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Roles of Materials Used in In-based Ohmic Contacts to n-type GaAs

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Recently, thermally stable, low resistance NiInW ohmic contacts to n-type GaAs have been developed using a standard evaporation and lift-off technique and annealing the contacts by a rapid thermal annealing method. By correlating the microstructure and the electrical properties, $In_xGa_{1-x}As$ phases, which were formed at the metal/GaAs interfaces, were found to primarily control the electrical properties. In this paper, in order to estimate the low limit of the barrier height possibly obtained at the metal/GaAs interface, In concentrations in the $In_xGa_{1-x}As$ phases were determined by analysing ternary InGaAs phase diagrams. Also, the role of Ni in determining the electrical properties and thermal stability was studied by observing the interfacial microstructure during heating process using cross-sectional transmission electron microscopy.

1. INTRODUCTION

Based on our observation that MoGeW contacts were converted from Schottky to ohmic behavior by the presence of indium impurities at the metal and GaAs inteface[1),2)], thermally stable, low resistance In-based NiInW ohmic contacts have been developed by depositing a small amount of In with the contact metals and annealing at temperatures higher than 800°C by a rapid thermal annealing (RTA) method[3)]. These contacts withstood 400°C annealing without degrading the electrical properties, a very desirable property for fabrication of GaAs integrated circuits. Correlating the electrical properties and the film microstructure of these contacts, ohmic behavior was first observed when formation of $In_xGa_{1-x}As$ phases on the GaAs substrate was observed after annealing at 700°C. Since the barrier heights of the metal/$In_xGa_{1-x}As$ contacts were measured to be lower than that of the metal/GaAs contacts[4)] and also the $In_xGa_{1-x}As$ phases grew epitaxially on the GaAs[2)], the effective barrier height (ϕ) is believed to be much lower than that (typically ~ 0.8eV) of the metal/GaAs contacts. Thus the electrical current flows primarily through the metal/$In_xGa_{1-x}As$/GaAs interfaces. The probable band diagram of this region is schematically shown in Fig. 1. The importance of the $In_xGa_{1-x}As$ phases in these contacts was also supported by the fact that the contact resistance (R_c) de-

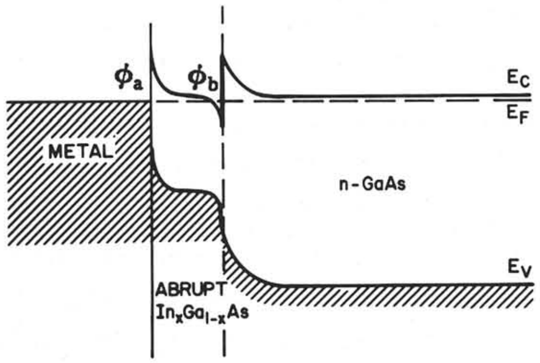


Fig. 1. Band diagram of metal/$In_xGa_{1-x}As$/GaAs contact.

creased with increasing the percentages of the GaAs interfaces covered by $In_xGa_{1-x}As$ phases[5)]. Among the In-based ohmic contact materials prepared by the conventional evaporation technique, the NiInW contact formed the largest $In_xGa_{1-x}As$ phases and yielded the lowest R_c. In addition, this contact demonstrated excellent thermal stability[3)].

There are several important questions concerning this NiInW ohmic contact. First, what is the lowest R_c value can we expect in this ohmic contact, if an $In_xGa_{1-x}As$ layer covers the entire GaAs surface? The R_c values are determined by the barrier height and the doping level at the metal/GaAs interfaces. If the doping levels in the $In_xGa_{1-x}As$ and GaAs regions are almost the same, the larger value of ϕ_a and ϕ_b will determine the the R_c value for the metal/$In_xGa_{1-x}As$/GaAs contacts, where ϕ_a and ϕ_b are the barrier heights of the metal/$In_xGa_{1-x}As$ and the $In_xGa_{1-x}As$/GaAs contacts, respectively, as shown in Fig. 1. When the $In_xGa_{1-x}As$ phases grow epitaxially on the GaAs substrate, ϕ_b is believed to be smaller than ϕ_a. On the other hand, if the In concentration in the $In_xGa_{1-x}As$ phases is large and lattice mismatch between the $In_xGa_{1-x}As$ phase and GaAs is large enough to induce crystal defects at the interface, ϕ_a is smaller than ϕ_b. Although relative importance of ϕ_a and ϕ_b is not known for the NiInW contacts, we concentrate, in the present study, on estimating the low limit of ϕ_a. Since the ϕ_a value is directly correlated with the In concentration (x) in $In_xGa_{1-x}As$, the ternary In-Ga-As phase diagrams were calculated to estimate the x values at various temperatures. A second question of interest is why the NiInW ohmic contacts provide the lowest R_c values among the In-based contacts. To understand the role of Ni on the $In_xGa_{1-x}As$ formation, the interfacial microstructure of the NiInW contacts during the heating process was studied by cross-sectional transmission electron microscopy(TEM).

2. EXPERIMENTAL PROCEDURE

Prior to metal deposition the wafers were chemically cleaned using a buffered HCl solution. The vacuum system was pumped down to $\sim 8 \times 10^{-6}$ Pa before metal deposition. To prepare the Ni/Ni-In/Ni/W ohmic contacts, Ni was deposited directly on the GaAs wafers by electron beam evaporation, Ni and In were deposited simultaneously (where In was deposited by RF induction heating), and then Ni and W were sequentially deposited by electron beam evaporation. The thickness of the first and third layers was 5 nm, that of the second coevaporated layer was 5 nm Ni and 5 nm In, and the top W layer was 30 nm thick. These samples were then heated for $\sim$ 1 sec by RTA in an Ar/H_2 atmosphere. Specimens for cross-sectional TEM were prepared by mechanical polishing and ion milling at liquid nitrogen temperature. Both JEOL-200CX TEM and Philips 400T TEM/STEM were used.

3. RESULTS AND DISCUSSION

A. In concentration in $In_xGa_{1-x}As$ phases

The In concentrations (x) in the $In_xGa_{1-x}As$ layer were calculated from the In-Ga-As phase diagrams at temperatures above 700°C, because ohmic behavior was observed

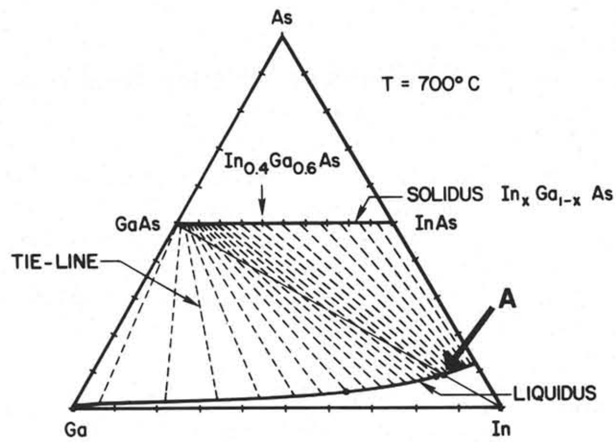


Fig. 2. Ternary In-Ga-As phase diagram at 700°C.

in the NiInW contacts at these high temperatures. (In this analysis Ni and W were assumed not to influence chemical reactions among In, Ga and As.) The InGaAs phase diagrams were calculated using an equation given by Antypas[6], where the activity coefficient in the liquid phase was calculated using Darken's quardratic equation[7] and the solid solution in equilibrium with the ternary liquid was assumed to be regular. An example of the phase diagrams is shown in Fig. 2. The dashed lines indicate tie-lines which connect two phases in thermal equilibrium at 700°C. At this temperature it is noted that the solid $In_xGa_{1-x}As$ phase and the liquid In-Ga-As phase coexist when the average composition is within the two phase region.

Referring to this phase diagram, reaction between In and GaAs at 700°C is considered. In order to make our interpretation clear, the microstructures expected during the heating process are shown schematically in Fig. 3. When In is deposited on the GaAs substrate at room temperature, In usually forms islands and no reaction with the GaAs was observed. Upon annealing at 700°C, In starts to react with the GaAs and In-rich In-Ga-As (liquid) phases and solid

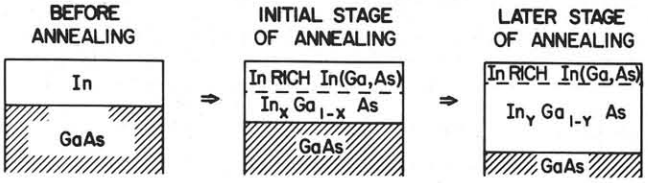
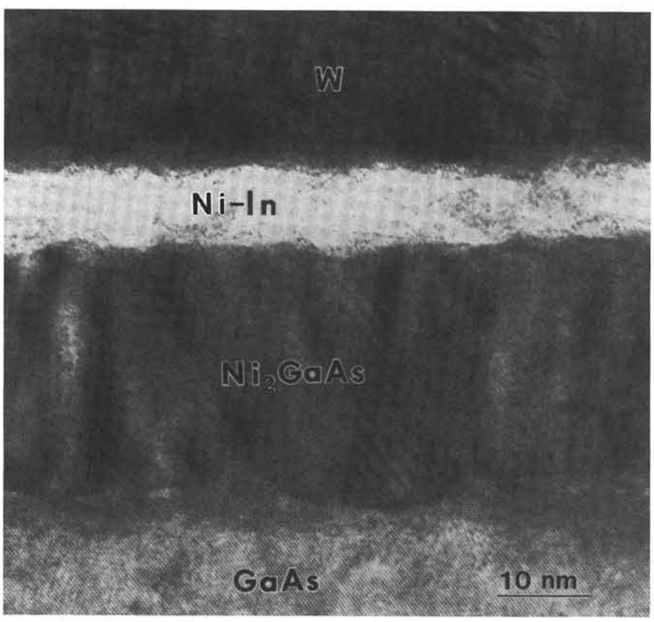


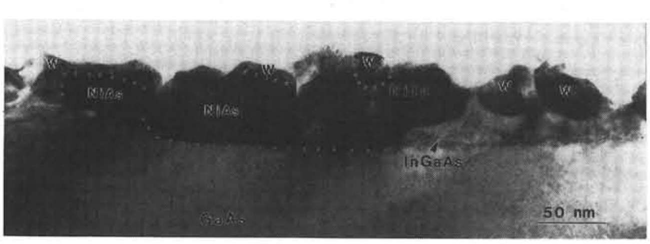
Fig. 3. Schematic illustration of microstructures during In/GaAs reaction.

$In_xGa_{1-x}As$ phases are expected. As the reaction progresses, the interface between the $In_xGa_{1-x}As$ and GaAs moves deeper into the GaAs substrate.

Note that for thin film/bulk reaction, the effective "average" composition (c_o) is the atomic percentage averaged within the "reacted" region (not the whole region) and shifts with progress of reaction. At the initial stages of reaction, c_o is very close to the "In" corner and a single (liquid) In-Ga-As phase is expected. When c_o moves into the two phase region along the line connecting "In" and "GaAs" of Fig. 2, the solid $In_xGa_{1-x}As$ phases precipitate out from the liquid In-Ga-As phase. Although the volume fraction of the solid phases is very small, the maximum In concentration (x_m) in the solid $In_xGa_{1-x}As$ phases is expected when the average composition is just inside the two phase region (indicated by A in Fig. 2). At 700°C annealing, x_m is ~ 0.4 from the tie-line. With progress of the reaction, the average composition shifts toward the GaAs region, the volume fraction of the solid $In_xGa_{1-x}As$ phases increases, and the x value in $In_xGa_{1-x}As$ approaches to zero. Therefore, the maximum In concentration expected in the $In_xGa_{1-x}As$ phase at 700°C is 0.4, which corresponds ϕ_a ~ 0.3eV. At higher annealing temperatures, the x_m value becomes smaller than 0.4 (e.g., 0.2 at 800°C). The present phase diagram analysis agrees well with the TEM and x-ray diffraction (XRD) results as given below.



(a)



(b)

Fig. 4. Micrographs of cross-sectional TEM for NiInW contacts annealed at 600°C (a) and 900°C (b).

B. Roles of Ni on $In_xGa_{1-x}As$ formation

To understand the roles of Ni on the $In_xGa_{1-x}As$ formation in the NiInW ohmic contacts, the interfacial microstructure during the heating process was examined by cross-sectional TEM. An as-deposited sample showed no reaction between the contact metals and the GaAs substrate. The first Ni layer was observed to cover uniformly the entire GaAs surface. Reaction between Ni with GaAs was first observed after 300°C annealing. Ni_2GaAs phases were observed on the GaAs surface. This phase was stable even after annealing at 600°C by RTA. The microstructure of the sample annealed at 600°C is shown in Fig. 4(a), where the Ni_2GaAs layer is observed to grow epitaxially on the (001) GaAs substrate and a Ni-In layer is formed between the Ni_2GaAs and W layers. Note that In did not react with GaAs even after annealing at such a high temperature. The atomic percentage of In in the Ni-In layer was calculated to be about 50% from the thickness ratio of Ni and In layers consumed to form this Ni-In layer. An orientation relationship between the Ni_2GaAs and the GaAs substrate was determined to be <0001>Ni_2GaAs // <111>GaAs and {1120}Ni_2GaAs //{110}GaAs. This orientation relationship agrees very well with the previous studies[8),9)]. A high density of micro-twins were observed in the Ni_2GaAs layer. By annealing the contacts above 700°C, the Ni_2GaAs phases started to partially decompose to the NiAs phases and simultaneously, formation of the $In_xGa_{1-x}As$ phases was observed locally at the GaAs interface. Growth of the $In_xGa_{1-x}As$ phases continued upon subsequent heating at higher temperatures and about 90% of the GaAs interface was covered by the $In_xGa_{1-x}As$ phases in the sample annealed at 900°C as seen in Fig. 4(b). The lattice mismatch between the $In_xGa_{1-x}As$ phase and the GaAs substrate was measured to be about 2 %, which corresponds an In concentration of about 0.3[10]. This In concentration is a little higher than that estimated from the InGaAs phase diagram. However, considering the experimental error for the lattice parameter measurement and the uncertainty in the actual annealing temperature, the agreement between the experiment and calculation is very good. A 1° orientation mismatch between these two crystals was also observed along the GaAs <110> zone axis.

The reason why the large $In_xGa_{1-x}As$ phases were found in the NiInW contact is primarily due to formation of Ni_2GaAs layer at the initial stages of annealing. The Ni_2GaAs compounds, observed to cover 100% the GaAs substrate below 600°C, blocked the In diffusion toward the GaAs substrate during heating process to 600°C. This is desirable to prevent In from diffusing deep into the GaAs substrate during the heating process. When the Ni_2GaAs phases decomposed to NiAs at temperatures above 700°C, the In started to diffuse from the Ni-In layer to the GaAs. Since heating time from 700 to 900°C by RTA is extremely short, shallow In diffusion into the GaAs was seen in Fig. 4(b), which is desirable to form large area $In_xGa_{1-x}As$ phases at the GaAs surface. Therefore, about 90% of the GaAs surface was covered by the $In_xGa_{1-x}As$ phases and the low R_c values were obtained in this contact at annealing temperatures in the range of 800 to 1000°C.

Also, the NiInW ohmic contacts showed excellent thermal stability after contact formation. From our previous studies of AuNiGe ohmic contacts, poor thermal stability was concluded to be due to formation of low melting poit β-AuGa phases[11]. In the present experiment, Ni_3In, NiAs compounds and $In_xGa_{1-x}As$ were observed in the NiInW contact after annealing at 900°C. The melting points of these phases are above 900°C and no evidence of existence of the unreacted In was obtained. The excellent thermal stability at 400 and 500°C observed in the previous experiment[3] is because the contact contains only refractory compounds.

4. SUMMARY

The maximum In concentration expected in the $In_xGa_{1-x}As$ phases, formed at the metal/GaAs interfaces of NiInW contacts, was determined by analysing the In-Ga-As ternary phase diagrams to be ~ 0.4 when the contact was formed by depositing In with Ni and W and annealing at temperatures above 700°C. This value agrees very well with the In concentration determined by TEM and XRD. This implies that a barrier height less than ~ 0.3eV is not expected in this contact. Nickel was found to form a uniform Ni_2GaAs layer at the initial stages of annealing. This layer was found to be critical to suppress deep In diffusion into the GaAs substrate during annealing and to form large area $In_xGa_{1-x}As$ phases at the GaAs interface, which produced low resistance. Excellent thermal stability observed in this ohmic contact was concluded to be due to the absence of low melting point phases after annealing at high temperatures. Unreacted In, which causes poor thermal stability of the In-based ohmic contacts, was eliminated by formation of high melting point Ni_3In compounds.

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