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Schottky barrier height of MnSb(0001)/GaAs(111)B contacts: Influence of interface structure

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The Schottky barrier height (SBH) of MnSb(0001)/*n*-GaAs(111)B diodes was investigated in terms of current–voltage characteristics for three different GaAs surfaces, GaAs ($\sqrt{19} \times \sqrt{19}$), GaAs (2×2), and sulfur passivated GaAs. We observed that the SBH and the ideality factor changed significantly depending on the GaAs surface structure prepared before the MnSb growth. The sulfur passivated sample was superior to the others in that it has a lower ideality factor and higher barrier. The SBH fell off linearly with increasing ideality factor n . The SBH of MnSb(0001)/*n*-GaAs(111)B was estimated to be 0.94 eV by extrapolating the linear relationship to $n=1$. © 2000 American Institute of Physics. [S0021-8979(00)02916-9]

I. INTRODUCTION

The hybrid structures consisting of a ferromagnetic material and a semiconductor have attracted a great deal of interest and new ideas such as a spin-polarized field effect transistor,¹ spin-valve transistor,² and spin-filter/aligner,³ have been brought into the semiconductor device concept. Recently spin-polarized light-emitting diodes at low temperature were reported using a diluted magnetic semiconductor (DMS) spin aligner⁴ or a ferromagnetic semiconductor injector.⁵ An essential requirement for these hybrid structure devices is the injection of spin-polarized electrons into the semiconductor. In particular, III–V compound semiconductors such as GaAs are believed to be the most useful candidates for spin related electronic devices.⁶ However, a high surface-state density of GaAs causes significant difficulties in implementing the spin device ideas. The high surface density pins the Fermi level near the midgap and affects the carrier lifetime and the spin relaxation at the metal/GaAs interface.⁷ Jonker *et al.* measured a carrier lifetime of the Fe/GaAs(001) interface at room temperature and reported the carrier lifetime enhancement because of a decrease in the density of the interface states by Fe–As bond formation at the interface.⁸ Moreover, the defects and the dislocation at the ferromagnet / semiconductor interface can cause spin-flip scattering, and as a result, spin dephasing. It is desirable to prepare a well-controlled ferromagnet/semiconductor interface to investigate the spin injection.

We have successfully grown epitaxial thin films of ferromagnetic MnSb(0001) on GaAs(111)B.⁹ MnSb is a ferromagnetic metal with a high Curie temperature of 585 K and has a large magnetic moment ($3.3 \mu_B/\text{Mn}$).¹⁰ Manganese pnictides, such as MnSb and MnBi, have been investigated intensively as materials with a large Kerr rotation angle for application of magnet-optical recording. MnSb has NiAs-type hexagonal structure and the lattice mismatch between the GaAs(111) plane and the MnSb(0001) plane is small (3.2%).¹¹ The magnetic easy axis of MnSb is parallel to the *a* axis at room temperature. But the easy axis changes from *a* axis to *c* axis with increasing Mn content¹² and we can control whether the magnetic easy axis is parallel or perpendicular to the plane. Therefore we choose MnSb as a ferromagnetic material on GaAs. The investigation of reflection high-energy electron diffraction (RHEED) and transmission electron microscopy (TEM) showed that an atomically flat heterointerface and no interdiffusion at the interface between MnSb and 2×2 reconstructed GaAs(111) were realized.⁹ Schottky barrier height (SBH) reflects mostly surface (interface) states at the metal-semiconductor (MS) contacts. For example, Hirose *et al.* reported the SBH of Sb/GaAs(100) depending on the surface reconstruction of GaAs.¹³ The sulfur passivation of the GaAs surface reduces the surface states and realizes the enhancement of photoluminescence intensity¹⁴ and controllable SBHs.¹⁵ In this article, we report SBH of MnSb(0001) on GaAs(111)B with three different surfaces, 2×2 and $\sqrt{19} \times \sqrt{19}$ reconstructed surfaces and the sulfur passivated surface. The relationship between SBH and the interfacial structure is discussed.

II. EXPERIMENTAL DETAILS

The sample growth was performed using molecular beam epitaxy (MBE). The base pressure of the chamber was in the low 10^{-11} Torr range. The substrate was *n*-GaAs(111)B ($n=0.9 \sim 1 \times 10^{18}/\text{cm}^3$). The surface struc-

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FIG. 1. RHEED patterns of GaAs(111)B and MnSb(0001) surfaces along $\langle 110 \rangle$ GaAs (a axis of MnSb). (a) GaAs ($\sqrt{19} \times \sqrt{19}$) and (b) MnSb on GaAs ($\sqrt{19} \times \sqrt{19}$), (c) GaAs (2×2) and (d) MnSb on GaAs (2×2), (e) sulfur passivated GaAs and (f) MnSb on sulfur passivated GaAs.

tures were confirmed by RHEED. In order to obtain a well-defined reconstructed surface of 2×2 and $\sqrt{19} \times \sqrt{19}$, a few tens of nm (typically 20 nm) Si-doped ($1 \times 10^{18} \text{ /cm}^3$) n -GaAs buffer layer was grown at 580°C after native oxide removal. To obtain 2×2 surface the substrate was cooled down to below 400°C with As flux, while obtaining $\sqrt{19} \times \sqrt{19}$ surface without As flux. Both RHEED patterns show sharp streaks with specular spots indicating that well reconstructed surfaces were realized [Figs. 1(a), and 1(c)]. The $\sqrt{19} \times \sqrt{19}$ surface, however, exhibited chevron-shaped features, which implied that pyramid-like structures or slight roughness may be formed. In order to obtain sulfur passivated GaAs, the GaAs substrates were soaked in an $(\text{NH}_4)_2\text{S}_x$ solution for 1 h. The wafer was rinsed in de-ionized water, dried with N_2 gas, glued with indium onto the molybdenum holder, and loaded into the MBE chamber immediately. After degassing at 400°C for 10 min, we confirmed that sulfur still remained on the GaAs surface by Auger electron spectroscopy (AES). No oxygen peaks were observed. The RHEED pattern with respect to 1×1 surface was clearly observed [Fig. 1(e)]. MnSb films 20 nm thick were epitaxially grown on these GaAs substrates at 300°C . During first 0.5 nm growth the reconstruction patterns of GaAs faded away and then transformed into a 2×2 reconstruction pattern of MnSb. The 2×2 reconstructed surfaces

FIG. 2. Current-voltage characteristics of MnSb(0001)/ n -GaAs(111)B (sulfur passivated) diodes with various mesa sizes. The current is raw data, not converted into the current density.

were observed for all samples. The main streaks had a separation that was almost the same as that of GaAs. It showed that the growth direction of the film was (0001) and the epitaxial relationship in plain was the a axis of MnSb // $\langle 110 \rangle$ GaAs. The RHEED patterns of MnSb on the 2×2 and the sulfur passivated GaAs surface were streaky [Figs. 1(d), and 1(f)] and that of MnSb on the $\sqrt{19} \times \sqrt{19}$ surface appeared streaky with slightly additional spots.

Different size diodes with the mesa area of 20×20 , 50×50 , 100×100 and $200 \times 200 \mu\text{m}^2$ were prepared using conventional photolithography and wet chemical etching. The SiO_2 isolation layer was sputter deposited and contact holes were made by photolithography and liftoff. Metal pads were deposited on the contact hole pattern in order to make electrical contacts to both the mesa area and the etched GaAs substrate surface; the contact holes for the GaAs surface were formed close to the mesa area in order to minimize voltage drop across the GaAs substrate. Back ohmic contacts were also formed by an indium alloying at 200°C . The current-voltage characteristics were measured using a HP4156 precision semiconductor parameter analyzer at room temperature in the dark. The voltage drop across the junction was measured using the contacts to the GaAs substrate and the mesa, while the current was driven through the contacts to the back of the substrate and the top of the mesa. Figure 2 shows typical forward current characteristics of MnSb(0001)/ n -GaAs(111)B diodes. The MnSb was grown on sulfur passivated GaAs. Each curve in Fig. 2 corresponds to one of the four different mesa sizes since the current axis is not converted into current densities. The SBH Φ_B and ideality factor n were obtained by the conventional thermionic emission analysis using a least-squares fitting of the straight region of semilogarithmic I - V curve.¹⁶ The Richardson constant A^* is $8.6 \text{ A/cm}^2/\text{K}^2$ for n -GaAs.

III. RESULT AND DISCUSSION

Figure 3 shows the SBH of MnSb/GaAs(111)B diodes as a function of the ideality factor n . The data are shown in Fig. 4 according to the GaAs surface structures or surface treat-

FIG. 3. Relationship between Schottky barrier height and ideality factor of MnSb(0001)/n-GaAs(111)B diodes. The MnSb was grown on (2×2) reconstructed (○), $\sqrt{19} \times \sqrt{19}$ reconstructed (□), and sulfur passivated (◇) GaAs substrates. The barrier heights Φ_B decrease proportional to ideality factor n . The solid line indicates a least-squares fit. The intrinsic SBH can be obtained as 0.94 eV by extrapolating to $n=1$.

ment, (a) GaAs 2×2, (b) GaAs $\sqrt{19} \times \sqrt{19}$ and (c) sulfur passivated GaAs. We found a linear relationship between the barrier heights and the ideality factors regardless of the GaAs surface condition. Such linear relationship was also reported in Ag/n-Si diodes, though their investigating range of the ideality factor was between 1.01 and 1.22.¹⁷ The barrier height decreases proportionally with the increasing ideality factor. Therefore we can obtain the intrinsic SBHs for the MnSb/GaAs(111)B diodes by extrapolating the lines to $n=1$. In Fig. 4, the best-fit line gives the barrier height of $\Phi_B^0 = 0.94 \pm 0.02$ eV for the intrinsic SBH of MnSb(0001)/n-GaAs(111)B. Taking into account an image force lowering of the barrier height for GaAs ($1 \times 10^{18} \text{ cm}^{-3}$), the barrier height is estimated to be 0.07 eV higher. Oshima *et al.* investigated Schottky barrier formation of epitaxial MnSb(0001)/n-GaAs(111)B by means of synchrotron radiation photoelectron spectroscopy (SRPES).¹⁸ The SBH was determined to be 0.93 eV from the As 3*d* core level shift due to MnSb growth, which is in good agreement with our result. Thus the extrapolating method of the Φ_B - n linear relationship enables us to estimate intrinsic SBH from I - V measurement of MS contacts. The SBH for MnSb/GaAs(111)B can be explained by the advanced unified defect model (AUDM).¹⁹ In this model, the defects responsible for the double donor and acceptor states are As antisites and Ga antisites, respectively, which play an important role in the Fermi level pinning in GaAs. The As antisites are located at 0.75 and 0.5 eV from the valence band maximum (VBM) and the Ga antisites are located near the VBM, which compensates donor electrons. The pinning of Fermi level depends on the number and position of these antisite defects and the Fermi level is pinned between these antisite states. This model shows that removing excess As will drive the Fermi level toward the VBM, that is, increase the SBH. Yang, Zhang, and Xie investigated the chemisorption of a Mn adatom on a GaAs surface and found that Mn will form a strong Mn-As bond.²⁰ As a result any excess As at the

FIG. 4. Relationship between Schottky barrier height and ideality factor of MnSb(0001)/n-GaAs(111)B diodes fabricated on (a) $\sqrt{19} \times \sqrt{19}$ reconstructed, (b) 2×2 reconstructed, and (c) sulfur passivated GaAs substrates. Two samples were prepared, respectively, which was shown by solid marks and open marks. The mesa areas of diodes are 20×20 (○, ●), 50×50 (□, ■), 100×100 (◇, ◆) and 200×200 μm^2 (△, ▲).

surface is consumed and the number of As antisites is reduced. The Fermi level is pinned at around 0.5 eV and the high SBH of about 0.94 eV is expected in the present MnSb/GaAs junctions.

The scatter of the ideality factors and the barrier heights implies that the metal/semiconductor (MS) interfaces may be inhomogeneous. The conventional thermionic emission

theory gives the SBH and the ideality factor independently, which gives no correlation between them. Tung reported that the MS contacts are greatly influenced by the existence of junction inhomogeneity, and modeled imperfect MS contacts by assuming laterally inhomogeneous barrier height.²¹ According to this model, the lower effective barrier height and the larger ideality factor can be described by the barrier height inhomogeneity. When n is close to unity (~ 1.3), a linear relationship can be qualitatively obtained from his formulation and extrapolating the line to $n=1$ gives the intrinsic barrier height. However, the slope of Φ_B - n line expected from the model was about twice as large as that of our experimental results. The ideality factor $n \gg 1$ is beyond the limit of an approximation and the barrier height is not proportional to the ideality factor. It may be necessary to take into account other effects in this model. Since the doping level of our sample was relatively high, a tunnel current may also influence the high ideality factor. However, the ratio of tunneling and thermionic current $J_{\text{tunnel}}/J_{\text{thermionic}}$ (at the doping level of $1 \times 10^{18} \text{ cm}^{-3}$ and at 300 K) is about 0.3 and the n is changed from 1 (ideal thermionic emission) to 1.1 by the contribution of the tunnel current.²² The tunnel current cannot explain the large n such as 2. The reason why the linear relationship between the barrier height and the ideality factor spreads over a wide range is under investigation.

We believe that the macroscopic inhomogeneity comes from the lateral distribution of microscopic defects because the scatter of the ideality factor depends on the surface condition of GaAs. The origin of the defects will be discussed below. The ideality factor dependency on the GaAs surface structure is a result of differences in the amount of low-barrier regions. As is shown in Fig. 4, the diodes with larger mesa area tend to have a higher (= worse) ideality factor and a lower barrier height. The larger mesa area is thought to have more low-barrier regions, which cause lower Φ_B and higher n . The order of decreasing ideality factor was GaAs ($\sqrt{19} \times \sqrt{19}$), GaAs (2×2), sulfur passivated GaAs. The As on the surface of GaAs ($\sqrt{19} \times \sqrt{19}$) is less than that of GaAs (2×2). Since many Ga atoms appear on the surface,²³ the Ga-Sb bond formation is expected at the early stage of the MnSb deposition. The GaSb formation may result in lower SBH regions in MS contact because GaSb has the smaller band gap (0.72 eV). Moreover, the $\sqrt{19} \times \sqrt{19}$ reconstructed surface tends to have roughness²⁴ and the pyramid-like structures may be formed on $\sqrt{19} \times \sqrt{19}$ reconstructed surface during decreasing temperature without As flux. These may lead to leaky characteristics in diodes. Such inhomogeneity lowers in SBH and increases the ideality factor for GaAs ($\sqrt{19} \times \sqrt{19}$). We prepared two samples for each surface. Figure 4 shows that the results of samples 1 and 2 are different, though they were expected to be similar. It can originate from the slight differences of the growth conditions, for example, the cooling rate after the growth of GaAs buffer layer. It may cause the difference of the As coverage or the hillock generation even if the RHEED pattern looks similar. Consequently, the inhomogeneity causes the wider distribution of diode properties. In the case of the sulfur passivated GaAs, the difference of samples 1 and 2 was relatively small. It is probably due to the fact that since sulfur

and Ga bond is strong and the surface states are decreased, the sulfur passivation makes a chemically stabilized surface.²⁵ Therefore the GaSb formation is prevented by the sulfur termination and it leads to the formation of a homogeneous MS contact, that is, the samples on sulfur passivated GaAs have the higher SBH and the lower ideality factor.

The top values of practical SBH are 0.86 eV at $n = 1.38$ for GaAs (2×2), 0.82 eV at $n = 1.47$ for sulfur passivated GaAs and 0.76 eV at $n = 1.63$ for GaAs ($\sqrt{19} \times \sqrt{19}$). The top value of GaAs (2×2) is larger than that of sulfur passivated GaAs. However, the diodes on sulfur passivated GaAs are superior to other samples in the distribution narrowness of the ideality factor and an average SBH. Thus the sulfur passivation of the GaAs substrate is useful in order to obtain higher and reproducible SBHs. On average, the SBH of about 0.8 eV corresponding to an ideality factor or about 1.5 was achieved by sulfur passivated GaAs ($n \sim 1 \times 10^{18} \text{ cm}^{-3}$).

IV. CONCLUSION

The Schottky barriers of MnSb(0001)/ n -GaAs(111)B were prepared on three different GaAs surfaces, namely, GaAs ($\sqrt{19} \times \sqrt{19}$), GaAs (2×2) and sulfur passivated GaAs. We found a linear relationship between the SBH and the ideality factor. The SBH of MnSb(0001)/ n -GaAs(111)B was estimated to be 0.94 eV by extrapolating the linear relationship to $n=1$. This value is in good agreement with the result from the SRPES, 0.93 eV. The extrapolation method of Φ_B - n linear relationship is useful to estimate the SBH from I - V measurement. The high SBH is caused by the chemisorption of a Mn adatom and the reduction of excess As on the GaAs surface because of the strong Mn-As interaction. The order of decreasing ideality factor was GaAs ($\sqrt{19} \times \sqrt{19}$), GaAs (2×2) and sulfur passivated GaAs. The ideality factor dependency on the GaAs surface structure is a result of differences in the amount of low-barrier regions. The GaSb formation at the interface is one of the origins of low-barrier regions because of the smaller band gap. Sulfur passivation is effective in preventing GaSb formation and gives a lower ideality factor and higher barrier heights.

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