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Influence of Ge and C for reaction in Ni/p$^+$-$Si_{1-x-y}Ge_xC_y$/Si(100) contacts

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1. Introduction

Realization of the low contact resistivity at metal/semiconductor interfaces is a key issue in the Si ultra-large scale integrated circuit technology. Nickel monosilicide (NiSi) has been previously reported to be one of promising candidates for the contact materials used in sub-100 nm CMOS devices [1] and we have recently demonstrated low contact resistivities on the order of 10^{-8} $\Omega\cdot cm^2$ for both n$^+$- and p$^+$-Si contacts using NiSi [2]. Another approach, based on the bandgap engineering, has been also performed to lower the contact resistivities: the introduction of SiGe intermediate layer between the metal and the Si substrate [3] Furthermore, it has been reported that C incorporation into the SiGe offers several advantageous effect, e.g. compensation of strain caused by the SiGe-Si lattice mismatch, blocking the diffusion of dopant impurities such as boron [4], and the band offset produced at the conduction band edge. In this paper, we have focused on Ni/Si(C) and Ni/SiGeC systems on Si(100) substrates and investigated the solid phase reactions which occur during silicidation annealing. Through the analysis for samples with various compositions, the effects of Ge and C on the structural and the electrical properties of Ni-silicide films have been examined.

2.Experimental

Substrates used were p-type Si(100) wafers with resistivities of 0.8-1.2 $\Omega\cdot$cm. p$^+$-$Si_{1-x-y}Ge_xC_y$ layers (x = 0-0.466, y = 0-0.012) with the thickness of about 300 nm were epitaxially grown on the substrate at 500-650°C by an ultraclean hot-wall low pressure chemical vapor deposition (LPCVD) system. A 20-nm-thick Ni film was deposited on the p$^+$-$Si_{1-x-y}Ge_xC_y$ layers at room temperature in an ultra-high vacuum chamber with a base pressure below 1×10^{-9} Torr, followed by annealing at 350°C for 30 min in the same chamber. Some samples were then annealed at 600-850°C for 30 sec in a nitrogen atmosphere as second-step annealing. X-ray diffraction (XRD) analysis, cross-sectional transmission electron microscopy (XTEM) were employed to reveal the crystallographic structure and the film morphology. The sheet resistance of the film was measured by a linear four-point probe method.

3.Results and Discussion

Figure 1 shows XRD profiles of Ni/p$^+$-$Si_{1-x-y}Ge_xC_y$ samples with various Ge and C composition after annealing at 850°C. In the samples without Ge, no specific peaks corresponding to poly-Ni($Si_{1-\alpha-\beta}Ge_\alpha C_\beta$) can detected, independently of the C composition. This is due to the fact that the $NiSi_2$(311) peak overlaps the Si(311) peak. Therefore, the phase transformation from NiSi to $NiSi_2$ occurs during the annealing and the $NiSi_2$ is epitaxially grown on the Si layer with 0.4% C, similarly to the case of the pure Si substrate [2]. On the other hand, diffraction peak patterns of poly-Ni($Si_{1-\alpha-\beta}Ge_\alpha C_\beta$) are observed in the samples containing Ge (x=0.143 and 0.466). This result indicates the increase in the NiSi-$NiSi_2$ phase transformation temperature, strongly suggesting the enhanced thermal stability of Ni($Si_{1-\alpha-\beta}Ge_\alpha C_\beta$) due to Ge incorporation. Figures 2(a) and 2(b) show XTEM images of Ni/p$^+$-$Si_{0.522}Ge_{0.466}C_{0.012}$/Si samples after annealing at 350°C and RTA at 850°C, respectively. In Fig. 2(a), a continuous poly-Ni($Si_{1-\alpha-\beta}Ge_\alpha C_\beta$) film conformable to the p$^+$-SiGeC layer is clearly observed. This film morphology was found to be drastic changed by 850°C-annealing, as shown in Fig. 2(b). Although the phase transition to $NiSi_2$ did not occur yet, the film agglomeration is obviously observed on the SiGeC surface. Furthermore, as seen in the vicinity of the SiGeC/Si interface, new phases of $NiSi_2$ with {111} facets were epitaxially grown into the Si substrate. This $NiSi_2$ phase formation is probably due to the Ni segregation to misfit dislocations pre-existing at the interface during the annealing.

Figure 3 shows the relationship between the sheet resistance and the annealing temperature for a various types of Ni/p$^+$-$Si_{1-x-y}Ge_xC_y$/Si samples. In the samples with Ge, the sheet resistance gradually increases with the annealing temperature and reaches the value of substrate resistance after 850℃-annealing. From the XTEM result shown in Fig. 2(b), it is likely that this sheet resistance increase was caused by the agglomeration of poly-Ni($Si_{1-\alpha-\beta}Ge_\alpha C_\beta$). Note that the value of sheet resistance keeps a low even after 750°C-annealing in the samples containing only C. Figure 4 shows a comparison between two film morphologies in a Ni/Si samples [2] and in the Ni/p$^+$-$Si_{0.996}C_{0.004}$/Si sample after 750℃-annealing. In the Ni/Si sample shown in Fig. 4(a), agglomeration of the silicide and large roughness at the silicide/Si interface are clearly observed, resulting in the exposure of Si surfaces. On the other hand, the sample with C shown in Fig. 4(b) exhibits continuous film morphology with a comparatively flat silicide/Si(C) interface. No silicide agglomeration and Si exposure were observed in this sample. This morphological difference accounts for the measured lower sheet resistance of the Ni/p$^+$-$Si_{0.996}C_{0.004}$/Si sample than those in the Ni/Si and the C incorporation into Si play a critical role in suppressing the agglomeration during the annealing.

4.Conclusions

We have investigated the structural and electrical properties of Ni/p$^+$-SiGeC/Si(100) systems with various Ge and C composition. Mainly three essential results have been obtained as follows.

- The incorporation of Ge raises the phase transformation temperature but enhances the agglomeration of the $Ni(Si_{1-\alpha-\beta}Ge_{\alpha}C_{\beta})$ phase.
- Abnormal $NiSi_2$ formation at the SiGeC/Si interface occurs in the sample with high contents of Ge, which might be due to the Ni segregation to the pre-existing misfit dislocations.
- C in the Si effectively suppresses the agglomeration of the monosilicide layer so that low sheet resistance values ann be obtained even after 750°C-annealing.

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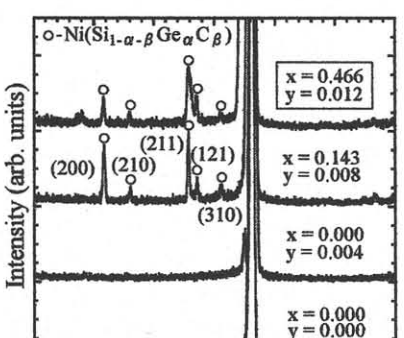

Fig. 1: XRD profiles of Ni/p$^+$-$Si_{1-x-y}Ge_xC_y$ samples annealed at 850°C.

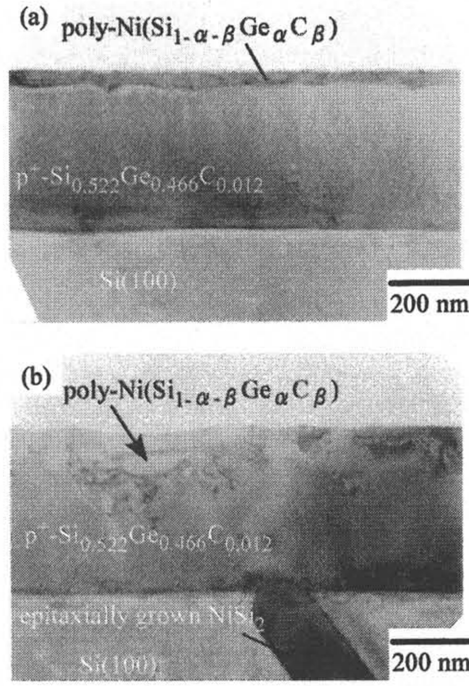

Fig. 2: XTEM images of the samples of Ni/p$^+$-$Si_{0.522}Ge_{0.466}C_{0.012}$/Si samples (a) after the first step 350°C annealing and (b) after RTA treatment at 850°C.

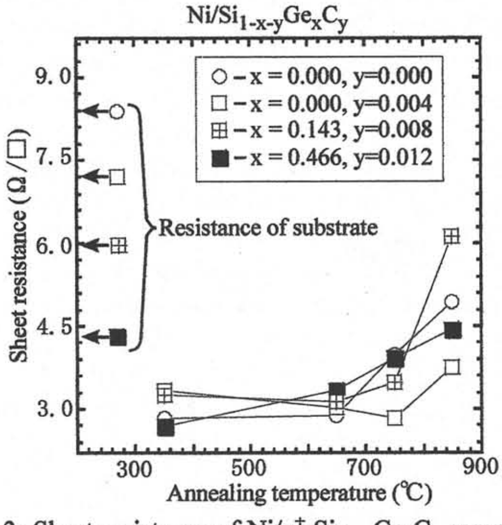

Fig. 3: Sheet resistance of Ni/p$^+$-$Si_{1-x-y}Ge_xC_y$ samples as a function of annealing temperature.

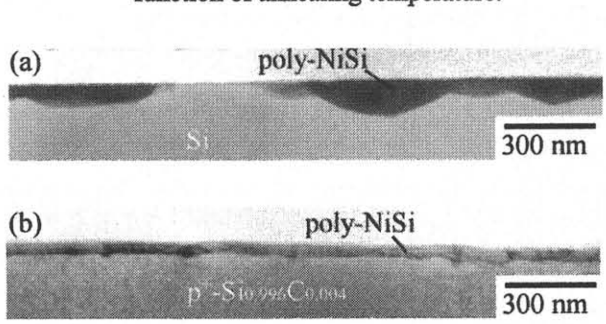

Fig. 4: XTEM images of (a) the Ni/Si sample and (b) the Ni/p$^+$-$Si_{0.996}C_{0.004}$/Si sample annealed at 750°C.