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Investigation of Elemental Composition and Bonding Structure at the Sb-Doped Ni-FUSI/SiO_2 Interface

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In advanced CMOS devices, among many kinds of gate electrodes, fully silicide (FUSI) has an advantage because of controllable threshold voltage. It was proposed that dopants segregate at the silicide/gate dielectrics interface and the thin dopant pileup layer would modulate the threshold voltage of gate electrode [1]. The dopant pileup had been investigated by macroscopic techniques such as AES and SIMS, but these techniques provide no information on detailed elemental compositions and bonding structures at the interface. Here, we have investigated the structure at the interface between Sb-doped Ni-FUSI gate electrode and SiO_2 dielectrics by the high-spatial resolution techniques such as EDX and EELS in STEM. A poly-Si film deposited on SiO_2 dielectric film was implanted with Sb, followed by activation annealing. After Ni deposition on poly-Si, silicidation was processed using rapid thermal annealing. EDX and EELS analyses were performed on a JEM2100F (JEOL) operating at 200 kV.

Fig. 1 shows HAADF-STEM images at the NiSi/SiO_2 interface. We found characteristic two regions about NiSi/SiO_2 interface structure. In Fig. 1(a), thickness of SiO_2 dielectrics was increased and thin high contrast layer was on SiO_2. We found that this high contrast layer is not Sb segregation but Ni simple substance, by EDX and EELS analyses. On the contrary, in Fig. 1(b), we didn't found the phenomena as in the region (a). The phenomena found at region (a) were well explained as follows. Some of native oxide would remain at poly-Si surface before Ni deposition. The position of the residual oxide at the surface of poly-Si would move to Si-substrate side together with the consumption of poly-Si, finally arrive at SiO_2 dielectric when NiSi formation was completed. Therefore, the thickness of SiO_2 would seem to be increased. At the place where the residual oxide would arrive at SiO_2 dielectric, the amount of Si supplied into NiSi side would be small, due to the lack of poly-Si and the increase of oxide layer. The amount of Ni diffused from Ni-rich silicide would be abundant, so Ni would exist as a simple substance without the reaction with Si.

In the region (b), we could detect only Sb segregation at NiSi/SiO_2 interface. Ni-L_3 ELNES at the Sb segregation layer shows a very small shoulder around 862 eV, while the ELNES of NiSi has no shoulder at this energy (Fig. 2). This small shoulder could be seen in the theoretical ELNES calculated for NiSb (by first-principles band structure calculation, Wien2K code), where Sb was substituted for Si in MnP-type NiSi. Since the structure of NiSi above the Sb segregation layer is also the MnP-type structure, it is suggested that Sb at NiSi/SiO_2 interface would exist in NiSi crystal being substituted for Si atoms. In Fig. 3, we find a coupling of states at about 8-10eV in unoccupied Ni d and Sb d calculated density of states (DOS) of NiSb (dotted line in Fig. 3), corresponding to the position of the small shoulder in Ni-L_3 ELNES at NiSi/SiO_2, in the same way as Ni_2Si reported in our previous study [2]. Therefore, it appears that the chemical bonding between Ni and Sb atoms in MnP-type NiSb structure has weak covalent character, which means that in the Sb segregation area at the bottom of Ni-FUSI, there is weak covalent bonding between Ni and Sb atoms.

References
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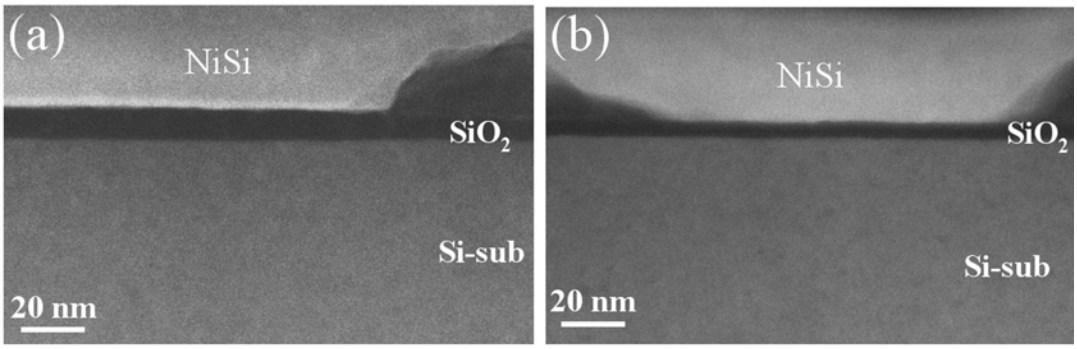

Fig. 1 HAADF-STEM images at $NiSi/SiO_2$ interface.

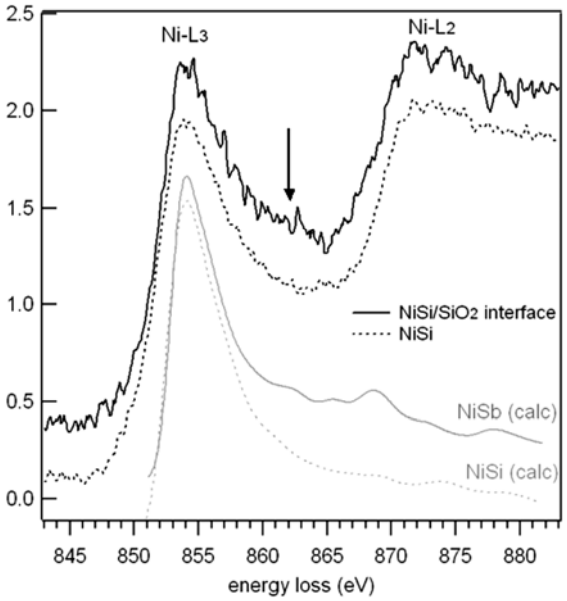

Fig. 2 Experimental Ni-$L_{2,3}$ and theoretical Ni-L_3 ELNES at $NiSi/SiO_2$ interface in the region (b) and NiSi for comparison.

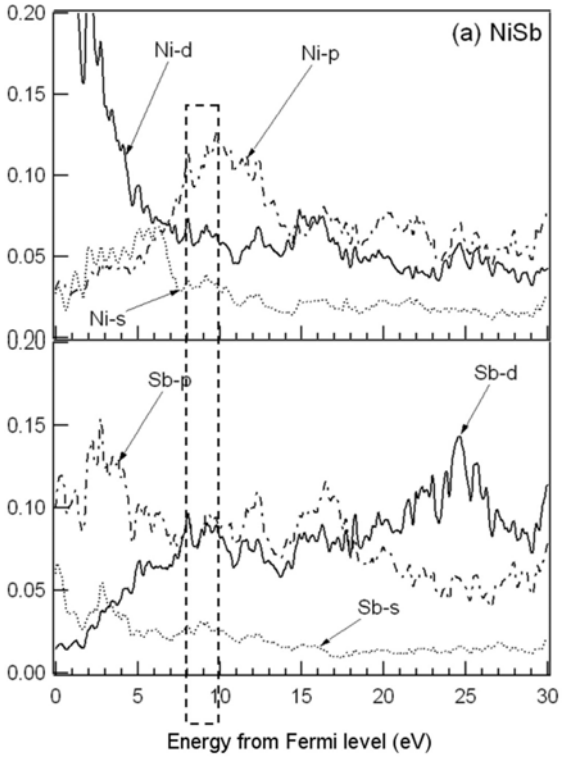

Fig. 3 Calculated unoccupied density of states (DOS) of MnP-type NiSb.

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