its potential distribution

$$\int_0^{-x_1} \frac{dx}{\delta} = \int_{\varphi_s}^{\varphi} \frac{d\varphi}{f(\varphi, \varphi_B)}, \tag{5}$$

where x_1 is distance from the GaN-vacuum interface, δ is known as the Debye screening length, and the function $f(\varphi_S, \varphi_B)$ is the same as defined previously,[14] where φ_S and φ_B are the parameters correlation with the potential energy at the GaN-vacuum interface.

In the $Ga_{0.5}Al_{0.5}N$ layer, the potential distribution can also be written as

$$\int_{-d_{\mathrm{GaN}}}^{-x_2} \frac{dx}{\delta} = \int_{\varphi_{s1}}^{\varphi} \frac{d\varphi}{f(\varphi, \varphi_G)}, \tag{6}$$

where x_2 is distance from the $Ga_{0.5}Al_{0.5}N$-GaN interface, d_{GaN} is the thickness of the GaN layer, $\varphi_G = (E_F - E_{Fi})/(k_B T)$, E_F and E_{Fi} are Fermi and quasi-Fermi energies of $Ga_{0.5}Al_{0.5}N$, respectively. $\varphi_{S1} = (\phi_{S1} - \phi_B)/(k_B T)$, φ_{S1} is the band bending at the $Ga_{0.5}Al_{0.5}N$-GaN interface ($x = -d_{\mathrm{GaN}}$).

The electric field E_S at the $Ga_{0.5}Al_{0.5}N$-GaN interface can also be obtained from

$$E_S = \frac{d\phi}{edx} = \frac{k_B T}{e\delta} \cdot \left. \frac{\delta d\varphi}{dx} \right|_{\varphi_S} = \frac{k_B T}{e\delta} \cdot f(\varphi_S, \varphi_B). \quad (7)$$

In the present model, it is supposed that the surface barrier depressing by electron accumulating occurs instantly when a field is applied to the FE structure. So the two WBGS layers can then be incorporated into a single layer by combining Eqs. (2)–(7), and the ultimate space charge distribution of the whole FE structure can be obtained.

To deal with the vacuum barrier, a more complicated and realistic image potential involving the image potential shifting[14] was introduced, and the potential barrier of the whole FE structure was calculated, as shown in Fig. 1, by the self-consistent method. In our calculations, the T is 300 K, which is a normal operation temperature, other parameters are the same as in our previous work.[14] So temperature effect could be neglected when operating at room temperature.

III. EVIDENCE OF ELECTRON ACCUMULATION IN QUANTUM WELL (QW)

To expound the experimental dual barrier mechanism for FE through two WBGS films, Semet *et al.*[8] thought that, unlike the one-layer FE structure, adoption of the two-layer structure induced the possibility for a fine control of the space charge value with the presence of subbands in the QW. That means the existence of the subbands increases the possibility of electron accumulation, which leads to a further reduction of the surface barrier. However, there was no plain evidence to show the physical process of electron tunneling in the dual-barrier model.[8] First, it is impossible to solve the steady local energy level for the unsteady electron accumulation in the two-step FE process; secondly, the values of the tunneling barrier and the quantum energy level cannot be determined distinctly in the dual-barrier model. In addition, this dual-barrier structure of field emission is related to a resonant tunneling diode (RTD), while in the present system, the "low bias" boundary of an RTD has been replaced by a vacuum with the effect of an image charge. There were a lot of theoretical and experimental investigations on RTD,[15,16] and the theory has become quite sophisticated. Early in 1987, Ando and iloh[17] used a matrix methods successfully calculated the energy levels of RTD. Here in this work, similar TM method is also used to compute the position of these energy levels in the field emission structure in this paper, hunting for the physics of the resonant FE structure.

Based on our self-consistent band bending model, as shown in Fig. 1, when a field of 0.05 V/nm is applied, the effective surface barrier calculated is 0.43 eV, in good agreement with experimentally measured data in the range of 0.25–0.53 eV.[8] It also corroborates the validity of our self-consistent band bending model.

Since the steady potential distribution of the FE structure has been constituted, the band structure characteristic of FE potential barrier can be presented by the calculated $T(E_x)$ with the electron incident energy. So it is easy to find the exact position of the energy levels in quantum, which can offer insights to understand the physics of the FE process. It is obvious in Fig. 2 that there are three distinct peaks when electrons tunnel through the dual-barrier potential well, indicating that three quantum energy levels localize in the FE structure when the electron incident energy is less than 0.8 eV. The results also show that the supposition that only two quantum states in the QM under zero field for the two-step FE mechanism[8] may not be appropriate. It can be seen clearly from Fig. 2 that there exists three distinct transmission peaks when zero filed is applied, and the positions of the transmission peaks keep almost unchanged in the fields less than 0.1 V/nm. However, they shift toward low energy sides, and even four peaks may appear with the field being further increased. Moreover, with increasement of the fields, the entire transmission increases by orders as shown in Fig. 2. This means that, consistent with experimental measurements, the calculated FE current will be even larger when the field is increased. The calculated results also show that the lowest quantum level for electron to accumulate lies above zero even at a field as high as 1 V/nm, which is in contrary with the conclusion in Ref. 8 that the level lies below zero, the reason may due to their simplified calculation procedure.

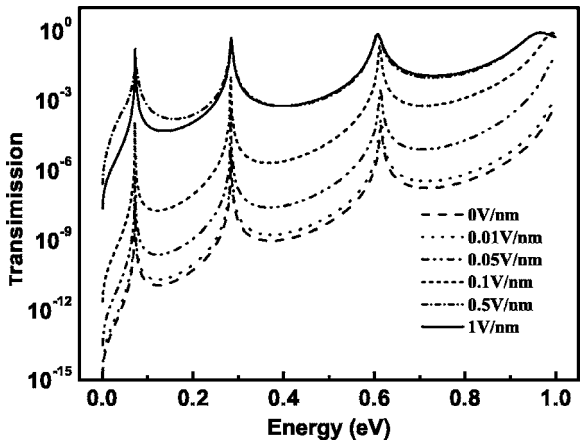

FIG. 2. Resonant transmission in the n-GaN/$Ga_{0.5}Al_{0.5}N$-GaN/vacuum structure with different fields applied (solid line: 0 V/nm; short dashed-dotted line: 0.01 V/nm; short dashed line: 0.05 V/nm; dashed-dotted-dotted line: 0.1 V/nm; dotted line: 0.5 V/nm; dashed line: 1 V/nm). Here d_1=2 nm and d_2=4 nm.

Since the quantum energy levels are self-consistently calculated as a result of electron accumulation, these levels should be the occupied states corresponding to the accumulation of electrons in the quantum well lower than the effective surface barrier. For example, at a field of 0.05 V/nm, the first barrier becomes 0.66 eV and the effective surface barrier is 0.43 eV. There exist two occupied states associated with the electron accumulation (see Fig. 1): E_1 at 0.071 eV and E_2 at 0.282 eV. They supply the ground of electron accumulation in the quantum well. The third energy level is at 0.617 eV above the effective surface barrier, from which the electrons will emit directly to vacuum by thermal field emission. Nevertheless, the third energy level may enhance the hot electron emission, which may lead to the emergence of resonant FE current. Of course, it is necessary to consider the temperature effect on the FE process. If the supposed 1%

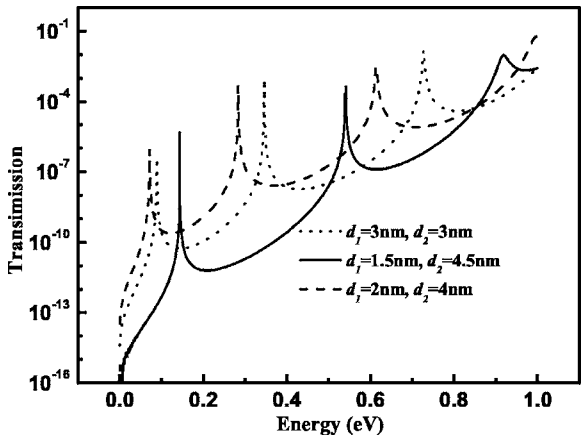

FIG. 3. Resonant transmission in three different n-GaN/$Ga_{0.5}Al_{0.5}N$-GaN/vacuum structures with the field of 0.05 V/nm applied. (dashed line: d_1=2 nm, d_2=4 nm; solid line: d_1=1.5 nm, d_2=4.5 nm; dotted line: d_1=3 nm, d_2=3 nm).

fluctuation of the effective barrier is 0.43 eV, then the scope of temperature for the validity of our calculations is about 300±50 K.

IV. STRUCTURE EFFECT FOR THE CONTROLLABLE FIELD EMISSION

To investigate the structure effect, it is necessary to compute electron tunneling transport in the FE structure, which affects the FE characteristic greatly. Figure 3 shows the calculated variation in the electron transmission for a 6 nm $Ga_{0.5}Al_{0.5}N$-GaN structure with the change in layer thickness proportion. Not only the magnitude of the transmission coefficients but also the positions of resonant tunneling peaks change tremendously when the individual layer thickness of the FE structure are altered. Comparing Fig. 2 with Fig. 3, it is easily found that the effect on the quantum energy level variation is more distinctly induced by the FE structure modulation than by increasing the field. It is well known that the quantum level can change the ground of the electron accumulation, which may lead to the effective surface barrier reduction. Seeing from Fig. 1, the effective surface barrier of the FE structure with 2 nm $Ga_{0.5}Al_{0.5}N$ and 4 nm GaN is 0.43 eV. Moreover, we also computed the effective surface barrier of the other two FE structures with a 0.05 V/nm field appiled, the effective barrier of 3 nm $Ga_{0.5}Al_{0.5}N$ and 3 nm GaN, is 0.446 eV, while the effective barrier of 1.5 nm $Ga_{0.5}Al_{0.5}N$ and 4.5 nm GaN is 0.501 eV. In addition, the experimental results also showed[6] that, with the effective surface barrier lowering, the FE current was increased by orders of magnitude and the threshold voltage was depressed enormously. It is suggested that the FE properties can be improved evidently by the structure modulated.

Figure 4 shows the calculated J-V curves of three different FE structures, where both the vacuum gap and the total thickness of the $Ga_{0.5}Al_{0.5}N$-GaN films are kept at the same values (10 nm and 6 nm, respectively). It can be seen clearly that an adjustment of the proportion of the film thickness can result in a variation in the FE current as large as 10^3! One

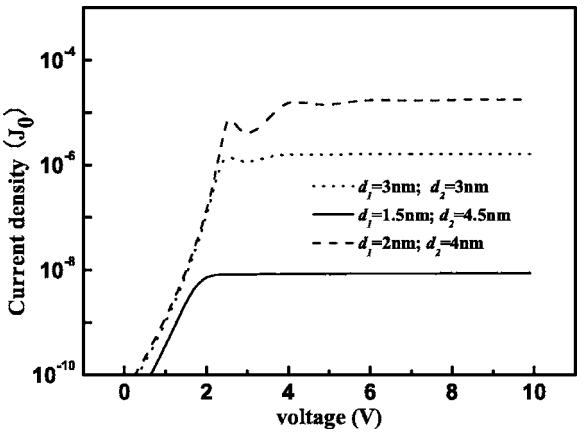

FIG. 4. FE current in three different n-GaN/$Ga_{0.5}Al_{0.5}N$-GaN/vacuum structures. (dashed line: d_1=2 nm, d_2=4 nm; solid line: d_1=1.5 nm, d_2=4.5 nm; dotted line: d_1=3 nm, d_2=3 nm).

may also see that up to 2.2 V, the FE current increases exponentially with increasing the voltage according to the F-N rule, which agrees well with the experimental results[8] in the range of $5\times10^5-1\times10^6$ V/cm. However, when the voltage is higher than 2.2 V, i.e., about 2.0×10^6 V/cm, the FE current keeps at an almost invariable value and there appear the resonant peaks, which is conceptually close to resonantly-enhanced field emission. Similar theoretical results were also reported for an emitter accumulation layer,[18–21] and experimental results were observed for FE from a cathode with DLC coating,[21,22] where the emergence of the resonant current peaks might be due to the subband occurring in the QW.

Why does the FE current change slightly in the high field intensity? It is obvious in Eq. (1) that the capability of drawing out electrons from the n-GaN substrate is limited for a certain FE structure. Figure 5 shows that, for applied voltages 2.2, 4.5, and 9 V, the transmission coefficients do not change significantly, the position of the quantum level remains almost unchanged, and the tunneling factor of the FE structure, J_T, probably reaches its maximum. Therefore, it is easy to understand the little variation in FE current at high voltages in Fig. 4.

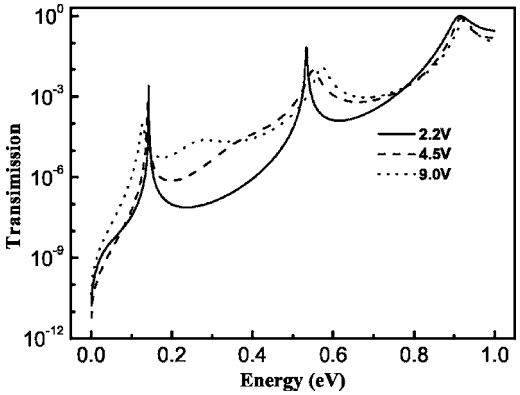

FIG. 5. Resonant transmission in the n-GaN/$Ga_{0.5}Al_{0.5}N$-GaN/vacuum structure with different voltages applied. (Solid line: 2.2 V; dashed line 4.5 V; dotted line: 9 V.) Here d_1=3 nm, d_2=3 nm, and the vacuum gap is 10 nm.

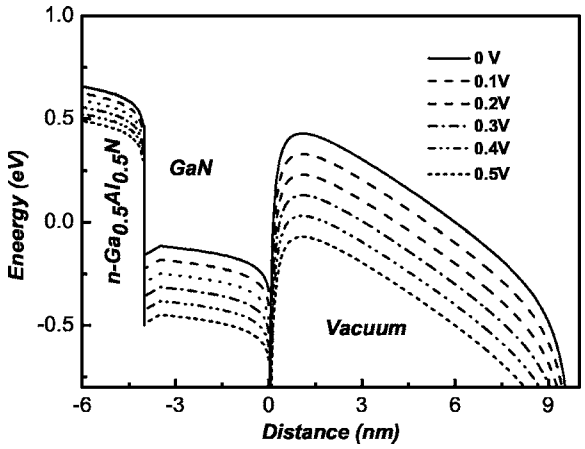

FIG. 6. Energy band diagram of the $Ga_{0.5}Al_{0.5}N$-GaN/vacuum FE structure when different bias voltage are applied between the n-GaN and the surface of the GaN. (Solid line: 0 V; dashed line: 0.1 V; dotted line: 0.2 V; dashed dotted line: 0.3 V; dashed dotted dotted line: 0.4 V; short dashed line: 0.5 V.) Here n-GaN is the substrate, $d_1=2$ nm and $d_2=4$ nm, and the vacuum gap is 10 nm, with a 0.1 V/nm field applied.

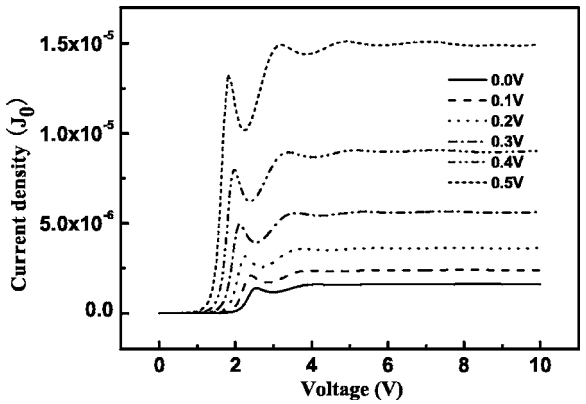

FIG. 7. FE current in the n-GaN/$Ga_{0.5}Al_{0.5}N$-GaN/vacuum structure with different biases applied to the $Ga_{0.5}Al_{0.5}N$-GaN. (Solid line: 0 V; dashed line: 0.1 V; dotted line: 0.2 V; dashed-dotted line: 0.3 V; dashed-dotted-dotted line: 0.4 V; short dashed line: 0.5 V.) Here $d_1=2$ nm and $d_2=4$ nm.

When the FE structure is made up of 3 nm GaN and 3 nm $Ga_{0.5}Al_{0.5}N$ films, in Fig. 4, the FE current only has a single resonant peak. When its structure is modulated to 2 nm $Ga_{0.5}Al_{0.5}N$ and 4 nm GaN, the FE current is evidently increased with two distinct resonant peaks. However, when the FE structure is constituted by 1.5 nm $Ga_{0.5}Al_{0.5}N$ and 4.5 nm GaN films, it is surprised to find that the FE current is remarkably decreased without any resonant peaks; moreover, the threshold voltage is increased. Engineering the order of 1 nm layers on the surface of a semiconductor is a very difficult problem; therefore, we do not further consider the FE structure of 1 nm $Ga_{0.5}Al_{0.5}N$-GaN and 5 nm GaN films.

It can be found from Eq. (1) that the remarkable structure effect of FE from the two semiconductor films should originate from the tunneling factor of the FE structure, J_T. By comparing the band structures of the three FE configurations, it can be approved clearly in Fig. 3 that there are deeper quantum levels in the quantum well for having the larger FE currents of the FE structure, and the deeper energy levels lead to the lower effective surface barriers, which will improve greatly the FE characteristic. Considering the total thickness of the FE structure is 6 nm, made up of 3 nm GaN and 3 nm $Ga_{0.5}Al_{0.5}N$ films, if the thickness of the $Ga_{0.5}Al_{0.5}N$ film varies from 3 nm to 0 nm or 6 nm, the FE structure changes from two-layer SSE to single-layer SSE (GaN or $Ga_{0.5}Al_{0.5}N$); but the experimental results show clearly that there is a better FE characteristic for two-layer SSE than single-layer SSE. Obviously, there exists an optimized structure from which the most excellent FE characteristics can be obtained, which is validated by our calculated results.

V. ACTUAL EFFECT ON FIELD EMISSION PROCESS OF THE EFFECTIVE SURFACE BARRIER

From the above calculated results and the previous experimental observations,[6–9] it is revealed that the effective surface barrier is a key factor to advance the FE character. To see the actual effect on field emission process of the effective surface barrier, a bias is applied between the n-GaN and the surface of the GaN, which can suppress forcibly the surface barrier. With a 0.1 V/nm field applied, seeing energy band of the $Ga_{0.5}Al_{0.5}N$-GaN/vacuum when different bias voltage added in Fig. 6, it is obvious that the surface barrier is evidently debased by the increased bias. So in Fig. 7, we calculate the FE properties with the change of the bias by the self-consistent band bending model. It can be seen clearly that the FE characteristic is greatly improved with increasing bias. The results show that, upon the application of only a 0.5 V bias on $Ga_{0.5}Al_{0.5}N$-GaN, the magnitude of the FE current is enhanced by about 10 times and the threshold voltage is decreased distinctly. The results supply a feasible scheme from the FE materials to the actual device. It also approves that depressing the effective surface barrier may be an important technical method to improve the FE characteristics. However, one may see from Fig. 5 that the shapes of the resonant FE current peaks are similar when different external voltages are added. It means that the external voltage only changes the effective surface barrier but does not affect the quantum levels.

VI. CONCLUSIONS

Based on the quantum self-consistent consideration, we present a quantitative model to investigate the structural enhancement mechanism of field emission from multilayer semiconductor films. The present results show that it is possible to evidently improve the FE characteristics by only the structure modulation. It may be a new key for FE research and application, with simple processes but huge gains, far beyond exploring or amending new materials to elevate the FE characteristics.

The structure effect on improving the FE characteristics is mainly due to two possibilities: the change in the band structure and the reduction of the effective surface barrier. The

detailed band structure is calculated by self-consistent quantum model. It gives a direct evidence of electron accumulation in QW which leads to the effective surface barrier reduction. Moreover, there is a clearer understanding of the physical process in the field emission from multilayer thin films by integrating the two-step mechanism to the self-consistent band structure model. The calculations of band structure also offered a more accurate scenario of energy levels in the quantum well. By compulsively depressing the surface barrier by additional bias applied to the FE structure, it is found that the FE characteristic can be greatly improved due to a lower effective surface barrier.

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