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Properties of Direct-Silicided WSi_2 Films

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Direct-silicided WSi_2 films grown on (100), (511), (110) and (111)Si substrates have been investigated concerning their resistivities and microstructures. The WSi_2 film formed on (511)Si substrate at 825°C has a 23μΩ·cm resistivity, i.e., the same value as the reported lowest WSi_2 film resistivity obtained by annealing at 1100°C for 30 minutes. It has been found by transmission electron microscopy observation that the film grew almost epitaxially on (511)Si substrate.

1. Introduction

WSi_2 film is used in polycide gate in MOS VLSIs. Although WSi_2 bulk resistivity was reported to be 12.5μΩ·cm, the film resistivity for standard deposition techniques, such as sputtering, CVD and thermal reaction, is usually higher than 60μΩ·cm, in spite of annealing at 900°C[1]. Reduction in the WSi_2 film resistivity is strongly required for further reduction in the polycide gate resistance.

The purposes of this study are to form WSi_2 films with low resistivities, as low as possible, and to clarify the dominant factors determining the WSi_2 film resistivity.

Direct-silicidation was used for forming low resistivity WSi_2 films at comparatively low formation temperature[2]. In this method, W is evaporated onto the Si substrate heated at a temperature sufficiently high for silicidation. Therefore, WSi_2 film grows directly on Si substrate, instead of metal W layer deposition.

In the present experiments, direct-silicided WSi_2 films were formed on (100), (511), (110) and (111)Si substrates. The crystal- and micro-structures for the films were observed using transmission electron microscopy and X-ray diffraction.

2. Experimental procedure

P-type (100), (511), (110) and (111)Si substrates were used. W evaporation onto the Si substrate at 640-880°C was performed using electron gun. Substrate temperature, Ts, was monitored using a thermocouple located at the back of the substrate. The substrate surface temperature typically increased by 100°C during W evaporation, mainly due to the variation in ultra-red ray transmissivity. Ts was defined as the middle of the surface temperatures, when evaporation started and finished. The error bar indicates the Ts variation during evaporation in the figures. The WSi_2 films were grown to a 900-1600Å thickness at a ~8Å/sec rate. The pressure in the evaporation chamber was less than 1×10^{-7} Torr before evaporation and less than

2×10^{-6} Torr during growth. For comparison, WSi_2 films were also formed by thermal reaction, i.e., depositing W on Si substrates at 200°C and subsequent in-situ anneal at 780-920°C for 4 minutes, the same as direct-silicidation growth time.

The sheet-resistivity was measured using a four-point probe. Average grain size $\bar{D}$ was obtained by measurements of typically 200 grains using transmission electron microscopy (TEM). The crystallographic orientation of the film was determined from X-ray diffraction patterns (XDPs) and electron diffraction patterns (EDPs).

3. Results

Electrical resistivity ρ dependence on Ts is shown in Fig. 1. In direct-silicided WSi_2 films on (511)Si substrates showed the lowest resistivities and the films on (111)Si substrates showed the highest resistivities. The ρ values for direct-silicided WSi_2 films were lower than those for in-situ annealed WSi_2 films. The lowest value was 23μΩ·cm for direct-silicided WSi_2 film on (511)Si substrate grown at Ts=825°C. The value is the same as the reported lowest WSi_2 film resistivity obtained by annealing at 1100°C for 30 minutes[3].

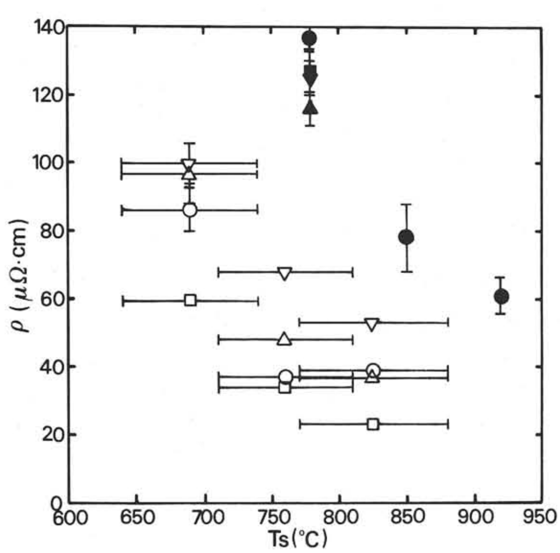

Fig.1. ρ dependence on Ts. The substrates are represented as O for (100)Si, □ for (511)Si, Δ for (110)Si and ∇ for (111)Si. Open symbols represent direct-silicidation and closed symbols represent in-situ annealing.

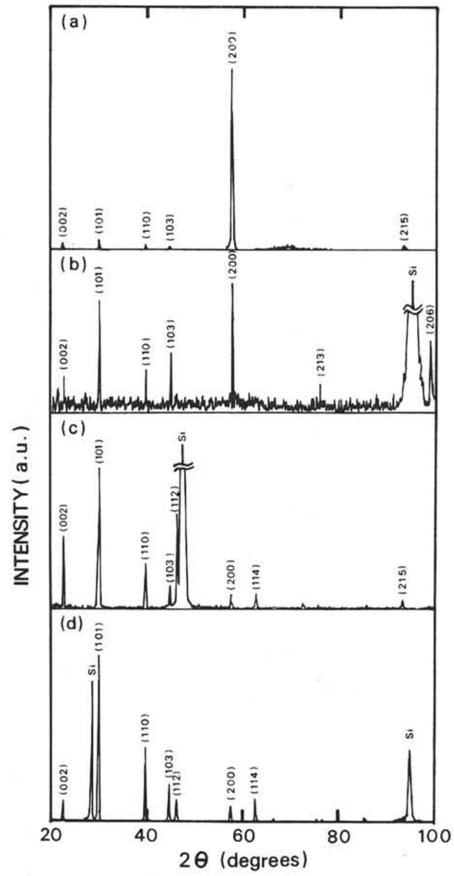

Fig.2. XDPs for direct-silicided WSi_2 films grown on (a) (100)Si at 760°C, (b) (511)Si at 825°C, (c) (110)Si at 825°C and (d) (111)Si at 825°C.

XDPs for some samples are shown in Fig. 2. All peaks were identified as those of tetragonal WSi_2 or Si. The WSi_2(200) peaks for the films on (100) and (511)Si substrates were markedly large, as shown in Figs. 2(a) and (b). For the films on (110) and (111)Si substrates, WSi_2(101) peaks were large instead of the WSi_2(200) peaks as shown in Figs. 2(c) and (d).

The X-ray rocking curve for WSi_2(200) peak of direct-silicided WSi_2 film formed on a (100)Si substrate showed that WSi_2 a-axis was almost perpendicular to the substrate surface. In the case of the film formed on (511)Si substrate at 825°C, the curve indicated that WSi_2 a-axis tilts ~10° from Si[511] toward Si[100].

EDPs for some samples are shown in Fig. 3. There are no ring patterns in the EDPs for all direct-silicided WSi_2 films on (511)Si substrates and direct-silicided WSi_2 film formed on (100)Si substrate at 760°C as shown in Figs. 3(a) and (b). Ring patterns exist in the EDPs for the other direct-silicided films as shown in Figs. 3(c) and (d). The EDPs for films formed by in-situ annealing were rings for typical polycrystals.

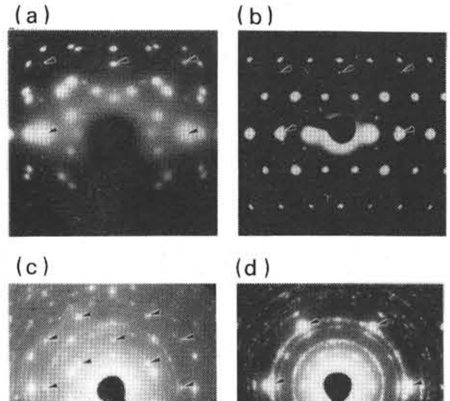

Fig.3. EDPs for direct-silicided WSi_2 films grown on (a) (100)Si at 760°C, (b) (511)Si at 825°C, (c) (110)Si at 825°C and (d) (111)Si at 825°C. Arrows are the patterns for the Si substrates.

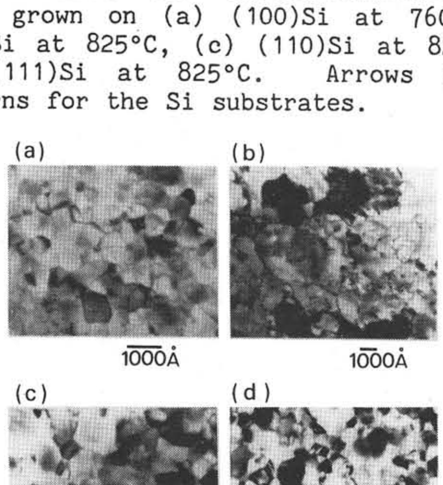

Fig.4. TEM bright field images for direct-silicided WSi_2 films grown on (a) (100)Si at 760°C, (b) (511)Si at 825°C, (c) (110)Si at 825°C and (d) (111)Si at 825°.

TEM images of some samples are shown in Fig. 4. The image for direct-silicided WSi_2 film formed on (511)Si substrate at 825°C shows single-crystalline zones several times as large as the film thickness including many defects, as shown in Fig. 4(b). The others, except direct-silicided films on (511)Si substrates, showed typical polycrystalline film images, as shown in Figs. 4(a), (c) and (d). Average grain size $\bar{D}$ values are shown in Table 1. It can be seen that $\bar{D}$ depends on substrate and formation method, as (511)Si>(110)Si>(100)Si>(111)>in-situ annealing.

4. Discussion

J. Torres et al reported that direct-silicided WSi_2 films on (100)Si substrates had two equivalent preferred orientations, i.e., Si[100]//WSi_2 a-axis, and Si[011]//WSi_2 c-axis or Si[0$\bar{1}$1]//WSi_2 c-axis[2]. These preferred orientations were also observed in the present experiment.

Direct-silicided WSi_2 film on (511)Si had a single preferred orientation. The relationship between Si and WSi_2 lattices is shown in Fig. 5, i.e., Si[0$\bar{1}$1]//WSi_2 c-axis, and WSi_2 a-axis tilts ~5° from Si[100] toward Si[511].

ρ depends on $\bar{D}$, as shown in Fig. 6. However, the ρ variation was unable to be explained merely by dependence on $\bar{D}$.

Table 1. Average grain size $\bar{D}$ (Å) for direct-silicided and in-situ annealed WSi_2 films.

	Direct-silicidation		
Substrate	Ts=690°C	Ts=760°C	Ts=825°C
(100)Si	321±17	525±32	814±83
(511)	356±20	696±43	1344±92
(110)	341±19	629±40	944±64
(111)	257±13	476±18	693±48

	in-situ annealing	
Substrate	Ts=850°C	Ts=920°C
(100)Si	428±34	704±36

Theoretical ρ-$\bar{D}$ dependence for one-dimensional polycrystals was proposed by Mayadas and Shatzkes, i.e.,

$$\rho=\rho_0\left\{1-\frac{3}{2}\alpha+3\alpha^2-3\alpha^3 ln\left(1+\frac{1}{\alpha}\right)\right\}^{-1} \qquad (1)$$

$$\alpha=\frac{l_0}{\bar{D}}\ \frac{R}{1-R} \qquad (2)$$

where ρ_0 is the intrinsic resistivity, l_0 is the mean free path for carriers within a grain and R is the reflection coefficient at grain boundaries[4]. For WSi_2, $\rho_0 \sim 12.5\mu\Omega\cdot cm$, $l_0 \sim 184Å$[5]. ρ-$\bar{D}$ curves for R=0.8, 0.85, 0.87 and 0.92 are drawn in Fig. 6. The data points for all direct-silicided WSi_2 films on (511)Si substrates and direct-silicided WSi_2 film on (100)Si substrate formed at 760°C are located between the curves for R=0.8 and 0.85. These films showed EDPs without ring pattern. The others are located between the curves for R=0.87 and 0.92. These results suggest that the grain orientations of film affect carrier reflection at the grain boundary.

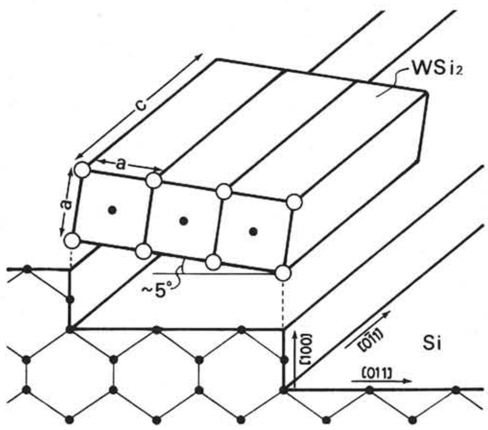

Fig.5. The relationship between Si and WSi_2 lattices for direct-silicided WSi_2 film on (511)Si substrate.

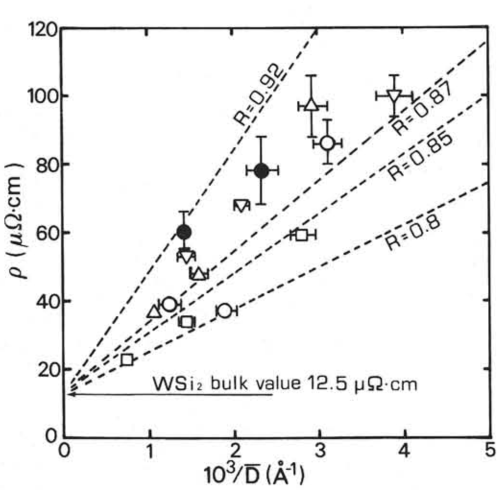

Fig.6. ρ dependence on $\bar{D}$. The same symbols in Fig. 1 are used. Broken lines are drawn based on Mayadas and Shatzkes model.

5. Conclusion

WSi_2 films formed by direct-silicidation have been investigated in terms of the film resistivity and microstructure dependences on Si substrate crystallographic orientation and formation temperature.

Direct-silicided WSi_2 film has grown almost epitaxially on (511)Si substrate at 825°C. Its electrical resistivity was $23\mu\Omega\cdot cm$, i.e., the same value as the reported lowest WSi_2 film resistivity reduced by annealing at 1100°C for 30 minutes.

Although WSi_2 film resistivity was controlled mainly by the grain size, the grain orientations are considered to contribute toward the resistivity.

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