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Low-barrier Hetero Junction to N-type Silicon Using Novel Ultrathin Epitaxial Silicide Consisting of Tungsten-encapsulating Silicon Clusters

N. Okada[1, 2], N. Uchida[2], and T. Kanayama[1, 2]

[1] Institute of Applied Physics, University of Tsukuba, 1-1-1 Tenodai, Tsukuba, Ibaraki 305-8573, Japan
[2] National Institute of Advanced Industrial Science and Technology, 1-1-1 Higashi, Tsukuba, Ibaraki 305-8562, Japan
Phone: +81-029-861-2512 E-mail: okada-naoya@aist.go.jp

1. Introduction

As the shrinkage of Si device dimensions, metallic contact to Si is becoming increasingly important, in particular for metal source/drain (S/D) structures. As a contact technique to Si, Transition metal (TM) silicides have been considered as the S/D material in Schottky barrier MISFETs. However, one difficulty in achieving high performance with these MISFETs is high contact resistance due to the Schottky barrier height (SBH) between the TM silicide S/D and the Si channel. We have to use proper silicide metals to reduce the SBH. However, no metal species was found to give low SBH for n-type Si, while Pt silicide was available for p-type Si [1, 2]. Mise et al. showed that Ni disilicide S/D with segregation of n-type and p-type dopants at atomically flat metal/Si interfaces can work for both type MISFETs [3]. It is necessary to develop new fabrication methods for a low-SBH junction with atomic accuracy because segregation of dopant atoms may induce fluctuation in effective channel lengths for short-channel MISFETs.

Recently, a hetero-epitaxial junction technique for Si has been developed by using the thin silicide film composed of W-encapsulating Si_{10} cage clusters (WSi_{10}) [4]. Resulting epitaxial layers of one-several nm thickness were observed by a scanning transmission electron microscope (STEM). From X-ray photoelectron spectra (XPS), the valence band edge of the WSi_{10} film was 0.49 eV below the Fermi level, indicating that the film had a semiconducting energy gap [4]. In this work, we discuss the electrical junction characteristics of WSi_{10} films on n- and p-Si substrates by current-voltage (*I-V*) and capacitance-voltage (*C-V*) measurements.

2. Experimental

The substrates used were n- and p-Si (100) with resistivity of ~8 Ωcm (P and B doped, respectively). The hetero-epitaxial WSi_{10} film (epi-WSi_{10}) was fabricated by deposition of $WSi_{10}H_x$ clusters onto clean Si substrates at 350°C and subsequent annealing at 500°C [4-6]. The clean Si substrates were prepared using flashing above 1200°C for several times in an ultrahigh vacuum. To investigate the electrical junction characteristics between WSi_{10} films and Si, W electrodes were sputtered at room temperature (RT) on WSi_{10} films (Fig. 1).

3. Results and discussion

Fig. 1 shows a cross-section high-resolution STEM image of a WSi_{10} film sandwiched between n-type Si (100) and W (W/epi-WSi_{10}/n-Si). The STEM observation shows that an epitaxial layer of one-several nm thickness was formed at the interface, and an amorphous WSi_{10} layer remained on top.

Typical *I-V* characteristics at RT are shown for the W/epi-WSi_{10}/n-Si, W/non-epi-WSi_{10}/n-Si and W/epi-WSi_{10}/p-Si in Fig. 2. The non-epi-WSi_{10} is the WSi_{10} film deposited at 350°C on HF-cleaned Si (100) substrates without the flashing process and subsequently annealed at 500°C. An ohmic property was observed on the W/epi-WSi_{10}/n-Si, while rectification properties were observed on the W/non-epi-WSi_{10}/n-Si and W/epi-WSi_{10}/p-Si. To estimate barrier heights (BHs) of the junctions, we measured the reverse bias C^{-2}-V curves of the W/non-epi-WSi_{10}/n-Si and W/epi-WSi_{10}/p-Si at RT, as shown in Fig. 3. From the curves, the built-in potential (V_{bi}) of non-epi-WSi_{10}/n-Si and epi-WSi_{10}/p-Si was calculated to be 0.27 ± 0.01 eV and 0.57 ± 0.02 eV, respectively. The BH was obtained to be 0.59 ± 0.01 eV and 0.79 ± 0.02 eV as a sum of the V_{bi} value and the energy difference ($\Delta\Phi_f$) between band edges and the Fermi level of the n- and p-Si substrates. The $\Delta\Phi_f$ was estimated from the carrier concentration of the n- and p-Si substrates. The junction of non-epi-WSi_{10}/n-Si was not ohmic but showed a rectification property. This is due to the Fermi level pinning by interface states between the non-epi-WSi_{10} and n-Si. In contrast, the ohmic property of the epi-WSi_{10}/n-Si is attributed to the fact that there is no interface state at the clean hetero epitaxial interface.

Temperature dependence of the BH obtained from *C-V* characteristics of the W/epi-WSi_{10}/n-Si is shown in Fig. 4. When the temperature was higher than 220 K, the *C* could not be measured by the presence of leakage current because the depletion layer disappeared. This indicates that the epi-WSi_{10} film is an n-type semiconductor with a band gap narrower than Si and has a high carrier concentration; i.e., the Fermi level is close to the conduction band edge, as shown in Fig. 5. The ohmic property of the W/epi-WSi_{10}/n-Si is caused by the tunnel current between the W and epi-WSi_{10} film. This band alignment is consistent with a large BH (~0.8 eV) of the epi-WSi_{10}/p-Si, in which a hetero p-n junction is formed. Below 220 K, the

C-V characteristics were observed for epi-WSi_{10}/n-Si and the BH was estimated to be ~0.4 eV. This behavior is attributed to complete depletion of the epi-WSi_{10} film resulting from carrier (electron) freezing.

4. Conclusions

The epi-WSi_{10}/n-Si showed an ohmic property, while the junction to p-Si had a good rectification property with a large barrier height of ~0.8 eV. Thus, the epi-WSi_{10} film is an n-type narrow-gap semiconductor, the Fermi level of which is close to the conduction band edge of Si, and forms a low-barrier hetero junction to n-Si.

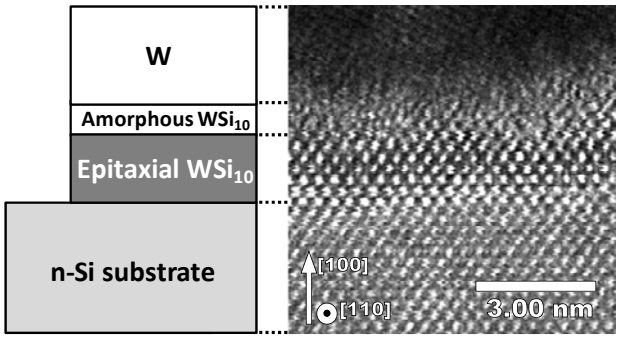

Fig. 1 Cross-section high-resolution STEM images of a WSi_{10} film formed on Si (100) viewed from the [110] direction, and schematic diagrams of sample configuration for *I-V* and *C-V* measurements.

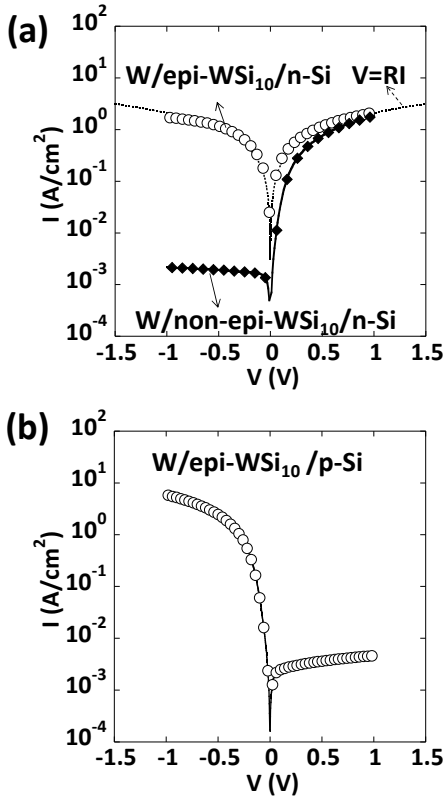

Fig. 2 *I-V* characteristics of (a) the W/epi-WSi_{10}/n-Si, W/non-epi-WSi_{10}/n-Si, and (b) W/epi-WSi_{10}/p-Si at RT.

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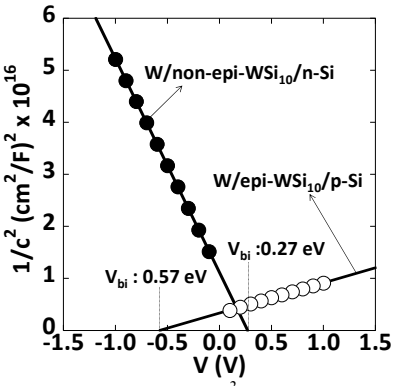

Fig. 3 The reverse bias C^{-2}-V curves of the W/non-epi-WSi_{10}/n-Si and W/epi-WSi_{10}/p-Si at RT.

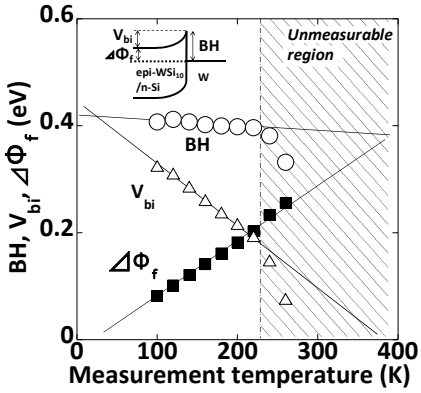

Fig. 4 Temperature dependence of the barrier height (BH), the built-in potential (V_{bi}), and the energy difference between conduction band and Fermi level ($\Delta\Phi_f$) of the n-Si obtained from *C-V* characteristics of the W/epi-WSi_{10}/n-Si.

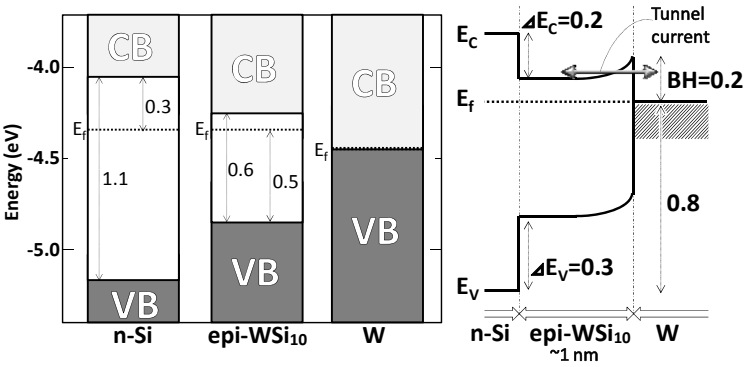

Fig. 5 Band diagrams of the W/epi-WSi_{10}/n-Si near RT estimated from *I-V* and *C-V* characteristics. The band gap of the epi-WSi_{10} film is derived from XPS (assuming the conduction band edge-E_f= 0.1 eV).