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Al/GaSb Contact with Slow Positron Beam

Hai-yun Wang, Hui-min Weng, C. C. Ling, Bang-jiao Ye, Xian-yi Zhou

a. Department of Modern Physics, University of Science and Technology of China, Hefei 230026, China; b. Department of Physics, The University of Hong Kong, Hong Kong, China

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Annealing study of the Al/GaSb system was performed by using a slow positron beam and the measurement of X-ray diffraction. The S parameter against positron energy data were fitted by a three layer model (Al/interface/GaSb). It was found there was a ~5 nm interfacial at the region between the Al layer and bulk in the sample of as-deposited. After the 400 °C annealing, this interfacial region extends to over 40 nm and S parameter dramatically drops. This is possibly due to a new phase formation induced by the atoms’ inter-diffusion at the interface. The annealing out of the open volume defects in the Al layer was revealed by the decrease of the S parameter and the increase of the effective diffusion length of the Al layer. Annealing behaviors of S and L of the GaSb bulk showed the annealing out of positron traps at 250 °C. However, further annealing at 400 °C induces formation of positron traps, which are possibly another kind of Vc-related defect and the positron shallow trap GaSb anti-site. The results of the X-ray diffraction experiment verified the conclusion of obtained by using positron technology.

Key words: Positron, Defect, Trapping, Al/GaSb, Interface

I. INTRODUCTION

Gallium antimonide is a III-V semiconductor having a narrow band gap, a high carrier mobility and a small effective carrier mass. This material is suitable for fabricating the high frequency electronic devices. Moreover, GaSb is the basic material for growing a variety of lattice matched optoelectronic materials working in the wavelengths of 0.8-4.3 μm [1]. Although, GaSb Schottky contact has a promising use in many fields, the defects in it, such as threading dislocations, stacking faults and stacking mismatch boundaries, degrade the characteristics of the GaSb-based devices, and thus influence on the electrical properties of GaSb Schottky contact. But fabricating reliable GaSb Schottky is not easy because of the Fermi level pinning close the valence band [2], and the insulating interfacial layer at the boundary [3]. Al has been reported in some studies to be good candidate for fabricating rectifying contact.

Positron annihilation spectroscopy is a powerful tool to detect vacancy-type defects in crystalline solids [4]. Recent developments in slow positron beam methods allow the investigation of such properties for thin films, layered structures. In this work, the Doppler broadening technique has been used to study the metal-semiconductor Al/GaSb interface on a slow positron beam. In this study, Al contacts onto Te-doped n-type GaSb samples (n~10^{18} cm^{-3}) have been made by electron beam evaporation. The depth profile of S parameter was obtained by varying the positron energies from 0-15 keV, thus the interfacial properties of the Al/n-GaSb contact and its annealing behavior, were investigated. The X-ray diffraction experiment was done to verify the positron experiments results.

II. EXPERIMENTAL

The GaSb samples used in this work is Te-doped LEC grown n-GaSb purchased from Wafer Technology U.K. Samples (dimensions about 1 cm x 1 cm) cut from the wafers were degreased with acetone and methanol, and then rinsed with deionization water. 8 mm diameter Al circular disc was deposited onto the sample surface in an electron beam evaporator at the pressure of 1.31 mPa. For the two series of Al/n-GaSb samples, their Al thicknesses were 100 and 200 nm, respectively. Annealing of samples was performed in a forming gas (N_2:H_2 80%-20%) atmosphere for a period of 30 min. The treatment conditions for all the samples were listed in Table I. Variable-energy positron measurements were performed for all specimens at the Nuclear Solid Lab. of the University of Science and Technology of China. The vacuum in the target chamber is 1.33 μPa. The Doppler broadening technique of annihilation radiation is applied to measurements. Photo-peak energy spectra of annihilation 511 keV γ-rays from the target were measured using a high purity Ge (HPGe)

<table>
<thead>
<tr>
<th>Sample</th>
<th>Al thickness/nm</th>
<th>Annealing</th>
</tr>
</thead>
<tbody>
<tr>
<td>F1K000</td>
<td>100</td>
<td>no</td>
</tr>
<tr>
<td>F1K250</td>
<td>100</td>
<td>250 °C, 30 min</td>
</tr>
<tr>
<td>F1K400</td>
<td>100</td>
<td>400 °C, 30 min</td>
</tr>
<tr>
<td>F2K000</td>
<td>200</td>
<td>no</td>
</tr>
<tr>
<td>F2K250</td>
<td>200</td>
<td>250 °C, 30 min</td>
</tr>
<tr>
<td>F2K400</td>
<td>200</td>
<td>400 °C, 30 min</td>
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</tbody>
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* Author to whom correspondence should be addressed. E-mail: wenghm@ustc.edu.cn
detector, which had an energy resolution of 1.2 keV (FWHM) at 514 keV γ-rays of $^{85}$Sr. The line-shape $S$ parameter is defined as the ratio of central region area to the total area under the annihilation peak. Each spectrum contains a total count of $5 \times 10^3$.

$$S = \frac{\int_{-a}^{a} c(E)dE}{\int_{-\infty}^{\infty} c(E)dE}$$

where $c(E)$ is the measured spectrum with the background subtracted, $(-a, a)$ is an energy region at the peak energy 511 keV, taking an energy shift of about 1 keV at both sides of the peak energy. The variation of the $S$ parameter is mainly influenced by the relative counts around the peak, so it provides the information about the positron annihilating with the lower momentum electrons. The atoms lack in the defect region will cause the increase of $S$ parameter for the larger fraction of lower momentum electrons.

All $S$-$E$ curves, which were the measured relative $S$ parameter as a function of positron implantation energy $E$, were analyzed using the VEPFIT program [5]. The fitted $L_{\text{eff}}$ indicates effective diffusion lengths of positron in material. It has the relationship with the trapping of defect in sample [6] as follow:

$$L_{\text{eff}} = \left( \frac{D_+}{\lambda_b + k_i} \right)^{1/2}$$

where $D_+$ is positron diffusion coefficient, $\lambda_b$ is the positron annihilation rate in the bulk, $k_i$ is the trapping rate in a concentration of defects $c_i$, and it is proportional to the defect-concentration: $k_i = \mu_i \times c_i$.

### III. RESULTS AND DISCUSSION

The $S$ parameter profiles of the as-fabricated Al/GaSb samples with 100 and 200 nm are shown in Fig. 1 (a) and (b) respectively. A three-layer model Al-interface-bulk was employed to analyze the $S(E)$ data of the Al/GaSb system, thus the resultant $S$ parameter is given by:

$$S(E) = f_s(E)S_s + f_{AI}(E)S_{AI} + f_i(E)S_i + f_B(E)S_B$$

where $S_j (j = s, AI, i$ or $b )$ are the $S$-parameters and the fractions of positron annihilating in surface and the corresponding layers of Al, interface and GaSb bulk. The fitted results of the $S$ parameters and the effective positron diffusion lengths $L_{AI}$ of the different layers are shown in Fig. 2. The fitted curves for different samples are shown in Fig. 1 and it is noticed that they give good representations to the experimental data. From Fig. 2, it is clearly shown that all the fitted $S$ parameters and $L_{\text{eff}}$ have the similar annealing trends regardless of the samples’ Al film thickness.

For the Al overlayer, $S_{AI}$ decreases with the increasing of the annealing temperature from 0.56-0.57 to 0.537, while its $L_{\text{eff}}$ increases from several nm to $\sim50$ nm. This is possibly due to the annealing out of the positron trapping vacancies in the Al film. The Al film deposited by electron beam evaporation is polycrystalline with grain size of about 100 nm [7]. With the increasing of the annealing temperature, the reforming process of the Al atoms improves the quality of the Al crystal, so many vacancies annealed out.

From the Fig. 2(b), for the interface, it can be seen that the $S_i$ has a value of $\sim0.59$ with the annealing temperature lower than 250 °C. As the annealing temperature increases to 400 °C, the $S_i$ abruptly drops to $\sim0.47$. While the fitted effective diffusion length increased from 15 nm to 50 nm. At first glance, the decreases of the $S_i$ and the increases of $L_{\text{eff}}$ are induced by the annealing out of the positron trapping center.

In the interface region, the defects can be induced by two processes. The first is atomic collision between Al and GaSb which can create some vacancies during the evaporation. These vacancies can be annealed out after lower temperature annealing. The slightly decreases of the $S_i$ and the slightly increases of the $L_{\text{eff}}$ in the range of annealing temperature from 0 °C to 250 °C indicate this fact. For the second, the mismatch between these two materials and the poor preparation of the GaSb surface can induce many dislocations and mismatch and so on. These kinds of defects will be annealed out with higher temperature annealing. So after 400 °C annealing, the $S_i$ decreases abruptly to $\sim0.47$ and the $L_{\text{eff}, i}$ increases significantly from 15 nm to $\sim50$ nm.

In fact, during the annealing, a chemical reaction occurs at interface region:

$$\text{xAl} + \text{GaSb} \rightarrow \text{Al}_x \text{Ga}_1 - x \text{Sb} + \text{xGa}$$

(4)

This makes the interface layer increases from several nm to 40 nm, which were the results of experiment data.
FIG. 2 The fitted values of the $S$ parameters and the positron diffusion length of the Al overlayer, the interfacial region and the GaSb bulk as a function of the annealing temperature. The fitting of the $S(E)$ data employed the three layer model. ○: 100 nm, △: 200 nm.

FIG. 3 The width of the interfacial region as a function of the annealing temperature. The triangles denote the 200 nm-Al coverage; the circles denote the 100 nm-Al coverage. ○: 100 nm, △: 200 nm.

fitted using the VEPFIT program, as showed in Fig.3.

It is noticed after the 400 °C annealing, the $S_i$ decreases to value of ~0.47, which is significantly smaller than those of $S_{Al}$ and $S_B$ at any annealing temperatures. However, at the same time, the value of $L_i$~50 nm after the 400 °C annealing is much smaller than the value of $L_B$~400 nm after the 250 °C annealing. This implies despite of the very low value of $S_i$ ~0.47 after the 400 °C annealing, there are significant amount of positron traps in the interfacial region. This leads us to speculate that the dramatically drop of the $S_i$ and the increase of the interfacial width upon annealing are also related to the formation of new phase at the interface originated to the inter-diffusion of atoms Al and Ga across the boundary. The new formed phase has a lower $S$ parameter. The Al/GaSb interface has been investigated by secondary ion mass spectroscopy (SIMS), Auger electron spectroscopy (AES) and soft X-ray photoemission spectroscopy although the results are divergent. Oueini et al. [8], Rouillard et al. [9], and Walters and Williams [10] have observed significant atomic inter-diffusion across the Al/GaSb interface, and Poole et al. [11] have observed an abrupt Al/GaSb boundary.

For the GaSb bulk layer, it is noticed that after the 250 °C annealing, the $S_B$ drops and the effective diffuse length $L_B$ increases from 100-200 nm to ~400 nm. It is also obvious that after 400 °C annealing, the $S_B$ increases, despite the magnitudes of increase for the two samples with different thickness are different. Moreover, the effective diffuse length $L_B$ significantly drops from 400 nm to 30 nm. In Ling et al.’s previous positron lifetime and temperature dependent Hall (TDH) stud-
ies of the electron irradiated LEC grown p-type GaSb [12,13], two different kinds of $V_{Ga}$-related defects having lifetimes of 280 and 315 ps were identified. These two components were attributed to the two $V_{Ga}$-related defects having different microstructures rather than the same $V_{Ga}$-related defect having different charge states and thus different degree of relaxation. The $V_{Ga,315}$ intensity decreases and the $V_{Ga,280}$ intensity increases with increasing annealing temperatures when the annealing temperature is below 300 °C. As the annealing temperature reaches 300 °C, the $V_{Ga,315}$ component disappears. Moreover, the concentration of the acceptor at $E_V + 34$ meV increases from $2 \times 10^{11}$ cm$^{-3}$ to $1.8 \times 10^{18}$ cm$^{-3}$ when the annealing at 400 °C. This acceptor was attributed to the GaSb anti-site. In present study, the initial decrease of $S_B$ and increase of $L_{+,B}$ are possibly the resultant effect of the annealing out of $V_{Ga,315}$ despite of the creation of $V_{Ga,280}$. The subsequent increase of $S_B$ and the significant drop of $L_{+,B}$ from 400 nm to 30 nm are possible due to the generations of the $V_{Ga,280}$ and the 34 meV acceptor, which acts as positron shallow trap.

In order to verify the positron experiments results, the Al/GaSb samples with 200 nm-Al thickness were examined by X-ray diffraction measurement. As shown in Fig.4, the Al (311) peak intensity increases with the increasing annealing temperatures. These implied that with the increasing of annealing temperature, in the reforming process of the Al atoms the crystal grain begins to have some orientation uniformity. The vacancies in Al layer were decreased and the quality of Al layer was improved. The improvement of Al layer also reduces the mismatch condition in the interface.

![FIG. 4 The results of X-ray diffraction of Al/GaSb samples with Al thickness of 200 nm.](image)

**IV. CONCLUSIONS**

Using a slow positron beam, annealing study of the Al/GaSb system was performed. The $S$ parameter against positron energy data were successfully fitted by a three layer model (Al/interface/GaSb). The annealing out of the open volume defects in the polycrystalline Al layer was revealed by the decrease of the $S$ parameter and the increase of the effective diffusion length of the Al layer, it caused by the reforming of Al atoms in this layer. For the as-deposited samples, a ~5 nm interfacial region with $S$ parameter larger than those of the Al layer and the bulk was identified. After the 400 °C annealing, this interfacial region extends to over 40 nm and its $S$ parameter dramatically drops. This is possibly due to the new defect formation induced by the atoms’ inter-diffusion at the interface. Annealing behaviors of $S_B$ and $L_B$ of the GaSb bulk showed the annealing out of positron traps (possibly the $V_{Ga}$-related defect) at 250 °C. However, further annealing at 400 °C induces formation of positron traps, which are possibly another kind of $V_{Ga}$-related defect and the positron shallow trap GaSb anti-site. Compared the results of the positron technology with that of the X-ray diffraction experiment, it is obvious that the later results verify the conclusion of the positron technology.

**V. ACKNOWLEDGMENT**

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