Schottky enhancement of reacted NiAl/*n*-GaAs contacts

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Schottky enhancement of reacted NiAl/*n*-GaAs contacts was demonstrated experimentally. The Schottky barrier height increases from 0.83 eV for the *as*-deposited contacts to 0.96 eV when the contacts were annealed at 400 °C for 1 min. Formation of a high Al content (Al,Ga)As layer at the interface upon annealing was rationalized in terms of a thermodynamic/kinetic model. A (200) dark field cross-sectional transmission electron microscopy image was used to show the presence of high Al content (Al,Ga)As at the interface.

Understanding the mechanisms for the enhancement of Schottky barrier height (SBH) is not only scientifically but also technologically important. It can, for instance, be used to improve the current integrated circuit industrial process for fabricating electronic devices, i.e., metal-semiconductor field-effect transistors (MESFETs). A high SBH would allow a larger positive gate bias for enhancement mode MESFETs, thus permitting the fabrication of digital logic circuits with improved noise margins and a relaxed tolerance on device threshold voltage uniformity.

A number of schemes have been used to increase the SBH. Basically, these schemes can be classified into two categories. One category grows a thin layer of semiconductor, i.e., Si, at the contact interface[1] and the other category counter dopes the *n*-GaAs with a *p*-type dopant, i.e., C or Zn.[2] However, the contacts made using all these schemes suffer from poor thermal stability. Sands *et al.*[3] showed that thermally stable contacts with higher SBH could be realized using the following contact structure: capped Ni(35 nm)/Al(68 nm)/Ni(10 nm)/*n*-GaAs. In their experiments, the layers were deposited by electron-beam evaporation. They obtained a value of SBH, ϕ_{Bn}, $\simeq$0.99 eV, after rapid thermal annealing of the fabricated layered structure at 650 ° for 20 s. The SBH was obtained from the current-voltage method. Subsequently, Chambers[4] grew a layer of NiAl on a substrate of *n*-GaAs at a substrate temperature of 500 °C using molecular-beam epitaxy (MBE). He obtained a value of $\phi_{Bn} \simeq 0.9$ eV using x-ray photoemission spectroscopy. Neither of these studies attempted to describe the cause of this Schottky barrier enhancement. However, both Sands *et al.*[3] and Chambers[4] speculated that the Schottky barrier enhancement was due to the exchange of Al and Ga at the interface, resulting in the formation of a thin (Al,Ga)As layer. Nevertheless, there was no definitive experimental evidence to show the existence of such an (Al,Ga)As layer. Moreover, Chen *et al.*[5] showed recently that the Schottky enhancement of a layered structure of Ni/Al/Ni/*n*-GaAs, upon annealing, can be attributed to a regrowth mechanism and not due to the exchange of Al and Ga at the interface.

The objectives of the present study are to (i) deposit films of NiAl on a substrate of *n*-GaAs using a sputter deposition method, (ii) determine the Schottky barrier height of the NiAl/*n*-GaAs contacts as a function of rapid thermal annealing temperature using the current-voltage ($I-V$) method, (iii) propose a mechanism to rationalize the formation of (Al,Ga)As at the metal/semiconductor interface which is responsible for the Schottky enhancement, and (iv) establish experimentally the existence of this phase.

Unintentionally doped ($\sim 3\times 10^{16}$ cm^{-3}) *n*-GaAs wafers with a (100) orientation were used as substrates in the present study. A standard photolithographic lift-off process was used for fabricating the contacts. The substrates were degreased with trichlorethylene, acetone, and methanol for 5 min each. The degreased wafers were then patterned with an array of 0.5 mm diameter dots using a standard lithographic technique. Prior to metal deposition, the patterned substrates were cleaned for 2 min by $NH_4OH:H_2O$ (1:2), followed by blow drying with N_2. Films of NiAl were deposited by sputter deposition to a thickness of 100 nm at an Ar pressure of 4 mTorr. The concentration of a 2 μm thick NiAl film sputter deposited on a glass plate under identical conditions was determined by EPMA to be 50±0.3 at. % Al. Annealing was carried out in a rapid thermal annealing furnace in an Ar ambient at 325 °C for 5 min, 400 °C for 1 min, 500 °C for 20 s, and 600 °C for 20 s. The backside ohmic contacts were formed by alloying In onto the *n*-GaAs substrate at a temperature of 400 °C for 1 min. The ohmic contacts were made prior to the Schottky metallization for samples annealed below 400 °C and after metallization for samples annealed above 400 °C.

The electrical measurements were made at room temperature. The current-voltage ($I-V$) measurements were performed with a Keithley model 236 electrometer. The $I-V$ characteristics were analyzed using the conventional thermionic-emission theory.[6] The relationship between the current and the applied forward voltage is given by the following equation:

$$I = SA^{**}T^2 \exp[-q(\phi_{Bn} - \Delta\phi_{Bn})/k_B T] \times [\exp(qV/nk_B T) - 1], \tag{1}$$

where S is the contact area, A^{**} is the effective Richardson

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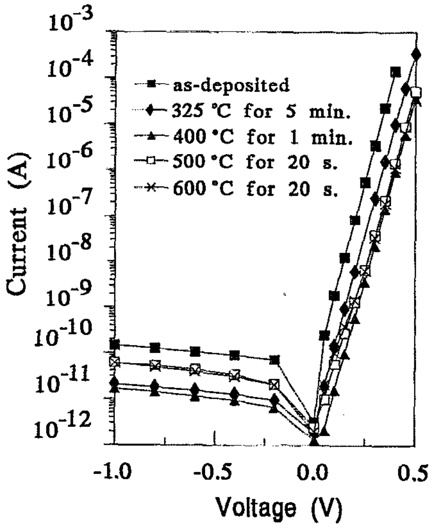

FIG. 1. The $I-V$ characteristics of the NiAl/n-GaAs contacts are shown for contacts after different thermal treatments. A linear relationships was found in the log $I-V$ characteristics under forward bias, over a wide range of the current measured, i.e., six orders of magnitude.

constant (8.64 A/cm^2 K^2 for n-GaAs), k_B is the Boltzmann constant, T is the temperature in K, ϕ_{Bn} is the Schottky barrier height, $\Delta\phi_{Bn}$ is the Schottky barrier lowering [(equal to $(qE/4\pi\varepsilon_s)^{1/2}$)[6]], E is the maximum electric field at the metal-semiconductor interface, ε_s is the permittivity of the semiconductor, and n is the ideality factor. The ideality factor must be close to unity in order to assure that thermionic emission is the dominant transport mechanism.

Transmission electron microscopy (TEM) examination of the reacted interfaces was carried out using a JEOL 200 CX.

The experimental $I-V$ data presented in Fig. 1 shows the existence of a linear region in a semilog plot of forward bias over six orders of magnitude for the applied voltage. The leakage current is below 1×10^{-7} A/cm^2 at a reverse bias of 1 V for all the contacts. Values of the SBH, ϕ_{Bn}, as well as the ideality factors, n, are summarized in Table I as a function of annealing temperature. The data clearly indicate that the Schottky behavior of the uncapped NiAl/n-GaAs contacts follows the thermionic-emission model. Ideality factors, equal to or less than 1.1, were determined on structures after annealing at temperatures as high as 600 °C for 20 s. The contacts, which become nonrectifying after being annealed at 650 °C for 20 s, are not listed in Table I. The maximum barrier height of the uncapped contact, 0.96 eV, is close to that of the capped Ni/Al/Ni/n-GaAs contact, 0.99 eV, annealed at 650 °C for 20 s obtained by Sands *et al.*[3] It is higher than that of the NiAl/n-GaAs contacts, 0.9 eV, grown by MBE at 500 °C by Chamber.[4] Chamber's Schottky barrier height was derived from a different experimental method which may account for the 0.06 eV difference between his result and the value reported here.

The processing used in the present study offers several practical advantages over those used by Sands *et al.*[3] and Chambers.[4] Sands *et al.* had to use an AlN cap as well as anneal their contacts at 650 °C to achieve Schottky barrier enhancement. In the present study, only a short anneal of the contacts at 400 °C for 1 min was necessary. This makes our processing technique compatible with the use of an Au—Ni—Ge ohmic contact. It is known that the Au—Ni—Ge contacts to n-GaAs requires annealing at 400 °C[7] to achieve a low contact resistivity. Secondly, sputter deposition can be adopted for most practical applications, eliminating the need for a MBE-based technology.

TABLE I. Schottky barrier heights and the ideality factors obtained for the reacted NiAl/n-GaAs contacts using the $I-V$ method.

Heat treatments	ϕ_{Bn}	n
As-deposited	0.83	1.03
325 °C/5 min	0.90	1.05
400 °C/1 min	0.96	1.06
500 °C/20 s	0.94	1.09
600 °C/20 s	0.89	1.14

We will use the thermodynamic and kinetic analysis proposed by Jan[8] to rationalize the formation of (Ga,Al)As at the metal/semiconductor interface which is responsible for the Schottky enhancement of the NiAl/n-GaAs contacts. The analysis proposed by Jan[8] was recently summarized by Chang.[9]

This analysis is applicable for the reciprocal system of NiGa—NiAl—AlAs—GaAs that exists in the quaternary Ga—Ni—Al—As system. The phase diagram of such a reciprocal system is given in Fig. 2. As shown in this figure, a two-phase equilibrium exists between the Ni(Ga,Al) phase denoted as β and the (Ga,Al)As phase denoted as α. This diagram was determined experimentally at 800 °C by Jan.[8] The dashed lines which connect the compositions of the coexisting α and β phases are referred to as the tie lines. Even though the diagram was determined at 800 °C, the phase diagrams at any other temperature may be calculated thermodynamically.[9] The calculated diagram at 800 °C is in agreement with the experimentally determined diagram.

It is clear from Fig. 2 that thermodynamic equilibrium does not exist at the NiAl/n-GaAs interface. Interfacial reaction will occur. Assuming diffusion to be the rate limiting

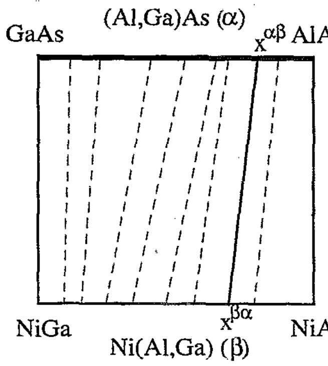

FIG. 2. The experimentally determined tie lines in a phase diagram of the GaAs—NiGa—NiAl—AlAs system at 800 °C were reported by Jan (see Ref. 8).

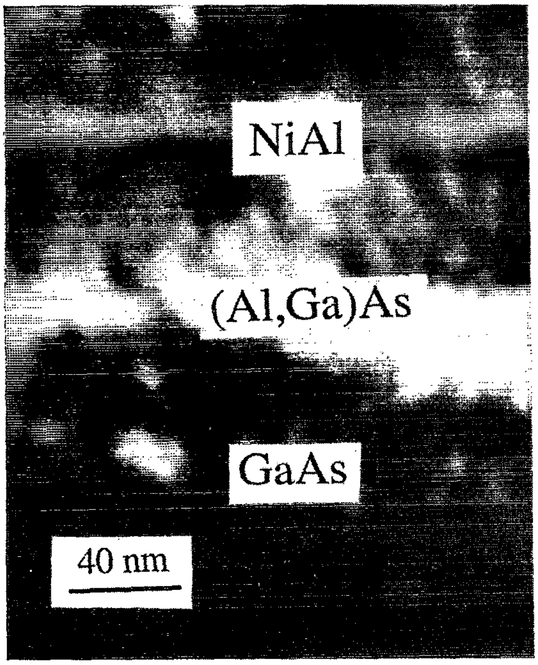

FIG. 3. (200) dark field XTEM images of the contact annealed at 700 °C for 20 s is used to determine the presence of a(Al,Ga)As phase. The (Al,Ga)As phase would be bright and the GaAs phase would be dark on the (200) dark field image.

step, the compositions of the coexisting phases at the metal/semiconductor interface is related to the interdiffusion coefficients of the α and β phases, as given by

$$\frac{x^{\alpha\beta}}{1-x^{\beta\alpha}}=\sqrt{\frac{\tilde{D}^{\beta}}{\tilde{D}^{\alpha}}}, \qquad (2)$$

where $x^{\alpha\beta}$ is the concentration of AlAs in the β phase at the α/β interfaces, $x^{\beta\alpha}$ is that of NiAl in the α phase at the α/β interface, $\tilde{D}^{\beta}$ is the interdiffusion coefficient of the β phase, and $\tilde{D}^{\alpha}$ is that of the α phase. Other assumptions involved in obtaining Eq. (2) are that the interdiffusion coefficients are composition independent and that the α/β interface is stationary. Values of $x^{\alpha\beta}$ and $x^{\beta\alpha}$ are the compositions of the α and β phases for a specific tie line, as shown in Fig. 2. The dark line shown in this figure is termed a diffusion path. The diffusion path states graphically that the concentration at the α/β interface is $x^{\alpha\beta}$ and $x^{\beta\alpha}$. The AlAs concentration in the α phase decreases from $x^{\alpha\beta}$ at the interface to zero far away from the interface, i.e., the bulk GaAs substrate. The NiAl concentration in the β phase, in a similar manner, increases from $x^{\beta\alpha}$ at the interface to 1, i.e., the bulk NiAl phase.

It is evident from Eq. (2) that if we know the values of $\tilde{D}^{\alpha}$ and $\tilde{D}^{\beta}$, we can readily calculate the concentrations of (Al,Ga)As and Ni(Al,Ga) at the NiAl/*n*-GaAs interface. Since $\tilde{D}^{\beta}$ is several orders of magnitude larger than $\tilde{D}^{\alpha}$,[10,11] the value of $x^{\alpha\beta}$ at the reacted NiAl/*n*-GaAs interface at 400 °C would be close to 1.0, i.e., the (Al,Ga)As formed at the interface is close to pure AlAs. In view of the fact that the Schottky barrier height to *n*-AlAl is ~1.0 eV,[12] a reacted NiAl/*n*-GaAs contact at 400 °C would exhibit a Schottky barrier enhancement.

The presence of (Ga,Al)As at the interface was demonstrated using a (200) dark field XTEM image.[13] The difference between the atomic scattering factor of Al and that of As is significant, while the atomic scattering factors of Ga and Al are quite similar. Therefore, the (Al,Ga)As phase would appear bright while the (Ga,As) phase would appear dark in the dark field image. A (200) dark field XTEM image of the NiAl/*n*-GaAs contacts annealed at 700 °C for 20 s are shown in Fig. 3. Figure 3 shows a bright thin layer formed at the interface, which is presumed to be the high Al content (Al,Ga)As phase. It is the presence of this phase which results in the Schottky barrier enhancement.

In summary, thermally stable NiAl/*n*-GaAs Schottky contacts, up to 600 °C for 20 s, have been realized. The contacts were made by sputter deposition from a NiAl target to substrates of (100) *n*-GaAs at a base pressure $\sim 2\times 10^{-7}$ Torr. The high Schottky barrier height 0.96 eV with an ideality factor of 1.1 deduced from the $I-V$ was measured for the contacts annealed at 400 °C for 1 min. The Schottky barrier enhancement is rationalized in terms of a thermodynamic/kinetic model for interfacial reactions within the reciprocal system of NiGa—NiAl—AlAs—GaAs that exists in the quaternary Ga—Ni—Al—As system. It is the presence of the AlGaAs aphase which results in the Schottky barrier enhancement. The existence of this phase at the reacted interface was verified using a (200) dark field XTEM image of a contact annealed at 700 °C for 20 s.

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