Ohmic contact technology in III nitrides using polarization effects of cap layers

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A technology for low-resistance ohmic contacts to III nitrides is presented. The contacts employ polarization-induced electric fields in strained cap layers grown on lattice-mismatched III-nitride buffer layers. With appropriate choice of the cap layer, the electric field in the cap layer reduces the thickness of the tunnel barrier at the metal contact/semiconductor interface. Design rules for polarization-enhanced contacts are presented giving guidance for composition and thickness of the cap layer for different III-nitride buffer layers. Experimental results for ohmic contacts with *p*-type InGaN and GaN cap layers are markedly different from samples without a polarized cap layer thus confirming the effectiveness of polarization-enhanced ohmic contacts. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1504169]

INTRODUCTION

Ohmic contacts with specific contact resistances in the $10^{-4}\ \Omega\,\mathrm{cm}^2$ range or smaller are imperative to minimize parasitic voltage drops and to increase the reliability and lifetime of optoelectronic devices such as light-emitting diodes and lasers.[1] Ohmic contacts in most semiconductors are achieved by heavily doping the contact region thereby reducing the tunnel-barrier thickness at the metal/semiconductor interface.

The wide band gap and large electron affinity of III nitrides compared to other III–V semiconductors such as GaAs generally result in high Schottky barriers for metal contacts to *p*-type and *n*-type material. In addition, the large thermal activation energy of *p*-type dopants in III nitrides[2] makes it difficult to create heavily doped layers with high free-hole concentrations. It is therefore particularly challenging to form low-resistance ohmic contacts to *p*-type III nitrides.

Several approaches have been used to fabricate low-resistance ohmic contacts to *p*-type III-nitride compounds such as deposition of high-work function metals with subsequent alloying at elevated temperatures,[3] deposition of conductive oxides,[4] and various types of surface treatments.[5]

A completely different approach to reduce the tunneling barrier width is based on the use of strained cap layers or superlattices pseudomorphically grown on top of the III nitride semiconductor of interest.[6–8] Strain-induced as well as spontaneous polarization result in electric fields that tilt the conduction and valence bands in the cap layers in such a way that tunneling of charge carriers through the barrier can be drastically enhanced. A significant advantage of this approach is its limited reliance on doping, the metallization type, and annealing conditions.

In this work, the theory of polarization-enhanced ohmic contacts using strained cap layers is discussed. Practical guidance is given for the selection of suitable cap/buffer layer combinations including the composition and thickness of the cap layers. Experimental results are presented that show the viability of polarization-enhanced ohmic contacts. InGaN caps on GaN, and GaN caps on AlGaN, significantly reduce the contact resistances as compared to contacts not utilizing cap layers.

THEORY

The magnitude of polarization fields in III nitrides is well known.[9–13] The piezoelectric polarization of a generalized wurtzitic III nitride cap layer $X_xY_{1-x}N$ (X and Y represent a group-III element such as Al, Ga, or In) pseudomorphically grown on a relaxed buffer layer depends on the strain in the basal plane of the Wurtzite crystal

$$\varepsilon_\perp(x)=[a_{\mathrm{buff}}-a(x)]/a(x)=\Delta a/a \tag{1}$$

with the equilibrium lattice constants of the buffer, a_{buff}, and the cap layer, $a(x)$ Values of the equilibrium lattice constant and strain for different III nitrides are given in Table I and Fig. 1. By taking into account second order effects, the piezoelectric polarizations along the c direction of strained binary layers can be written as[12,13]

$$P^{\mathrm{pz}}_{\mathrm{AlN}}=[-1.808\varepsilon_\perp+5.624\varepsilon_\perp^2]\ \mathrm{C\,m^{-2}} \quad \text{for } \varepsilon_\perp<0, \tag{2a}$$

$$P^{\mathrm{pz}}_{\mathrm{AlN}}=[-1.808\varepsilon_\perp-7.888\varepsilon_\perp^2]\ \mathrm{C\,m^{-2}} \quad \text{for } \varepsilon_\perp>0, \tag{2b}$$

$$P^{\mathrm{pz}}_{\mathrm{GaN}}=[-0.918\varepsilon_\perp+9.541\varepsilon_\perp^2]\ \mathrm{C\,m^{-2}}, \tag{2c}$$

$$P^{\mathrm{pz}}_{\mathrm{InN}}=[-1.373\varepsilon_\perp+7.559\varepsilon_\perp^2]\ \mathrm{C\,m^{-2}} \tag{2d}$$

with the piezoelectric polarization in a strained *ternary* layer (in $\mathrm{C\,m^{-2}}$) given by a Vegard law

$$P^{\mathrm{pz}}_{X_xY_{1-x}N}(x)=xP^{\mathrm{pz}}_{XN}[\varepsilon_\perp(x)]+(1-x)P^{\mathrm{pz}}_{YN}[\varepsilon_\perp(x)]. \tag{3}$$

The spontaneous polarization can be expressed by[12]

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TABLE I. Cap/buffer layer combinations for polarization-enhanced ohmic contacts to Ga-faced wurtzitic III-nitride semiconductors. Upper-diagonal elements are combinations resulting in a compressively strained cap layer suitable for *p*-type contacts to $X_xY_{1-x}N$ compounds. The diagonal elements of the table contain the respective in-plane lattice constants taken from Ref. 12. The lower-diagonal elements of the table correspond to possible combinations decreasing the contact resistances for *n*-type material

	Cap layer					
Buffer layer (Ga face)	AlN	$Al_xGa_{1-x}N$	$Al_xIn_{1-x}N$	GaN	$In_xGa_{1-x}N$	InN
AlN	3.1095 Å					
$Al_xGa_{1-x}N$		(3.1986 $-0.0891x$) Å				
$Al_xIn_{1-x}N$			(3.5848 $-0.4753\,x$) Å			
GaN				3.1986 Å		
$In_xGa_{1-x}N$					(3.1986 $+0.3862\,x$) Å	
InN						3.5848 Å

$$P^{\mathrm{sp}}_{\mathrm{Al}_x\mathrm{Ga}_{1-x}N}(x)=[-0.09x-0.034(1-x)+0.019x(1-x)]\ \mathrm{C\,m^{-2}}, \tag{4a}$$

$$P^{\mathrm{sp}}_{\mathrm{In}_x\mathrm{Ga}_{1-x}N}(x)=[-0.042x-0.034(1-x)+0.038x(1-x)]\ \mathrm{C\,m^{-2}}, \tag{4b}$$

$$P^{\mathrm{sp}}_{\mathrm{Al}_x\mathrm{In}_{1-x}N}(x)=[-0.09x-0.042(1-x)+0.071x(1-x)]\ \mathrm{C\,m^{-2}}. \tag{4c}$$

To obtain the electric field $\mathcal{E}^{\mathrm{pol}}$ in the cap layer caused by the spontaneous and piezoelectric polarization fields $P^{\mathrm{sp}}_{\mathrm{cap}}$, $P^{\mathrm{sp}}_{\mathrm{buff}}$, and $P^{\mathrm{pz}}_{\mathrm{cap}}$, it is assumed that the free charge density inside the sample is negligible; therefore $\nabla\mathbf{D}=0$ with $\mathbf{D}$ being the dielectric displacement field. The displacement fields $\mathbf{D}_{(i)}$ in the cap and buffer layers may be written as[14]

$$\mathbf{D}_i=\varepsilon_0\varepsilon_i\,\mathcal{E}_i+\mathbf{P}^{\mathrm{sp}}_i+\mathbf{P}^{\mathrm{pz}}_i \quad (i=\mathrm{cap},\mathrm{buff}), \tag{5}$$

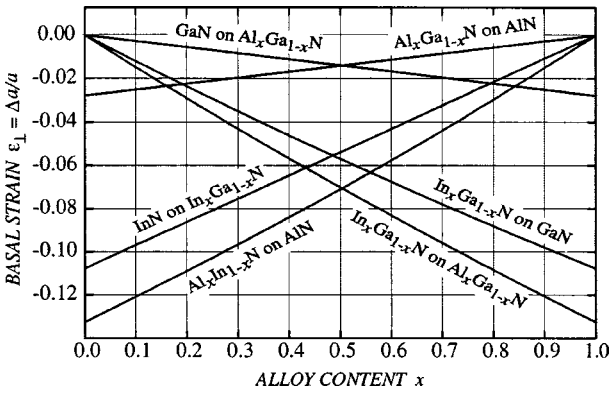

FIG. 1. Elastic strain ε in the basal plain of Ga-faced $X_{1-x}Y_xN$ compounds pseudomorphically grown as cap layers on top of relaxed III-nitride buffer layers. Negative values of $\varepsilon_\perp$ indicate compressive strain.

where ε_0 is the dielectric permittivity of vacuum; $\varepsilon_{\mathrm{cap}}$ and $\varepsilon_{\mathrm{buff}}$ are the relative dielectric constants in the cap and buffer layer, respectively, and may be obtained from the relationship $\varepsilon_{X_xY_{1-x}N}(x)=x\varepsilon_{XN}+(1-x)\varepsilon_{YN}$. Using the boundary condition $D_{n,\mathrm{cap}}=D_{n,\mathrm{buff}}$ at the cap/buffer interface with D_n denoting the component of $\mathbf{D}$ normal to the interface, $\mathcal{E}^{\mathrm{pol}}\equiv\mathcal{E}_{\mathrm{cap}}$ is given by

$$\mathcal{E}^{\mathrm{pol}}=\frac{1}{\varepsilon_0\varepsilon_{\mathrm{cap}}}(-P^{\mathrm{pz}}_{\mathrm{cap}}-P^{\mathrm{sp}}_{\mathrm{cap}}+P^{\mathrm{sp}}_{\mathrm{buff}})+\frac{\varepsilon_{\mathrm{buff}}}{\varepsilon_{\mathrm{cap}}}\mathcal{E}_{\mathrm{buff}}. \tag{6}$$

The field $\mathcal{E}_{\mathrm{buff}}$ will be screened by free charge carriers as soon as the tilted conduction or valence bands in the buffer layer come close to the Fermi level; this condition allows to obtain an upper limit for $\mathcal{E}_{\mathrm{buff}}$ according to

$$\mathcal{E}_{\mathrm{buff}}d_{\mathrm{buff}}\leqslant\frac{E_{G,\mathrm{buff}}}{e}, \tag{7}$$

where e is the elementary electric charge and $E_{G,\mathrm{buff}}$ and D_{buff} denote the band gap energy and the thickness of the buffer layer, respectively. For GaN and thicknesses $d_{\mathrm{buff}}>300$ nm the value of the field $\mathcal{E}_{\mathrm{buff}}$ is about 10^7 V/m or smaller; this may be neglected compared to typical values $P^{\mathrm{pz}}_{X_xY_{1-x}N}/(\varepsilon_0\varepsilon_{X_xY_{1-x}N})\geqslant 10^8$ V/m in strained III nitrides.[11–13] Equation (6) may therefore be approximated

$$\mathcal{E}^{\mathrm{pol}}\approx\frac{1}{\varepsilon_0\varepsilon_{\mathrm{cap}}}(-P^{\mathrm{pz}}_{\mathrm{cap}}-P^{\mathrm{sp}}_{\mathrm{cap}}+P^{\mathrm{sp}}_{\mathrm{buff}}). \tag{8}$$

It turns out that for *compressive strain* ($\varepsilon<0$, see Fig. 1), $\mathcal{E}^{\mathrm{pol}}$ as obtained from Eq. (8) points along the *negative c* direction of the Ga-faced wurtzite crystal, that is, towards the substrate. In the case of *p*-type III-nitride materials this results in a *decrease* of the tunnel barrier thickness and will therefore be beneficial to attain smaller specific contact resistances. Table I summarizes possible cap/buffer layer combinations resulting in compressive strain in the cap layer.

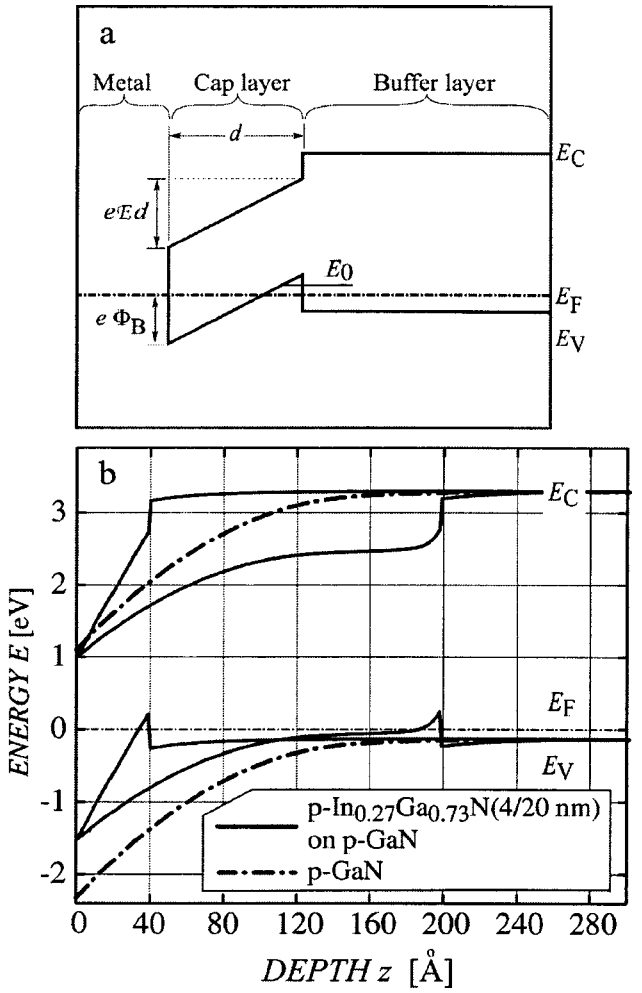

FIG. 2. (a) Schematic band diagram for a polarization-enhanced contact employing a strained *p*-type III-nitride cap layer pseudomorphically grown on top of a relaxed III-nitride buffer layer. E_0 denotes the groundstate energy of a 2DHG formed in the triangular barrier at the interface between cap and buffer layer, d is the cap layer thickness, $\mathcal{E}$ is the electric field in the strained cap layer, and Φ_B is the Schottky barrier height. (b) Self-consistently calculated band diagram for Ni contacts to bulk *p*-type GaN and to polarization-enhanced structures consisting of strained *p*-$In_{0.27}Ga_{0.73}N$ cap layers ($d=4$ nm and $d=20$ nm) on top of relaxed *p*-GaN. The dopant concentration was assumed to be 10^{19} cm^{-3}.

For strong enough electric fields or sufficiently thick cap layers, the formation of a two-dimensional hole gas (2DHG) at the interface between the cap and the buffer layers will occur. The density $p_{2\mathrm{DHG}}$ of the two-dimensional hole gas can be calculated by numerically solving the condition for the constancy of the Fermi level [see Fig. 2(a)]:

$$e\Phi_B + e d_{\mathrm{cap}}\mathcal{E}_{\mathrm{tot}} + (E_0 - E_V) + (E_F - E_0) = 0. \tag{9}$$

In Eq. (9), d_{cap} denotes the thickness of the cap layer, $\mathcal{E}_{\mathrm{tot}}$ is the total electric field in the cap layer, Φ_B is the Schottky barrier height, E_V is the valence band energy at the cap/buffer layer interface; E_F and E_0 are the Fermi energy and the energy of the 2DHG groundstate, respectively. The terms on the left-hand side in Eq. (9) are given by

$$e\Phi_B = E_{G,\mathrm{cap}} - e(\Phi_M - \chi_{\mathrm{cap}}), \tag{10a}$$

$$\mathcal{E}_{\mathrm{tot}} = \mathcal{E}^{\mathrm{pol}} + \frac{e p_{2\mathrm{DHG}}}{\varepsilon_{\mathrm{cap}}\varepsilon_0}, \tag{10b}$$

$$E_0 - E_V = \frac{3}{2}\left[\frac{3}{2}\frac{e^2\hbar}{\varepsilon_{\mathrm{cap}}\varepsilon_0\sqrt{m^*}} p_{2\mathrm{DHG}}\right]^{2/3}, \tag{10c}$$

$$E_F - E_0 = \frac{\pi\hbar^2}{m^*} p_{2\mathrm{DHG}}. \tag{10d}$$

In Eq. [10(a)], $E_{G,\mathrm{cap}}$, χ_{cap} are the band gap energy and the electron affinity of the cap layer, Φ_M is the work function of the contact metal; here we use the work function of Ni $\Phi_M = 5.2$ eV. The ternary band gap energy can be obtained from

$$E_{G,X_xY_{1-x}N} = xE_{G,XN} + (1-x)E_{G,YN} - bx(1-x), \tag{11}$$

where a bowing parameter $b=2.5$ eV[10] is used; the ternary electron affinity may be obtained from linear interpolation of the respective binary values according to

$$\chi_{X_xY_{1-x}N} = x\chi_{XN} + (1-x)\chi_{YN}. \tag{12}$$

In Eq. [10(c)], $E_0 - E_V$ is calculated using the Fang–Howard approximation[15] for energy states in a triangular well. The effective hole mass m^* in the cap layer is $1.0 \times m_0$, and $\hbar$ is Planck's constant divided by 2π. $E_F - E_0$ in Eq. [10(d)] is calculated using the high-density approximation of the Fermi–Dirac distribution and the two-dimensional density of hole states $\rho_{2D} = m^*/(\pi\hbar^2)$.

Tunneling from the contact metal into the cap layer requires the existence of unoccupied valence band states in the cap layer. This condition allows one to calculate the minimum thickness of the cap layer

$$d_{\mathrm{min}} = -\frac{\Phi_B - E_0/e}{\mathcal{E}_{\mathrm{tot}}} \approx -\frac{\Phi_B}{\mathcal{E}_{\mathrm{tot}}}. \tag{13}$$

corresponding to the minimum thickness required for the formation of a 2DHG. The approximation in Eq. (13) is valid if quantum-size effects in the triangular potential well at the cap/buffer layer interface are neglected, in analogy to the approach in Ref. 16. Thus, Eq. (13) is the solution of Eq. (9) for $p_{2DHG}=0$, the onset of the 2DHG.

Figure 2(b) shows self-consistently calculated band diagrams[17] for $In_{0.27}Ga_{0.73}N$ cap layers on GaN with two different cap layer thicknesses, $d=4$ nm and $d=20$ nm, as well as the band diagram of bulk *p*-type GaN. We assumed a uniform Mg dopant concentration of $N_{\mathrm{Mg}}=10^{19}$ cm^{-3} with an acceptor activation energy of $E_a=50$ meV in the capping layer obtained by extrapolating the values of E_a given in Ref. 18 towards larger In contents. Nickel was used in the calculation as the contact metal.

It can be seen that for the thicker cap layer, the Schottky barrier width approaches that of bulk *p*-type GaN; therefore no reduction of the specific contact resistance compared to *p*-type GaN can be expected.

Figure 3 shows the dependence of the electric field $\mathcal{E}^{\mathrm{pol}}$ for various cap/buffer layer configurations. Also included is the dependence of d_{min} on the electric field in the cap layer calculated from Eq. (13) assuming $\mathcal{E}_{\mathrm{tot}}=\mathcal{E}^{\mathrm{pol}}$ and using the barrier heights Φ_B of Ni on GaN ($\Phi_B=2.3$ V), InN (Φ_B

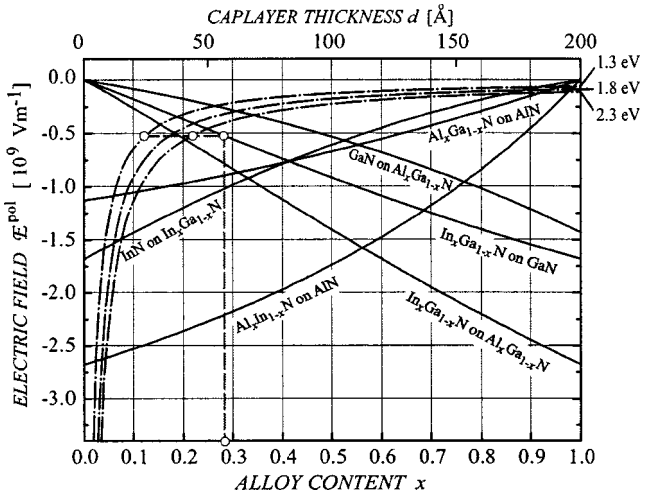

FIG. 3. Polarization-induced electric field $\mathcal{E}^{pol}$ in Ga-faced $X_{1-x}Y_xN$ cap layers pseudomorphically grown on different buffer layers (strain relaxation due to critical thickness effects is not taken into account). Negative values indicate that the $\mathcal{E}^{pol}$ vector points towards the buffer layer. The dashed-dotted curves correspond to the cap layer thickness d_{min} given by Eq. (9) using Schottky barrier heights $e\Phi_B$ for Ni on GaN ($e\Phi_B=2.3$ eV), on InN ($e\Phi_B=1.3$ eV), and on AlN ($e\Phi_B=1.8$ ev) . As an example, the dashed lines indicate how to determine the thickness d_{min} of an $In_{0.27}Ga_{0.73}N$ cap layer on GaN.

$=1.3$ V), and AlN ($\Phi_B=1.8$ V). As an example, the minimum thickness of an $In_{0.27}Ga_{0.73}N$ cap layer on a GaN buffer layer can be determined to be between 2 and 4 nm.

According to the WKB approximation the tunneling probability T^* through a triangular barrier for holes with energy $E=0$ is given by

$$T^* = \exp\left[-\frac{4\Phi_B^{3/2}\sqrt{2m^*e}}{3\hbar|\mathcal{E}_{tot}|} \right]. \tag{14}$$

By using the slope of the valence band at $z=0$ in Fig. 2(b) to estimate the electric field $\mathcal{E}_{tot}$ a tunneling probability $T^* \approx 10^{-8}$ can be obtained for the cap layer with thickness $d=4$ nm, which is much larger than the value $T^* \approx 10^{-24}$ for the 20-nm-thick cap layer. It is therefore prudent to not exceed the minimum cap layer thickness d_{min} by more than a factor of 2.

The cap layer will change the barrier height as compared to a no-cap layer situation. Note, however, that the barrier thickness is much more important than the barrier height. This is because the thickness can vary by a larger factor than the barrier height and also because the tunneling probability has a stronger dependence on the thickness as compared to the barrier height [see Eqs. (13) and (14)]. Therefore, it is reasonable to assume that the change in barrier height will be of minor importance.

The electric fields $\mathcal{E}^{pol}$ shown in Fig. 3 are similar or even larger than the critical fields $\mathcal{E}_c$ in InN ($\mathcal{E}_c \approx 1\times10^8$ V/m), GaN ($\mathcal{E}_c \approx 3\times10^8$ V/m), and AlN ($\mathcal{E}_c \approx 9\times10^8$ V/m) obtained from a power law relationship.[19] For doped samples, however, $\mathcal{E}^{pol}$ will be reduced by free charge carriers and ionized impurities. In addition, if d_{min} approaches the critical thickness of the cap layer for pseudomorphic growth, the onset of elastic strain relaxation will result in further reduced fields $\mathcal{E}^{pol}$. Therefore, minimum cap layer thicknesses obtained from Fig. 3 have to be regarded as a lower limit.

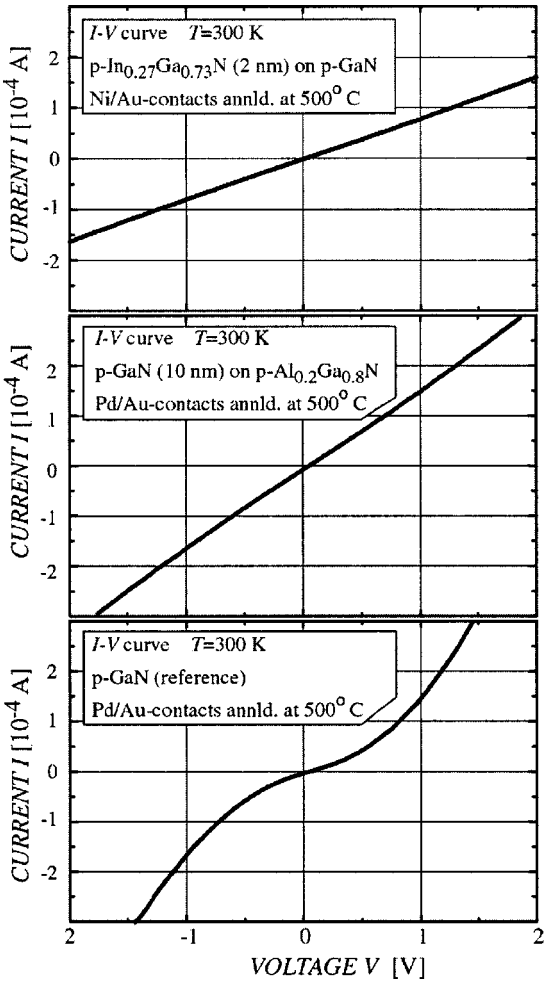

FIG. 4. $I-V$ curves for ohmic contacts to *p*-type GaN and for polarization-enhanced contacts utilizing InGaN-on-GaN or GaN-on-AlGaN cap layer structures. The data are obtained for TLM pads with a separation of 10 μm.

EXPERIMENTAL RESULTS

Several experiments were conducted to confirm the validity of polarization-enhanced contacts. Here we report on the marked difference in the $I-V$ characteristic obtained for samples with and without a cap layer. Detailed experimental studies on contact resistances have been reported elsewhere.[6,7]

Metallic contacts (Ni/Au and Pd/Au) were deposited by electron beam evaporation using lift-off photolithographic techniques. The contacts were square-shaped pads (200 μm $\times$200 μm) separated by 2, 4, 6, 8, 10, and 15 μm wide gaps. To remove surface oxide layers, the samples were treated with a buffered-oxide etch or in a solution containing 20% HF and 80% H_2O. Subsequently, the contacts were annealed in a rapid thermal annealing furnace at 500 °C in either nitrogen (Pd/Au contacts) or oxygen (Ni/Au contacts) ambient. The contact resistances were determined from $I-V$ measurements using the transfer length method (TLM).

Figure 4 shows the $I-V$ curves of samples with an

$In_{0.27}Ga_{0.73}N$ cap layer on a GaN buffer, a GaN-on-$Al_{0.2}Ga_{0.8}N$ superlattice structure and a *p*-type GaN reference sample. The thicknesses $d=2$ nm of the InGaN cap layer and $d=10$ nm of the GaN cap layer agree well with the respective minimum thicknesses d_{min} that can be obtained from Fig. 3.

Inspection of Fig. 4 shows that excellent ohmic $I-V$ characteristics were found for both samples containing cap layers. However, the $I-V$ characteristic for the *p*-type GaN reference sample is markedly nonlinear. This clearly indicates the advantageous effect of polarization fields in the cap layers. Specific contact resistances of $\rho=6\times10^{-3}\ \Omega\,cm^2$ for the InGaN cap layer and $7\times10^{-4}\ \Omega\,cm^2$ for the GaN cap layer were determined. Additional experimental results have been reported elsewhere.[6,7]

The two experimental examples reported here, namely the InGaN cap on GaN layers and the GaN cap on AlGaN layers have great practical importance. It is expected that the InGaN cap layer can be applied to light emitting diodes (LEDs) emitting in the visible spectrum. Such LEDs usually have GaN upper cladding layers. Furthermore, the GaN cap layer on AlGaN buffers will be useful for UV LEDs and lasers. Such devices usually have AlGaN upper cladding layers.

CONCLUSION

A technology for low-resistance ohmic contacts to III nitrides is presented. Strong polarization fields exist in III nitrides pseudomorphically grown as thin nonlattice-matched cap layers on top of relaxed III-nitride buffer layers. The corresponding electric fields in Ga-faced cap layers are calculated for different cap/buffer layer combinations and are on the order of $10^9\ V\,m^{-1}$. It is shown that a GaN cap on AlGaN, an InGaN cap on GaN, and other material combinations are suited for low-resistance *p*-type ohmic contacts to III nitrides.

For a proper choice of cap and buffer layer, the tunneling barrier thickness at the contact metal/semiconductor interface is drastically reduced as a result of band tilting in the cap layer region. For *p*-type contacts, enhanced by polarization effects, the hole tunneling probability through the surface barrier is increased by more than ten orders of magnitude compared to bulk *p*-type GaN without cap layer.

The beneficial effect of cap layers is demonstrated experimentally for an $In_{0.27}Ga_{0.73}N$-on-GaN structure and a GaN-on-$Al_{0.2}Ga_{0.8}N$ structure. As opposed to a *p*-type GaN reference sample, excellent linearity of the $I-V$ characteristics independent of the choice of contact metallization was achieved for the polarization-enhanced contacts. The specific contact resistances obtained from the TLM-method were $\rho=6\times10^{-3}\ \Omega\,cm^2$ for the InGaN cap layer and $7\times10^{-4}\ \Omega\,cm^2$ for the GaN cap layer.

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