Surface, structural, and electrical properties of C54 $TiSi_2$ thin films grown on *n*-Si (100) substrates by using high-temperature sputtering and one-step annealing

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The surface, the structural, and the electrical properties of C54 $TiSi_2$ thin films grown on *n*-Si (100) substrates by using a high-temperature sputtering and one-step annealing method were investigated to produce Ohmic contacts with low specific contact resistances. Atomic force microscopy images showed that the surfaces of the annealed C54 $TiSi_2$ thin films grown on the *n*-Si (100) substrates became smooth due to the increase in the substrate temperature. Scanning electron microscopy images, energy dispersive X-ray fluorescence, and X-ray diffraction patterns showed that thin layers were C54 $TiSi_2$ polycrystalline films. Current-voltage measurements showed that the specific contact resistance of the C54 $TiSi_2$/*n*-Si (100) heterostructures decreased dramatically with increasing substrate temperature. These results indicate that C54 $TiSi_2$ thin films grown on the *n*-Si (100) substrates by using the high-temperature sputtering and one-step annealing method hold promise for potential applications in Si-based ultra-large-scale integration devices.

1. Introduction

$TiSi_2$ thin films have attracted much attention because of their potential applications in electronic devices [1, 2]. $TiSi_2$ thin films have been extensively used in ultra-large-scale integrated devices as contacts and gate electrodes because of their low resistivities, good thermal stability, and minimal contact resistance. $TiSi_2$ exists in two phases: a metastable C49 base-centered orthorhombic phase that is formed at a lower temperature and a stable face-centered orthorhombic C54 phase into which the C49 phase is transformed at higher temperatures [3]. However, when the dimensions of the devices are reduced to shrink below 1 μm, there is the inherent problem due to the resistivity of C49 $TiSi_2$ being dramatically higher than the resistivity of C54 $TiSi_2$ [4–6]. Thus, when the C49 $TiSi_2$ phase is formed during the growth process of $TiSi_2$ thin films, since the size of the crystals in the C49 $TiSi_2$ thin film is smaller than the fine linewidth of the electrode, the density of the C49 $TiSi_2$ thin film within the fine linewidth of the electrode is high. Some works suggested preamorphized methods of doping with impurities of As, Ge, Sb, or Mo into the Si substrates to improve the electrical properties of the contact interfaces [7–9]; however, the optimum formation conditions of C54 $TiSi_2$ thin films have not yet been clarified [10, 11]. Even though some works concerning the dependence of structural and electrical properties on substrate temperature for annealed C54 $TiSi_2$ thin films grown on *p*-Si substrates have been performed [12], systematic studies of the surface, the structural, and the electrical properties of C54 $TiSi_2$ thin films formed by simple methods are still very important for applications in electronic devices.

In this paper, we report on the systematic data on the surface, the structural, the electrical, and the contact properties of C54 $TiSi_2$ grown on *n*-Si (100) substrates by using the high-temperature sputtering and one-step annealing method. Atomic force microscopy (AFM) measurements were performed to characterize the surface microstructural properties of the C54 $TiSi_2$ layers grown on Si substrates under various growth conditions, and scanning electron microscopy (SEM), energy dispersive X-ray fluorescence (EDX), and X-ray diffraction (XRD) measurements were carried out in order to investigate the structural properties of the annealed $TiSi_2$ thin films. Current-voltage (I-V) measurements were performed to investigate the electrical properties of the C54 $TiSi_2$/*n*-Si (100) heterostructures.

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2. Experimental details

The $TiSi_2$ thin film samples used in this study were grown on (100)-oriented n-Si substrates by using the DC magnetron-sputtering deposition method. Polycrystalline Ti with a purity of 99.99% was used as a source target material and was precleaned by repeated sublimation. The resistivity of the Si substrate used in this experiment was approximately between 10 and 15 Ω·cm. The substrate was etched in a solution of H_2SO_4 and H_2O_2 (4:1) at 40°C for 5 min and the etched in a mixture of HF and H_2O (1:10) at room temperature for 5 min. After the cleaned Si substrate had been dried at 100°C in a nitrogen atmosphere for approximately 10 min, it was mounted into a chamber. The substrate temperature for the growth of the Ti thin film was changed from 27 to 350°C. A thermal annealing process in the temperature range between 450 and 750°C was performed to form the $TiSi_2$ thin film.

3. Results and discussion

Fig. 1 shows AFM images of C54 $TiSi_2$ thin films grown on Si (100) substrates at (a) 27, (b) 100, (c) 200, and (d) 250°C by using sputtering methods and annealed at 650°C for 60 s. The root-mean-square average surface roughnesses of the $TiSi_2$ thin films grown at 27, 100, 200, and 250°C are 157.8 Å, 29.5 Å, 36.7 Å, and 57.1 Å, respectively, as shown in Fig. 2. The images in Fig. 1 also indicate that the surfaces of the $TiSi_2$ thin films grown on the n-Si (100) substrates at 100, 200, and 250°C were much smoother than the surface grown at 27°C and that the surfaces of the $TiSi_2$ thin films grown on the n-Si (100) substrates by using a high-temperature sputtering method can be improved in comparison with those grown by using a room-temperature sputtering method.

Fig. 3 shows the cross-sectional SEM image of the $TiSi_2$ thin films grown on the n-Si (100) substrate at 200°C and subsequently annealed at 650°C for 60 s. Even though the growth of the $TiSi_2$ thin films was performed at substrate temperatures between 27 and 250°C, only the structural properties of the $TiSi_2$/n-Si(100) heterostructures grown at a substrate temperature of 200°C are reported because they had the best surface morphologies among the several samples, which was confirmed by the AFM images. When the substrate temperature was 200°C, the Ti layer almost disappeared after the annealing treatment resulting in the formation of a $TiSi_2$ thin layer, as shown in Fig. 3, which was confirmed by EDX measurements. The result of the EDX spectrum confirmed that samples consisted of Ti and Si and that the composition ratio of Ti to Si for the sample was approximately 1:2. Fig. 4 shows the XRD pattern of the $TiSi_2$ thin films grown on the n-Si (100) substrate at 200°C and subsequently annealed at 650°C for 60 s. The peaks corresponding to the C54 $TiSi_2$ thin film are clearly observed in Fig. 4. These SEM, EDX, and XRD results indicate that the formed films grown on the n-Si (100) substrates at 200°C and subsequently annealed at 650°C for 60 s are polycrystalline C54 $TiSi_2$.

Fig. 5 shows that the sheet resistance of the $TiSi_2$ thin films on n-Si (100) substrates at (a) 27, (b) 100, and (c) 200°C by using sputtering methods as a function of the annealing temperature. The sheet resistance decreased with increasing substrate and annealing temperatures. The dramatic decrease in the sheet resistance originates from the more formation of C54 $TiSi_2$ thin film with increasing substrate temperature. Therefore, the increases of the substrate and annealing temperatures reduce the sheet resistance of the C54 $TiSi_2$ thin film.

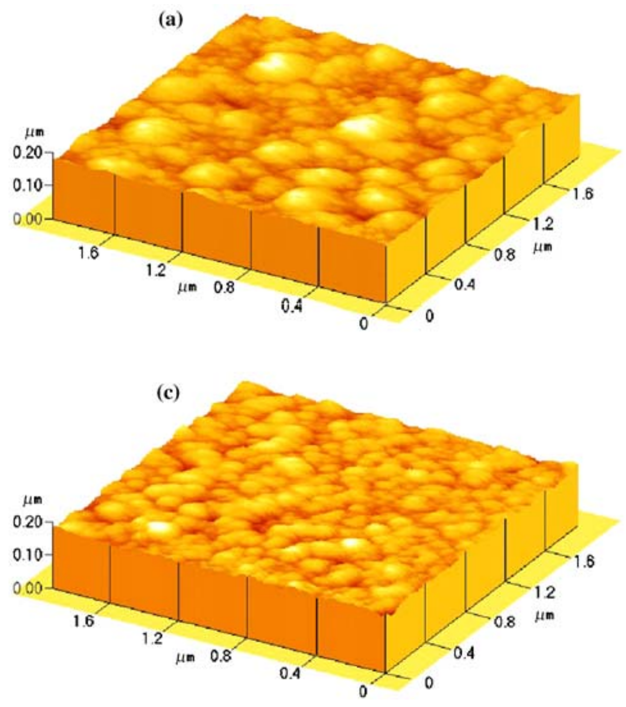

Figure 1 Atomic force microscopy images of the C54 $TiSi_2$ thin films grown on n-Si (100) substrates by sputtering at (a) 27°C, (b) 100°C, (c) 200°C, and (d) 250°C and subsequently annealed at 650°C for 60 s.

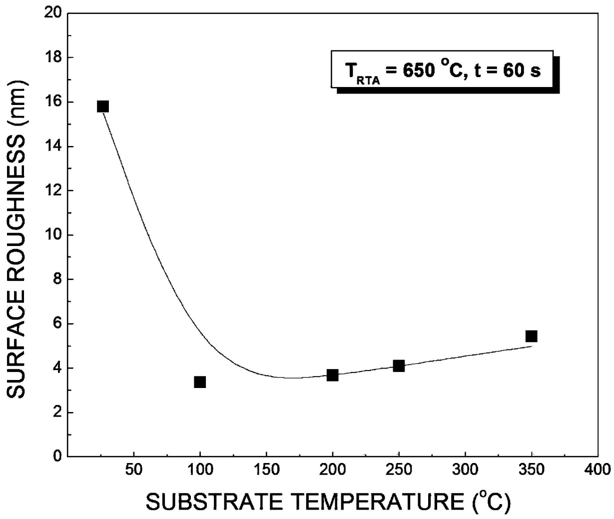

Figure 2 Surface roughness of the C54 $TiSi_2$ thin films grown on *n*-Si (100) substrates and annealed at 650°C for 60 s as a function of the substrate temperature.

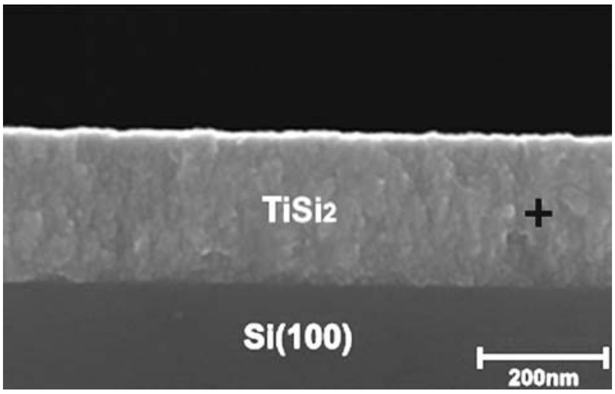

Figure 3 Cross-sectional scanning electron microscopy image of the $TiSi_2$ thin film grown on the *n*-Si (100) substrate at 200°C and subsequently annealed at 650°C for 60 s. +represents the position for the energy dispersive X-ray fluorescence measurements.

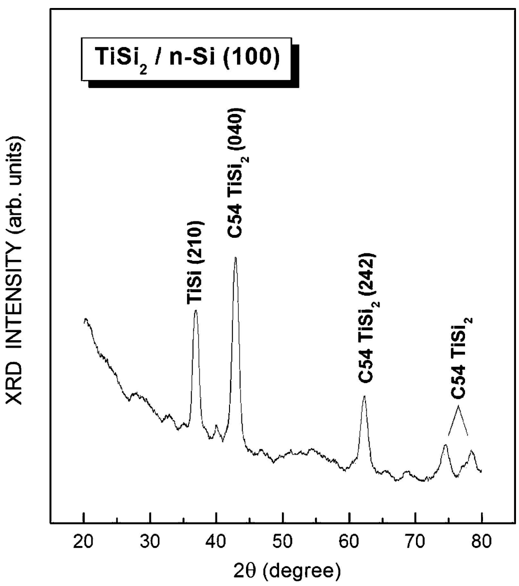

Figure 4 X-ray diffraction pattern of the $TiSi_2$ thin film grown on the *n*-Si (100) substrate at 200°C and subsequently annealed at 650°C for 60 s.

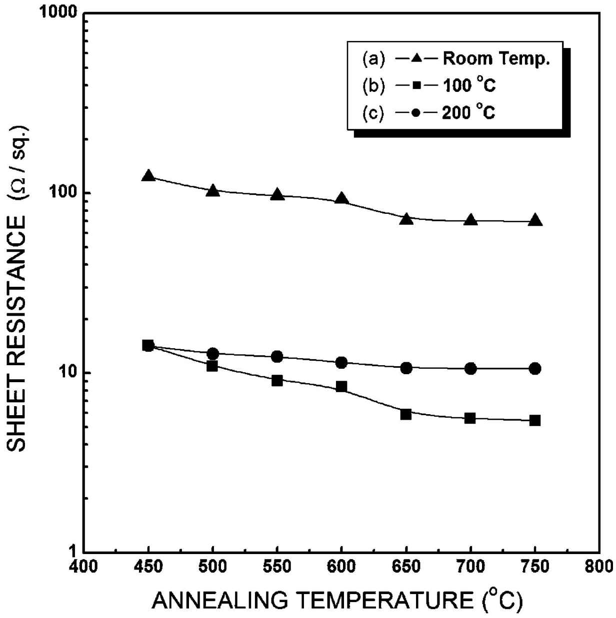

Figure 5 Sheet resistance of the C54 $TiSi_2$ thin films grown on *n*-Si (100) substrates by sputtering at (a) 27°C, (b) 100°C, and (c) 200°C as a function of the annealing temperature.

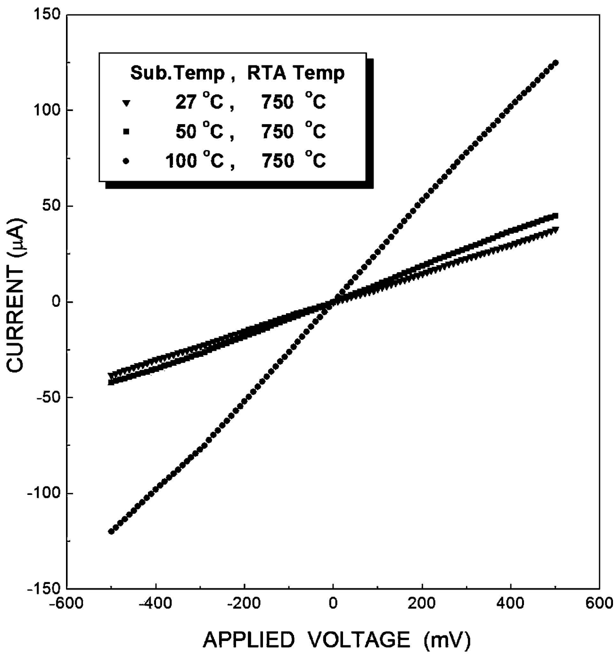

Figure 6 Current-voltage curves for the C54 $TiSi_2$ thin films grown on *n*-Si (100) substrates at 27°C, 50°C, and 100°C, and annealed at 750°C for 60 s.

Fig. 6 show the I-V curves for C54 $TiSi_2$ thin films grown on *n*-Si (100) substrates at 27, 50, and 100°C, and annealed at 750°C for 60 s. These I-V curves indicate that the C54 $TiSi_2$/*n*-Si (100) heterostructures have ohmic properties and that their resistances decreases with increasing substrate temperature. To clarify the electrical properties of the C54 $TiSi_2$/*n*-Si (100) heterostructures, we determined the specific contact resistances as a function of the substrate temperature, as shown in Fig. 7. The specific contact resistances decrease dramatically with increasing substrate temperature. The specific contact resistance for the C54 $TiSi_2$/*n*-Si (100) heterostructure grown at 200°C,

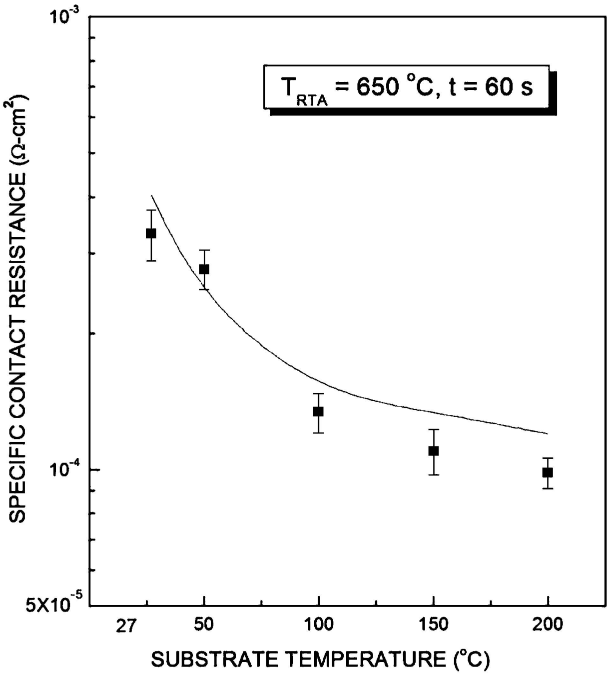

Figure 7 Specific contact resistance of the C54 $TiSi_2$ thin films grown on *n*-Si (100) substrates and annealed at 650°C for 60 s as a function of the substrate temperature.

4.89×10^{-5} Ω·cm², was significantly lower than that of the one grown at 27°C, 4.74×10^{-4} Ω·cm². This dramatic decrease in the specific contact resistance due to the increase of the substrate temperature might be related to the enhancement of the surface morphology, which was observed by the AFM measurements.

4. Summary and conclusions

$TiSi_2$ thin films were grown on *n*-Si (100) substrates by using a high-temperature sputtering method, followed by one-step annealing, and the surface, the structural, and the electrical properties of the C54 $TiSi_2$/*n*-Si (100) heterostrutures were investigated using AFM, SEM, EDX, XRD, and I-V measurements. The results of the AFM measurements showed that the surface morphology of the $TiSi_2$ thin films became smoother with increasing substrate temperature, and SEM, EDX, and XRD measurements showed that the formed samples were polycrystalline $TiSi_2$ thin films. I-V curves showed that the specific contact resistance decreased dramatically with increasing substrate temperature. These results suggest that high quality C54 $TiSi_2$ thin films can be grown on *n*-Si (100) substrates by using the high-temperature sputtering and one-step annealing method.

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