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Research Article

Temperature Dependence of the Energy Band Diagram of AlGaN/GaN Heterostructure

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Temperature dependence of the energy band diagram of AlGaN/GaN heterostructure was investigated by theoretical calculation and experiment. Through solving Schrodinger and Poisson equations self-consistently by using the Silvaco Atlas software, the energy band diagram with varying temperature was calculated. The results indicate that the conduction band offset of AlGaN/GaN heterostructure decreases with increasing temperature in the range of 7 K to 200 K, which means that the depth of quantum well at AlGaN/GaN interface becomes shallower and the confinement of that on two-dimensional electron gas reduces. The theoretical calculation results are verified by the investigation of temperature dependent photoluminescence of AlGaN/GaN heterostructure. This work provides important theoretical and experimental basis for the performance degradation of AlGaN/GaN HEMT with increasing temperature.

1. Introduction

AlGaN/GaN high electron mobility transistor (HEMT) has attracted great interest for high temperature, high frequency, and high power applications due to its intrinsic material advantages, such as wide band gap, high breakdown electric field, high electron saturation velocity, and high two-dimensional electron gas (2DEG) concentration [1–3]. Although the performance of AlGaN/GaN HEMT has made remarkable progress [4–7], the reliability, especially at high temperature, has been and remains a major constraint in realizing the true potentials of such devices [8–10]. Improvements of reliability require a better understanding of the degradation mechanism. The performance degradation of AlGaN/GaN HEMTs with increasing temperature can be largely attributed to the effect of temperature on 2DEG transport properties [10–12]. The intrinsic physical reason for that is the energy band diagram of AlGaN/GaN heterostructure varies with temperature, which should be fully investigated. However, there have been few reports on the temperature dependence of the energy band structure of AlGaN/GaN heterostructures until now. Wang et al. [13] calculated the energy band diagram of AlGaN/GaN heterostructure at room temperature, 250°C and 500°C, just to explain that the 2DEG density decreases with increasing temperature. But there is not detailed analysis and discussion. In this work, the temperature dependence of the energy band structure of AlGaN/GaN heterostructure was investigated by theoretical calculation and experimental verification.

2. Theoretical Calculation

The AlGaN/GaN heterostructure used in this study consists of a 2 μm thick GaN buffer layer and a 25 nm thick AlGaN barrier layer, as shown in Figure 1. The Al composition of the AlGaN layer is 0.3. The n-type doping level in both GaN and AlGaN layers is set to be $1 \times 10^{16}\ \mathrm{cm}^{-3}$, to keep consistent with the level for unintentionally doped samples

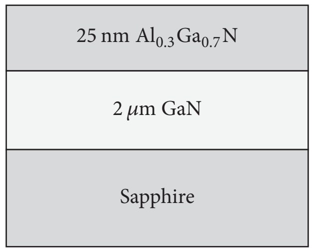

Figure 1: Schematic of AlGaN/GaN heterostructure.

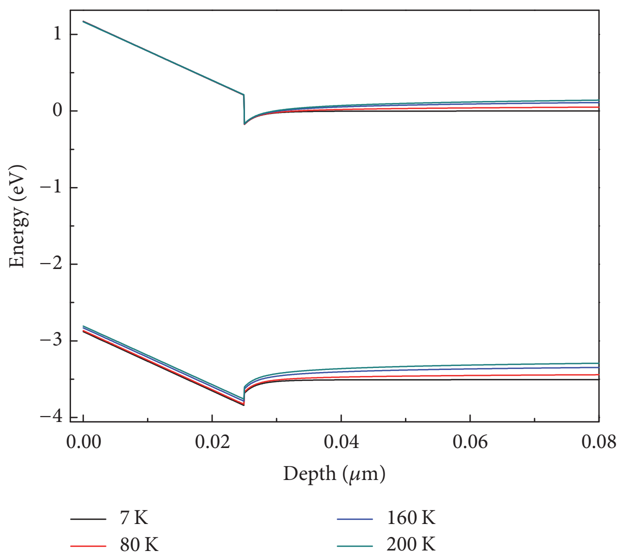

Figure 2: The energy band diagrams of AlGaN/GaN heterostructure at different temperature.

in experiment. Considering the screening effect caused by defects, the polarization charge densities are assumed to be 40% of the calculated values [14].

Through solving the Schrodinger and Poisson equations self-consistently by using the Silvaco Atlas software [15], the temperature dependent energy band diagram of AlGaN/GaN heterostructure can be calculated. The calculation results with temperature lower than 200 K are shown in Figure 2. It can be seen that the conduction and valence band energies of both GaN and AlGaN layers increase with increasing temperature, especially in the GaN layer. Compared with the conduction band, the valence band shows larger shift with varying temperature. So, the energy band gaps of GaN and AlGaN layers decrease with increasing temperature. This is consistent with temperature dependent band gap shrinkage effect [16, 17].

Besides the energy band gaps, the conduction band offset of AlGaN/GaN heterostructure also changes with temperature. The conduction band profile near the AlGaN/GaN interface with varying temperature is shown in Figure 3. It can be seen that the conduction band offset between AlGaN and GaN layers decreases with increasing temperature, which means that the depth of the quantum well at AlGaN/GaN interface becomes shallower and the confinement of that

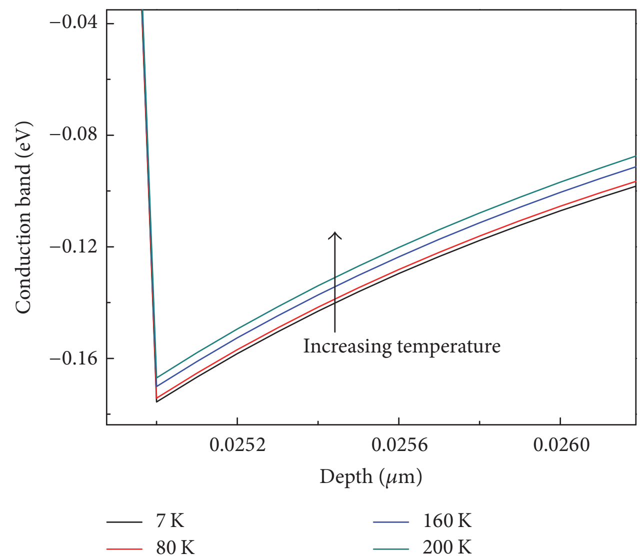

Figure 3: The conduction band profile of the AlGaN/GaN interface for different temperature.

on 2DEG reduces. In addition, the 2DEG concentration in unintentionally doped AlGaN/GaN heterostructures shows a direct proportional relationship to the conduction band offset, according to the following equation [13]:

$$n_s(x) = \frac{\sigma(x)}{e} - \left(\frac{\varepsilon_0 \varepsilon(x)}{d_{\mathrm{AlGaN}} e^2}\right)\left[e\phi_b(x) + E_F(x) - \Delta E_c(x)\right], \tag{1}$$

where $\sigma(x)$ is the polarization-induced bound charge, $\varepsilon(x)$ is the relative dielectric constant of AlGaN, d_{AlGaN} is the thickness of the $Al_xGa_{1-x}N$ barrier layer, $e\phi_b(x)$ is the Schottky barrier of the gate contact on top of AlGaN, $E_F(x)$ is the Fermi level with respect to the GaN conduction-band-edge energy, and $\Delta E_c(x)$ is the conduction band offset at AlGaN/GaN interface. So, the 2DEG concentration decreases with increasing temperature due to the reduction of the conduction band offset ΔE_c. The same temperature dependence of the 2DEG concentration has been measured by Khan et al. [18]. Therefore, the performance of AlGaN/GaN HEMT will degrade with increasing temperature [19]. The detailed temperature dependence of the energy band gaps and conduction band offset in AlGaN/GaN heterostructure is shown in Figure 4.

3. Experimental Verification

In order to verify the theoretical calculation, we investigated temperature dependent photoluminescence (PL) of AlGaN/GaN heterostructure, which can directly reflect the energy band structure of the measured samples. In this work, PL measurements were performed on the $Al_{0.3}Ga_{0.7}N$/GaN heterostructure between 7 K and 200 K. The light source was a He-Cd laser with a wavelength of 325 nm.

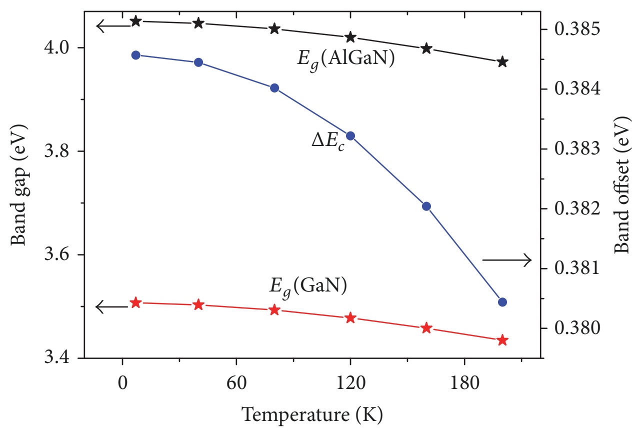

Figure 4: Temperature dependence of the energy band gaps of AlGaN and GaN and the conduction band offset of AlGaN/GaN heterostructure.

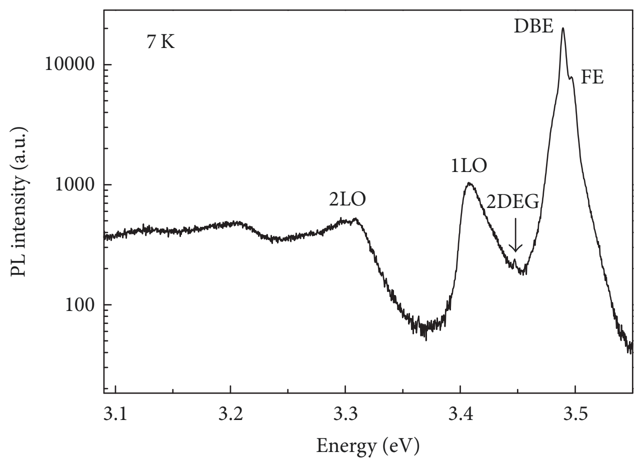

Figure 5: PL spectrum of AlGaN/GaN heterostructure at 7 K.

Figure 5 shows the PL spectrum of the AlGaN/GaN heterostructure at 7 K. The free exciton (FE) and donor bound exciton (DBE) emissions in GaN are located at 3.498 eV and 3.489 eV, respectively, and are much stronger than other peaks. These two emissions are near-band-edge emissions, which can directly reflect the band gap of corresponding material. The broad peaks at 3.408 eV and 3.309 eV are attributed to the one and two longitudinal optical (LO) phonon replicas of the GaN FE emission, respectively. The weak peak at 3.448 eV is attributed to recombination between 2DEG and photoexcited holes. Due to the strong built-in internal electric field near AlGaN/GaN heterointerface, the photoexcited holes diffuse rapidly into the flat-band region of GaN. Therefore, the probability of recombination between 2DEG and photoexcited holes is low and its intensity is very weak.

Figure 6 shows the PL spectra of AlGaN/GaN heterostructure with varying temperature in the range of 7 K to 160 K. The inset shows the PL spectrum at 200 K. It can be seen from Figure 6 that the GaN FE and DBE emissions exhibit obvious red shift with increasing temperature, indicating the reduction of the band gap of GaN layer. This is consistent with the result of theoretical calculation. The intensity of the 2DEG PL peak is very weak and decreases with increasing temperature. As shown in the inset of Figure 6, this peak disappears when the temperature reaches 200 K. Different from the GaN FE and DBE peaks, the 2DEG PL peak shows unobvious shift with increasing temperature. It demonstrates that the energy separation between the ground state of 2DEG and the valence band of flat-band region in GaN layer does not change obviously with varying temperature in the range of 7 K to 200 K. Additionally, the energy separation between GaN FE and 2DEG PL peak gradually decreases with increasing temperature, which indicates the depth of quantum well at AlGaN/GaN interface becomes shallower. Therefore, the confinement of the interface quantum well on 2DEG decreases with increasing temperature. It is also consistent with the theoretical calculation results.

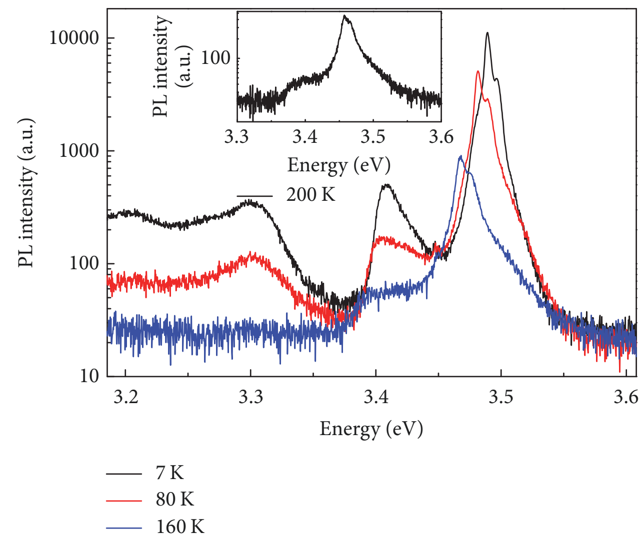

Figure 6: PL spectra of AlGaN/GaN heterostructure in the temperature range of 7 K to 160 K. The inset shows the PL spectrum of AlGaN/GaN heterostructure at 200 K.

4. Conclusions

In summary, temperature dependence of the energy band diagram of AlGaN/GaN heterostructure was investigated. Through theoretical calculation and experiment verification, it is confirmed that the band gaps of both AlGaN and GaN layers and the conduction band offset of AlGaN/GaN heterostructure decrease with increasing temperature in the range of 7 K to 200 K. So the depth of quantum well at AlGaN/GaN interface becomes shallower and the confinement of that on 2DEG reduces. This work provides important theoretical and experimental basis for the performance degradation of AlGaN/GaN HEMT with increasing temperature.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

Acknowledgments

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