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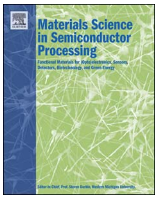

Modulation of Fermi level pining position at metal/*n*-Ge interface by semimetal $Ge_{1-x}Sn_x$ and Sn interlayers

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ABSTRACT

We have investigated the dependence on the metal work function of Schottky barrier height (SBH) of metal/$Ge_{1-x}Sn_x$/*n*-Ge Schottky diode and have discussed the mechanism of SBH reduction by insertion of a $Ge_{1-x}Sn_x$ interlayer. The SBH of metal/$Ge_{1-x}Sn_x$/*n*-Ge Schottky diodes for various metal electrodes of Zr, Al, and Au were estimated. Even after the insertion of $Ge_{1-x}Sn_x$ layer at various metal/*n*-Ge interface, the dependence of SBH on the metal work function is weak as well as direct metal/*n*-Ge contact. We also found that the SBH decreases by 0.1–0.2 eV by the insertion of a $Ge_{1-x}Sn_x$ or Sn layer regardless of the metal work function. This result means that the SBH is determined only by the interfacial semimetal $Ge_{1-x}Sn_x$ layer. Considering that density of states at the E_F and momentum of electrons in semimetal $Ge_{1-x}Sn_x$ and α-Sn are small, those epitaxial interlayers would suppress the metal induced gap state at the metal/Ge interface as well as the disorder induced gap states. Additionally, we demonstrated the reduction of the metal/*n*-Ge contact resistivity by introduction of a $Ge_{1-x}Sn_x$ interlayer.

1. Introduction

Germanium (Ge) is one of the most attractive semiconductors for channel material of next-generation metal-oxide-semiconductor field effect transistor (MOSFET). Because of small carrier effective mass of both electrons and holes in Ge and its small energy bandgap, Ge-channel MOSFET is expected to realize high-performance with low power consumption [1].

One of the challenges for realizing high-performance Ge-channel MOSFET is the reduction of parasitic resistance which mainly consists of source/drain resistance and metal/Ge contact resistance. The contact resistivity is essentially dominated by the Schottky barrier height (SBH) at the metal/semiconductor interface and the impurity concentration in the semiconductor. For an ideal case, SBH linearly depends with a slope of unity on the work function of a metal electrode [2]. However, for the practical case of metal/Ge contact, the Fermi level of metal is pinned near the valence band edge of Ge regardless of the kind of metal and SBH hardly depends on the metal work function. This phenomenon is called Fermi level pinning (FLP) [3,4]. Due to this strong FLP, SBH of metal/*n*-type Ge contact usually shows a value as high as 0.5–0.6 eV and a high contact resistivity at metal/*n*-Ge interface is one of serious problems for the practical application of Ge-channel MOSFET. Therefore, the development of technology for controlling SBH is necessary in order to reduce the contact resistivity.

Origins of FLP phenomenon at metal/semiconductor interface are discussed mainly with two interface state models. One is called metal induced gap state (MIGS) [5], which is attributed to the penetration of the electron wave function in metal into semiconductor with the quantum-mechanical effect. Another model is disorder induced gap state (DIGS), which is attributed to the disorder of atomic arrangement at the metal/semiconductor interface [6]. Based on these models, some technologies for controlling SBH of metal/Ge contact have been proposed, using wide bandgap interlayer [7,8], epitaxial metal/Ge contact [9,10], amorphous metal nitride interlayer [11], and so on. However, for the practical application, technology for controlling SBH of metal/Ge contact has to be still developed in order to realize a low enough contact resistivity.

Recently, we are focusing on the insertion of a germanium tin ($Ge_{1-x}Sn_x$) thin layer at metal/Ge interface to control the SBH. $Ge_{1-x}Sn_x$ has a diamond structure identical to that of Ge. An epitaxial layer of $Ge_{1-x}Sn_x$ on Ge enables the termination of dangling bonds on the Ge surface, and we expect the suppression of DIGS. Furthermore, semimetal $Ge_{1-x}Sn_x$ and α-Sn would suppress MIGS. Recently, Nishimura *et al.* reported the possibility that using a metal with a

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low electron density can weaken MIGS phenomena at the metal/Ge interface [12], supporting our suggestion partly. From the viewpoint of quantum mechanics, the quantity of electrons which penetrates into semiconductor should be determined by the quantity of incident electrons, the momentum of electrons, and the penetration probability. The penetration probability of electron is dominated by the energy bandgap of semiconductor. In addition, the quantity and the momentum of incident electrons are equivalent to the density states of electrons at the Fermi level in a metal. In semimetal $Ge_{1-x}Sn_x$ and α-Sn case, density states of electrons at Fermi level (E_F) is relatively small compared to typical metals, because E_F is very close to the conduction band minimum (E_C) in α-Sn, that means a small quantity of incident electrons and a small momentum of electrons.

Previously, we have achieved the epitaxial growth of a $Ge_{1-x}Sn_x$ layer with a Sn content up to 47% by a low temperature growth at 50 °C and the strain control [13]. We also reported that the SBH of aluminum (Al)/$Ge_{1-x}Sn_x$/*n*-Ge diode can be reduced with increasing the Sn content of the $Ge_{1-x}Sn_x$ interlayer [14]. Considering the practical application for Ge-channel MOSFET, deep understanding of the effect $Ge_{1-x}Sn_x$ interlayer on the SBH reduction will essentially contribute to the development of metal/*n*-Ge contact with an ultralow contact resistivity. However, the reason for the SBH reduction by introduction of $Ge_{1-x}Sn_x$ interlayer is still under discussion. In this study, we investigated the dependence on the metal work function of SBH of metal/Ge contact with a $Ge_{1-x}Sn_x$ interlayer. Additionally, from the result of this experiment, we discussed the mechanism of the SBH reduction by introduction of a $Ge_{1-x}Sn_x$ interlayer.

2. Experimental procedure

In this study, Schottky diodes with a metal/$Ge_{1-x}Sn_x$/Ge structure were fabricated as follows: substrate used was *n*-type Ge(001) with a resistivity of 2–3 Ω cm. After chemical cleaning using deionized water (DIW) and diluted hydrofluoric acid (DHF) solution, the Ge substrate was thermally cleaned at 430 °C in an ultra-high vacuum chamber with a pressure below 10^{-6} Pa. Subsequently, a 3-nm-thick $Ge_{1-x}Sn_x$ layer was deposited with molecular beam epitaxy (MBE) system on the Ge substrate at 50 °C. A Sn content of the $Ge_{1-x}Sn_x$ layer was estimated to be 42% using X-ray photoelectron spectroscopy. After the sample was taken out atmosphere, the surface oxide of the $Ge_{0.58}Sn_{0.42}$ layer was chemically removed using DIW and DHF solution. Immediately, a top electrode of zirconium (Zr), Al, or gold (Au) layer was formed on the $Ge_{0.58}Sn_{0.42}$ surface in high vacuum chamber. We prepared three kinds of metal electrode to change the work functions; those of Zr, Al, and Au are 4.05, 4.28, and 5.10 eV, respectively [15]. Finally, Al electrode was formed on the backside of the samples. For comparison, metal/Sn/*n*-Ge and metal/*n*-Ge Schottky diodes were fabricated. The Sn layer was deposited by electron beam evaporation in ultra-high vacuum chamber. The deposition temperature was room temperature, and the thickness of the Sn layer was 3 nm.

The epitaxial growth of a deposited $Ge_{0.58}Sn_{0.42}$ layer with a highly flat surface was confirmed using in-situ reflection high energy electron diffraction (RHEED), in-plane-XRD measurement, and atomic force microscopy (AFM) observation. Fig. 1**(a)–(d)** shows RHEED patterns after the deposition of $Ge_{0.58}Sn_{0.42}$, in-plane-XRD profile of the $Ge_{0.58}Sn_{0.42}$/Ge(001) sample, surface AFM image and surface line profile of the $Ge_{0.58}Sn_{0.42}$ layer, respectively. From the RHEED pattern after the deposition of $Ge_{0.58}Sn_{0.42}$, periodical sharp streaks indicating the epitaxial growth on Ge substrate were clearly observed. From the in-plane-XRD profile of $Ge_{0.58}Sn_{0.42}$/Ge(001) sample, we can also observe a weak diffraction peak related to the $Ge_{1-x}Sn_x$ overlapping on the strong diffraction peak of Ge substrate. In the AFM image, a flat and smooth surface was observed after the $Ge_{0.58}Sn_{0.42}$ deposition. These results indicate that the low temperature growth at 50 °C of an enough thin $Ge_{1-x}Sn_x$ layer are effective to epitaxial growth of uniform and flat $Ge_{1-x}Sn_x$ layer even with a Sn content of a few tens of percent. From the obtained RHEED pattern of a pure Sn layer, obscure halo pattern was observed, meaning that the existence of an amorphous Sn layer on Ge substrate.

3. Results and discussion

3.1. Dependence of SBH on metal work function

We measured the current density-voltage (*J*-*V*) characteristics for Zr, Al, and Au/$Ge_{0.58}Sn_{0.42}$/*n*-Ge(001) Schottky diodes to estimate SBHs. The measurement temperature was ranging from 200 to 300 K. *J*-*V* characteristics of Zr, Al, and Au/$Ge_{0.58}Sn_{0.42}$/*n*-Ge(001) Schottky diodes measured at 300 K are shown in Fig. 2. The rectifying property due to thermionic emission conduction can be seen in *J*-*V* characteristics of all Schottky diodes. In addition, these *J*-*V* characteristics hardly depend on the kind of metal electrodes even though the difference of the work functions between Zr and Au is as large as 1 eV. This implies that the dependence of the SBH on the metal work function is not significant in these samples.

In order to quantitatively estimate the SBHs, the saturation current density and the ideality factor were estimated from the forward *J*-*V* characteristics using the equations of the thermionic emission conduction. The current density at a metal/semiconductor interface is expressed as [2]:

$$J = J_S\left\{\exp\left(\frac{qV}{nk_BT}\right) - 1\right\} \tag{1}$$

$$J_S = A^*T^2\exp\left(-\frac{q\Phi_{Bn}}{k_BT}\right) \tag{2}$$

where J_S is the saturation current density, q is the elementary charge, *n* is the ideality factor, k_B is the Boltzmann constant, *T* is the measurement temperature, A^* is Richardson's constant, and Φ_{Bn} is the SBH. In this study, we estimated SBH using the forward *J*-*V* characteristics. This is because the forward current of a Schottky diode often reflects the property of thermionic emission conduction well, while the reverse current would include unignorable component related to tunneling current attributed to defects near the interface region. Additionally, when we estimated the SBH, the total current was separated into the areal and peripheral current components, based on the following equation [16]:

$$I_{total} = J_AA + J_PP, \tag{3}$$

where J_A is the areal current density, *A* is the contact area, J_P is the peripheral current density, and *P* is the contact perimeter length. We used only extracted J_A component for the SBH estimation. We consider that J_A reflects essential property of the current conduction at metal/Ge contacts and the peripheral current conducted at the contact edge would include any leakage current due to various unintentional reasons. The Arrhenius plots of J_S of Schottky diodes are shown in Fig. 3. The ideality factors for each diode are also shown. $_S$ *in the voltage region where the ideality factor is close to unity, 0.05–0.1 V. In that region, the J-V characteristics are on straight line*. The current density close to *V*=0 does not show a straight line in the logarithm plot. In this study, we estimated J_S in the voltage region where the ideality factor is close to unity, 0.05–0.1 V. In that region, the *J*-*V* characteristics are on straight line.The current density close to *V*=0 does not show a straight line in the logarithm plot. In this study, we estimated J_S in the voltage region where the ideality factor is close to unity, 0.05–0.1 V. In that region, the *J*-*V* characteristics are on straight line. For these case, the ideality factors of all Schottky diodes are close to unity in the region from 200 to 300 K. This means that thermionic emission conduction is the most dominant in all current components for the forward *J*-*V* characteristic at the interfaces. The SBHs of all diodes were estimated from the slopes of the Arrhenius plots of J_s/T^2 using