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Effects of a cap layer on built-in electric fields of $Al_xGa_{1-x}N$/GaN heterostructures non-destructively probed by Franz-Keldysh oscillations

H. Takeuchi[1,a], Y. Yamamoto[1], Y. Kamo[1], T. Oku[1], and M. Nakayama[2]

[1] R & D Department, High Frequency and Optical Device Works, Mitsubishi Electric Corporation, 4-1 Mizuhara, Itami, Hyogo 664-8641, Japan
[2] Department of Applied Physics, Graduate School of Engineering, Osaka City University, 3-3-138 Sugimoto, Sumiyoshi-ku, Osaka 558-8585, Japan

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Abstract. We have investigated electric field strengths in the $Al_xGa_{1-x}N$ layer, F_{AlGaN}'s, of $Al_xGa_{1-x}N$/GaN heterostructures with and without a GaN cap layer using photoreflectance (PR) spectroscopy. Franz-Keldysh oscillations (FKOs) from the $Al_xGa_{1-x}N$ layer are clearly observed in the PR spectra. It is found from analysis of the FKOs that stacking of the cap layer causes a remarkable enhancement of F_{AlGaN}. This fact demonstrates that the FKO profile is a non-destructive probe for a change of built-in electric field strength induced by a cap layer. Numerical calculations of F_{AlGaN} based on a Schrödinger-Poisson equation clarify that the magnitude of the enhancement of F_{AlGaN} is dominated by the cap-layer thickness.

PACS. 78.40.Fy Semiconductors – 78.67.Pt Multilayers; superlattices – 77.65.-j Piezoelectricity and electromechanical effects

1 Introduction

Group III-nitride heterostructures are featured by the fact that piezoelectric polarization and spontaneous polarization originating from the wurtzite crystal structure [1,2] considerably influence electronic and optical properties, which is also utilized in device applications. In clarifying physical properties of III-nitride heterostructures, it is, therefore, necessary to characterize the heterostructures in advance taking account of the polarization effects. Furthermore, the above-mentioned characterization is useful to optimize the heterostructures used for electronic and optical devices. Recently, electronic characteristics of $Al_xGa_{1-x}N$/GaN-based high-electron-mobility transistors [3] have been improved by the incorporation of an n-type GaN (n-GaN) cap layer, which stabilizes the interface of the $Al_xGa_{1-x}N$ Schottky layer and improves pulsed current-voltage characteristics [4]. In III-nitride heterostructures, stacking of a given layer produces polarization charges, which results in changes of built-in electric fields and potentials. In fact, using photocurrent measurement, Yu et al. [5] found that the cap layer enlarges the effective Schottky barrier height. The assessment with use of the photocurrent measurement, however, lacks versatility owing to the problem that destructive processes such as evaporation of metal for electrodes are essential to measure photocurrent. In contrast, photoreflectance (PR) spectroscopy, which is contactless in principle, can non-destructively probe an electric field through the analysis of Franz-Keldysh oscillations (FKOs) [6,7]. Consequently, PR characteristics of the III-nitride heterostructures have been intensively studied so far. Actually, several groups performed measurements of the FKOs from the III-nitride heterostructures [8–11], whereas the earlier works overlooked the important information on the PR characteristics related to the electric-field changes induced by the incorporation of a cap layer. Previous studies of electroreflectance (ER) spectroscopy [12,13], which is similar to PR spectroscopy in the modulation mechanism of reflectance, also did not take account of the point described above. These situations in the research field of III-nitride heterostructures indicate that the detailed analysis of FKOs observed by PR spectroscopy is still essential in semiconductor physics.

In the present paper, we report on the effects of a cap layer on PR characteristics of $Al_xGa_{1-x}N$/GaN heterostructures and demonstrate that PR measurements can quantitatively diagnose changes of electric field strengths induced by stacking of a cap layer in III-nitride

[a] e-mail: Takeuchi.Hideo@db.MitsubishiElectric.co.jp

heterostructures. We have examined both $Al_xGa_{1-x}N$/GaN heterostructures with an n-GaN cap layer and an $Al_xGa_{1-x}N$/GaN heterostructure without the cap layer. The PR spectra of the samples show that the cap layer lengthens the period of the FKOs from the $Al_xGa_{1-x}N$ layer, which indicates that the electric field strength in the $Al_xGa_{1-x}N$ layer, F_{AlGaN}, is enhanced by the presence of the cap layer. The samples are also characterized by X-ray diffraction (XRD) measurements in order to estimate the Al composition. The enhancement of F_{AlGaN} induced by the cap layer is compared with a change of F_{AlGaN} caused by a difference in Al composition. We elucidate the relation between F_{AlGaN} and the structure parameters such as the thickness and doping density of the cap layer with use of numerical calculations based on a Schrödinger-Poisson equation.

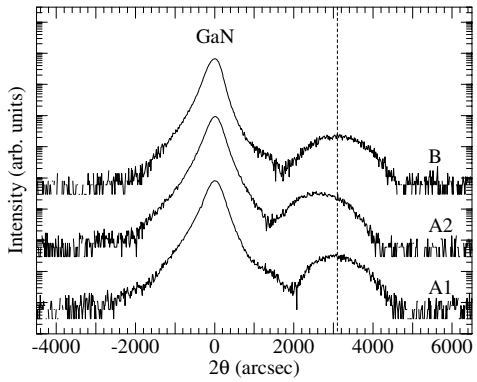

Fig. 1. XRD patterns of samples A1, A2, and B around the Bragg angle of the GaN-(0004) reflection. Position of the dashed line: calculated Bragg angle of the $Al_{0.2}Ga_{0.8}N$-(0004) reflection.

2 Samples and experimental procedures

Three samples of $Al_xGa_{1-x}N$/GaN heterostructures, A1 and A2 with an n-GaN cap layer and B without an n-GaN cap layer, were grown on Si-face semi-insulating 4H-SiC substrates by metal organic vapor phase epitaxy. Samples A1 and A2 are designed as follows from the top: an n-GaN (thickness of 5 nm, doping density of 5.0×10^{17} cm^{-3}) cap layer, an undoped $Al_{0.2}Ga_{0.8}N$ (27 nm) layer, an undoped GaN (2.2 μm) buffer layer, and an AlN layer. Sample B has the same structure mentioned above except for the lack of the cap layer. All the PR measurements were performed at room temperature. The probe beam illuminating the epitaxial layers was monochromatic light with a spectral width of 1.2 nm. The power density was wavelength-dependent: from 5 to 15 μW/cm^2. The pump beam with a wavelength of 262 nm and an average power density of 4.0 mW/cm^2 was provided from a diode-pumped Q-switched laser at a repetition rate of 1 kHz. The reflectance component R and modulated reflectance component ΔR were recorded by a dc voltmeter and a lock-in amplifier, respectively.

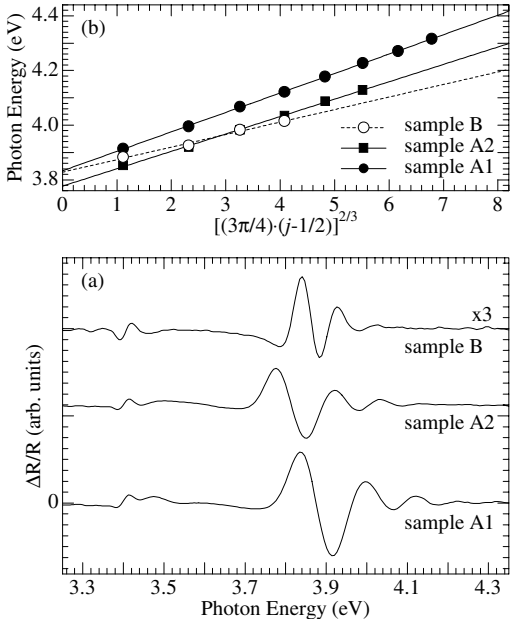

Fig. 2. (a) PR spectra of samples A1, A2, and B at room temperature. (b) Positions of the extrema in the FKOs plotted according to equation (1). Lines: fitting results. Symbols: measured data.

3 Results and discussion

At first, we evaluate the Al composition of the $Al_xGa_{1-x}N$ layer for each sample using the XRD method because it influences F_{AlGaN} through the piezoelectric polarization produced by the lattice mismatch [1,2]. Figure 1 shows the θ-2θ XRD patterns around the Bragg angle of the GaN-(0004) reflection for the CuKα_1 line. The side peaks around 3000 arcsec are assigned to the (0004) reflection of $Al_xGa_{1-x}N$. The position of the dashed line corresponds to the calculated Bragg angle of the $Al_{0.2}Ga_{0.8}N$-(0004) reflection on the assumption of the pseudomorphic growth of the $Al_{0.2}Ga_{0.8}N$ layer on the GaN layer. The elastic and lattice constants used were cited from reference [14]. As shown in Figure 1, the $Al_xGa_{1-x}N$-reflection-peak angles of samples A1 and B agree with the calculated Bragg angle. In contrast, the $Al_xGa_{1-x}N$-reflection peak of sample A2 is shifted to the low angle side by 360 arcsec, so that the Al composition is estimated to be 0.18.

Next, we focus on how the presence of the cap layer affects the PR spectra shown in Figure 2a. The characteristic signals at the photon energy of 3.42 eV are attributed to the PR signals from the GaN layers because the fundamental exciton-transition energy of GaN is 3.414 eV [14]. Consequently, the oscillations starting from 3.72 eV are assigned to the FKOs from the $Al_xGa_{1-x}N$ layer. The effect of the cap layer appears in the period of the FKOs; namely, the FKO periods of samples A1 and A2 are much longer than that of sample B. We also note that the initial energy of the FKOs is shifted to the low energy side

in sample A2, which is explained by the relatively low Al composition characterized by the XRD patterns.

In order to quantify the effect of the cap layer, we estimate F_{AlGaN} using the following relation between the position of the extremum in the FKOs, $\hbar\omega_j$, and its index j [15]:

$$\hbar\omega_j = \hbar\Theta\left[(3\pi/4)\,(j-\varphi/\pi)\right]^{2/3} + E_0. \qquad (1)$$

Here, E_0 is the critical point energy and $\hbar\Theta$ given by $(e^2\hbar^2 F_{\mathrm{AlGaN}}^2/2\mu)^{1/3}$ is the electro-optic energy determining the FKO period. The interband reduced mass μ in $Al_xGa_{1-x}N$ can be regarded as the reduced mass for the transition from the A-valence band to the conduction band because it is the lowest-energy optical transition [16]. The values of μ used are 0.189 for sample A2 and 0.191 for samples A1 and B in free electron-mass units [14]. The phase factor φ is usually given by $\pi/2$ in a bulk crystal [15]. We reported that the interference effect peculiar to a layered structure works on φ [17]; however, in the present samples, the interference effect is negligible owing to the thin cap layer. According to equation (1), the positions of the extrema in the FKOs are plotted and fitted in Figure 2b. The values of F_{AlGaN} are estimated to be 424, 357, and 219 kV/cm for samples A1, A2, and B, respectively. Even in sample A2, the Al composition of which is lower than that of sample B, F_{AlGaN} is larger than F_{AlGaN} in sample B. This fact means that the enhancement of F_{AlGaN} induced by the cap layer exceeds the reduction caused by the decrease in the Al composition. Thus, it is proved that the presence of the cap layer leads to the enhancement of F_{AlGaN}.

Finally, we clarify the relation between F_{AlGaN} and the physical parameters (thickness and doping density) of the cap layer by numerically calculating the Schrödinger-Poisson equation [18]. Here, we deal with the quantities at equilibrium corresponding to absence of the illumination of light. The equilibrium electric field is different from the electric field estimated from the FKOs because the latter is considerably reduced by the photovoltaic effect resulting from the light illumination [17,19]. We could not include the photovoltaic effect in the present calculation since the surface recombination velocities of GaN and $Al_xGa_{1-x}N$, which affect the photovoltaic effect [17], have not been systematically studied.

Figure 3a shows the Fermi energy (dashed line) and conduction-band potential energy (solid curve) as a function of distance from the surface calculated for the n-GaN (5 nm, 5.0×10^{17} cm^{-3})/$Al_{0.2}Ga_{0.8}N$ (27 nm)/GaN (500 nm) heterostructure. The polarization charges were modeled as fixed sheet charges, which is usually used as a model for calculations of electronic properties of $Al_xGa_{1-x}N$/GaN heterostructures [20,21]. The parameters employed are as follows: the band-gap energy of $Al_xGa_{1-x}N$ at room temperature given by $E_g(x) = 6.2x + 3.4(1-x) - 1.0x(1-x)$ (eV), conduction-band-offset energy of $\Delta E_c = 0.7[E_g(x) - E_g(0)]$, dielectric constant of $\epsilon(x) = 8.9 - 0.4x$, surface Fermi level of GaN $\phi_s = 0.95$ eV [21], and polarization charge density at the n-GaN/$Al_{0.2}Ga_{0.8}N$ ($Al_{0.2}Ga_{0.8}N$/GaN) interface of

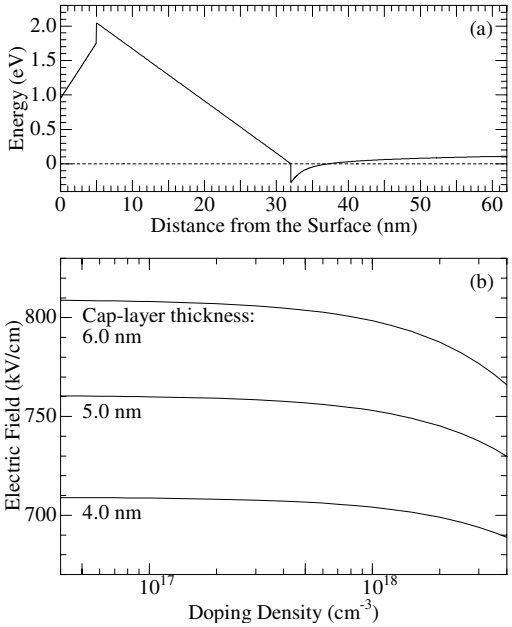

Fig. 3. (a) Fermi energy (dashed line) and conduction-band potential energy (solid curve) as a function of distance from the surface calculated for the n-GaN (5 nm, 5.0×10^{17} cm^{-3})/$Al_{0.2}Ga_{0.8}N$ (27 nm)/GaN (500 nm) heterostructure. (b) F_{AlGaN} as a function of cap-layer doping density calculated at the cap-layer thicknesses of 4.0, 5.0, and 6.0 nm.

$\sigma_p^{-(+)} = -(+)1.79$ μC/cm^2 [1]. As shown in Figure 3a, the n-GaN cap layer has a potential slope rising toward the $Al_{0.2}Ga_{0.8}N$ layer, which reflects the inherent polarization. The product of the slope and cap-layer thickness corresponds to enhancement of the effective Schottky barrier height given by the potential-energy difference between the $Al_{0.2}Ga_{0.8}N$ conduction band and Fermi level at the n-GaN/$Al_{0.2}Ga_{0.8}N$ interface. The potential of the $Al_{0.2}Ga_{0.8}N$ layer shows a linear dependence on the distance; therefore, F_{AlGaN} is position-independent. The values of F_{AlGaN} calculated at various cap-layer thicknesses are plotted in Figure 3b as a function of doping density of the cap layer. It is obvious that F_{AlGaN} is sensitive to the cap-layer thickness. This is because the effective Schottky barrier height depends on the cap-layer thickness as mentioned above. In contrast, F_{AlGaN} hardly depends on the doping density lower than 10^{18} cm^{-3}, which is due to the relatively high polarization charge density. To put it concretely, the ionized donor density of 5.0×10^{17} cm^{-3} in the 5-nm-thick cap layer corresponds to the sheet charge density of 4.0×10^{-2} μC/cm^2, which is much lower than $|\sigma_p^{-(+)}|$. Since the cap-layer-thickness dependence of F_{AlGaN} results from the polarization, it is concluded that the polarization effects can overcome the doping effect.

We also discuss consistency between the present calculation and PR characterization on the enhancement of F_{AlGaN} induced by the cap layer. It is reasonable to assume that the photovoltaic effect is in the almost same magnitude between samples A1 and B because the cap

layer is thin and the photovoltaic effect is mainly determined only by the $Al_{0.2}Ga_{0.8}N$ and GaN buffer layers. We, therefore, focus on the difference in F_{AlGaN} between the samples with and without the cap layer, instead of comparing the absolute values. We calculated F_{AlGaN} for the $Al_{0.2}Ga_{0.8}N$ (27 nm)/GaN (500 nm) heterostructure. In the calculation, the value of ϕ_s employed for $Al_{0.2}Ga_{0.8}N$ is 1.42 eV [21]. The value of F_{AlGaN} calculated for the $Al_{0.2}Ga_{0.8}N$ (27 nm)/GaN (500 nm) heterostructure is 535 kV/cm, which is smaller by 222 kV/cm than the value for the n-GaN (5 nm, 5.0×10^{17} cm^{-3})/$Al_{0.2}Ga_{0.8}N$ (27 nm)/GaN (500 nm) heterostructure as shown in Figure 3b. It is noted that the values of F_{AlGaN} are estimated from the FKOs to be 424 and 219 kV/cm for samples A1 and B, respectively; namely, the difference between the two values is 205 kV/cm. The experimental and theoretical results on the difference in F_{AlGaN} indicate that the present calculation reasonably explains the experimentally characterized change of F_{AlGaN} induced by the cap layer.

4 Summary

We have investigated the PR spectra and XRD patterns of three $Al_xGa_{1-x}N$ (27 nm)/GaN (2.2 μm) heterostructures with and without an n-GaN (5 nm, 5.0×10^{17} cm^{-3}) cap layer. It has been found in the PR spectra that stacking of the cap layer lengthens the period of the FKOs from the $Al_xGa_{1-x}N$ layer, which indicates that the profile of the FKOs is sensitive to the presence of the cap layer. The analysis of the FKOs has revealed that the electric field strength in the $Al_xGa_{1-x}N$ layer, F_{AlGaN}, is larger in the samples with the cap layer than F_{AlGaN} in the sample without the cap layer. The enhancement of F_{AlGaN} induced by the cap layer is so large that it exceeds the effect of the Al-composition difference that mainly modifies the piezoelectric field: $x = 0.20$ and 0.18 in the present case. We, therefore, conclude that stacking of the cap layer enhances F_{AlGaN} and that the PR characterization is applicable to quantitatively probe the electric-field change induced by the cap layer in III-nitride heterostructures. We have also numerically calculated the Schrödinger-Poisson equation in order to evaluate the effects of the cap layer on F_{AlGaN}. The cap-layer thickness strongly influences F_{AlGaN} while the doping density less than 10^{18} cm^{-3} hardly changes F_{AlGaN}. This indicates that the cap-layer thickness is the main factor determining the change of F_{AlGaN} in the present samples. The change of F_{AlGaN} without and with the cap layer is reasonably explained by the numerical calculation.

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