Extended Abstracts of the 2007 International Conference on Solid State Devices and Materials, Tsukuba, 2007, pp. 1038-1039

F-10-1

Dependence of Electrical Characteristics on Interfacial Structures of Epitaxial $NiSi_2$/Si Schottky Contacts Formed from Ni/Ti/Si System

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1. Introduction

Formation of silicide/Si contacts with an ultra flat interface on ultra shallow source/drain junctions is required for future Si MOSFETs. However, there is a problem of the inhomogeneity of the interfacial structure due to grain boundaries of generally used polycrystalline silicides. Additionally, there is concern that the fluctuation of the Schottky barrier height (SBH) will become obvious due to the fluctuation of interface orientations between polycrystalline silicide grains and a Si substrate with shrinkage of contact area to the size of silicide grains.

Epitaxial $NiSi_2$ on Si substrate is one of promising candidates to realize not only the homogeneous interface structure [1-4] but also the uniform electrical characteristic due to a single SBH. We previously reported the formation of epitaxial $NiSi_2$ layers having an ultra flat interface without {111} facets by solid phase reaction of Ni/Ti/Si(001) system [1, 2]. In this study, we investigated electrical characteristics of epitaxial $NiSi_2$/Si Schottky contacts formed from Ni/Ti/Si system and clarified the dependence of them on the interfacial structure between epitaxial $NiSi_2$ layers and Si substrates.

2. Experiments

After chemical cleaning of Si(001) substrates, it was loaded into an ultra high vacuum (UHV) chamber. A 2-nm-thick Ti layer and a 9-nm-thick Ni layer were successively deposited. Samples were then annealed at 300ºC or 350ºC for 30 min in the same UHV chamber. Some samples were additionally annealed at a temperature ranging from 650ºC to 850ºC for 30 sec in a N_2 ambient by using the rapid thermal annealing (RTA) system. Both n- and p-type Schottky diodes whose contact area size was $500\times500\ \mu m^2$ were fabricated.

3. Results and Discussion

Figures 1(a)-1(d) shows scanning electron microscopy (SEM) images of center and edge regions of contact area in Schottky diodes. In the sample annealed at 350ºC for 30 min, the epitaxial $NiSi_2$/Si interface consists of a lot of domains surrounded {111} facets (Fig. 1(a) and 1(b)). These {111} facets at the interface decrease with increase in annealing temperature [2, 3]. In the sample annealed at 750ºC, there are no {111} facets at the center region of the epitaxial $NiSi_2$/Si interface (Fig. 1(c)), while {111} facets are formed at the edge region of the contact (Fig. 1(d)).

Figure 2 shows forward current-voltage (I-V) characteristics of both n- and p-type Schottky diodes annealed at 750ºC for various measurement temperatures. I-V curves for both samples show good thermionic emission current characteristics. The saturation current, J_s and the ideality factor, n were estimated from I-V characteristics [5]. Figure 3 shows Arrhenius plots of $\ln(J_s/T^2)$. These plots exhibit good linear characteristics, and SBHs for all samples were estimated by same method. We also estimated SBH from capacitance-voltage (C-V) characteristics with the reverse-biased condition.

Figure 4(a) and 4(b) show the annealing temperature dependence of SBH estimated from I-V and C-V characteristics for n- and p-type Schottky diodes, respectively. In n-type contact, SBHs estimated from both I-V and C-V characteristics decrease with increase in annealing temperature. Tung *et al*. reported SBHs of 0.65 eV and 0.40 eV for the interface between epitaxially grown $NiSi_2$ on n-Si(111) and n-Si(001), respectively [6, 7]. The annealing temperature dependence of SBHs for n-type diodes in our study can be explained by the transformation of the interfacial structure in epitaxial $NiSi_2$/Si contacts and the reduction of SBH at central area of the contact.

In the case of the p-type diode formed at 350ºC, with many {111} facets, SBHs of both I-V and C-V exhibit comparable values and agree with previously reported SBH of 0.47 eV for the epitaxial $NiSi_2$(111)/p-Si(111) interface [6]. However, the discrepancy of SBH values estimated from I-V and C-V characteristics becomes large in samples with the uniform $NiSi_2$(001)/Si(001) interface as shown in Fig. 1(c) and 1(d). High SBH values estimated from C-V characteristics agrees with the SBH of 0.74 eV for the epitaxial $NiSi_2$(001)/p-Si(001) interface [7]. Low SBH values estimated from I-V characteristics are accounted for by much larger current density of the $NiSi_2$(111)/p-Si(111) interface than the $NiSi_2$(001)/p-Si(001) interface due to its low SBH. The current density ratio of $NiSi_2$(111)/p-Si(111) to $NiSi_2$(001)/p-Si(001) is estimated to over 10^7 even at room temperature because of the exponential dependence of the current density on SBH. Therefore, I-V characteristics of p-type diodes annealed over 750ºC are dominated by the current component through {111} facets at the edge region, while the area ratio of {111} facets to the $NiSi_2$(001)/Si(001) interface occupying almost contact is estimated to about 10^{-3}.

4. Conclusions

We investigated electrical characteristics of epitaxial

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NiSi$_2$/Si Schottky contacts, which have various interface structures. Locally formed {111} facets having low SBH strongly affect I-V characteristics of epitaxial NiSi$_2$/p-Si(001) contacts. Results in this study also promise simultaneous realization of low contact resistance for both n- and p-type contacts with low SBHs by controlling the interfacial structure of epitaxial NiSi$_2$/Si contacts.

Acknowledgement

This work was partly supported by the MEXT, Grant-in-Aid for Scientific Research for Priority Area, No. 18063012, 2006.

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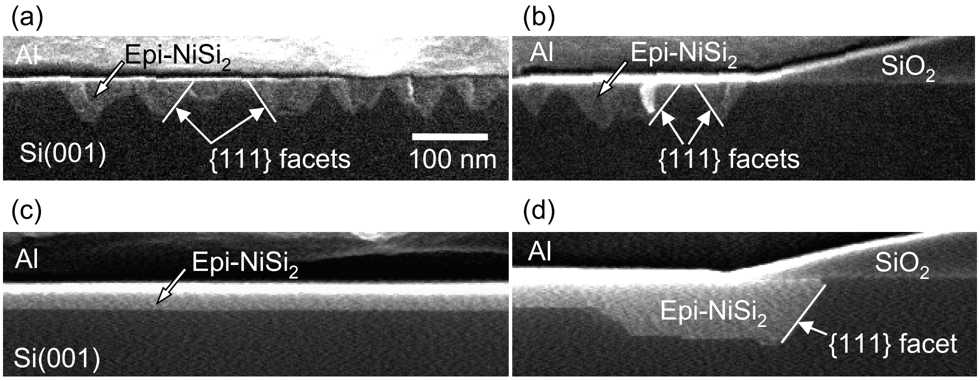

Fig. 1 SEM images of contact area in epitaxial NiSi$_2$/Si Schottky diodes; (a) center and (b) edge regions of the sample annealed at 350ºC and (c) center and (d) edge regions of one annealed at 750ºC.

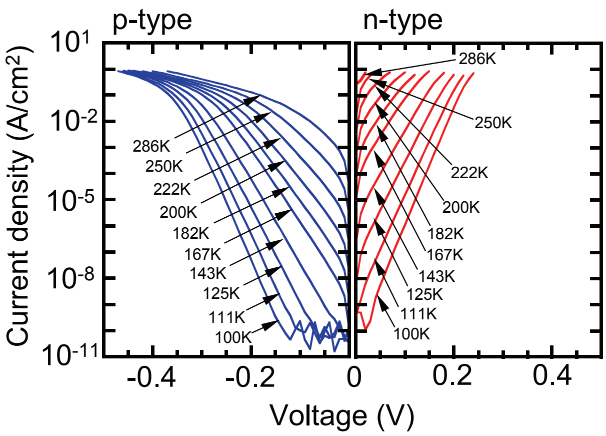

Fig. 2 Forward I-V characteristics of n- and p-type epitaxial NiSi$_2$/Si Schottky diodes annealed at 750ºC for various measurement temperatures ranging from 100 K to 286 K.

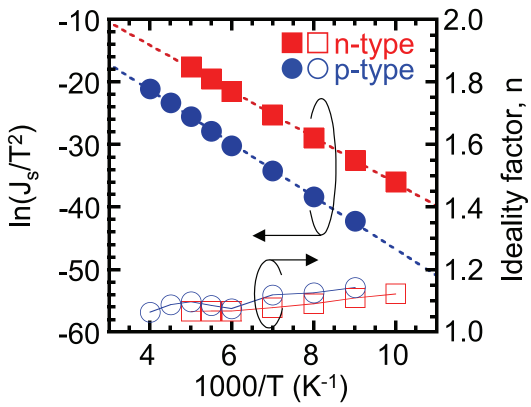

Fig. 3 Arrhenius plots of ln(J_s/T^2) estimated from I-V characteristics of n- and p-type Schottky diodes annealed at 750ºC. Ideality factors are also shown.

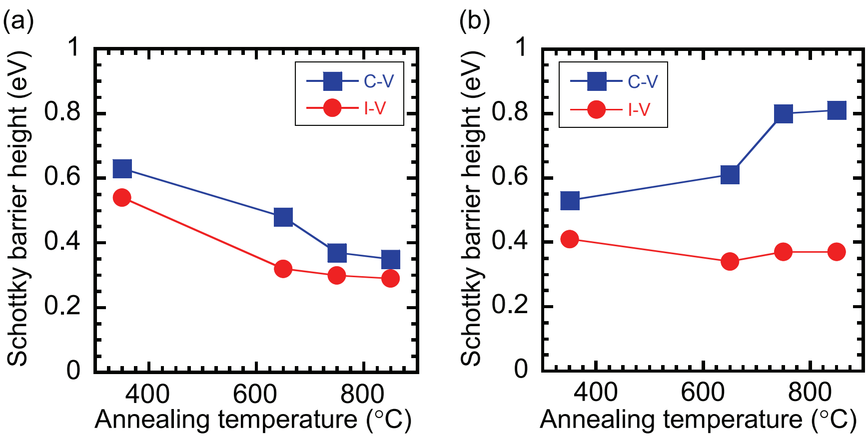

Fig. 4 Annealing temperature dependence of SBH estimated from I-V and C-V characteristics of (a) n- and (b) p-type epitaxial NiSi$_2$/Si Schottky diodes.