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Electrical and Compositional Properties of $TaSi_2$ Films

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Tantalum silicide ($TaSi_2$) thin films were sputter deposited on p- and n-type silicon substrates using ultrapure $TaSi_2$ targets. The $TaSi_2$/Si samples were annealed in nitrogen or forming gas or oxygen containing steam at temperatures in the range of 400–900°C. The sheet resistances of $TaSi_2$/Si were measured by four-point probe before and after anneal. The structure of these films was investigated using x-ray diffraction (XRD) methods. It has been found that the sheet resistance decreases with the increase in annealing temperature and also with the increase in film thickness. X-ray diffraction patterns show changes in the morphological structure of the films. Oxidation characteristics of the films have been investigated in the temperature range of 400–900°C in oxygen containing steam ambient. The oxidation time ranged from 0.5 to 1.5 h. No oxide formation of the tantalum silicide films was observed in this investigation. This has been attributed to the high purity of $TaSi_2$ sputter targets used in the preparation of the films.

Key words: Tantalum silicide, annealing, sputtering, sheet resistance, oxidation

INTRODUCTION

With continuously decreasing device dimensions in silicon-integrated circuit technology, the relatively high sheet resistance of doped polycrystalline silicon as the gate metal has become a limiting factor for device performance. This has led to increased interest in incorporating refractory metal silicides into the device fabrication process. The potential benefits of smaller integrated-circuit dimensions can be realized only if measures are taken to prevent parasitic effects from dominating the electrical characteristics. One of the most urgent needs is to find a low-resistivity substitute for heavily doped polycrystalline silicon (poly-Si) at the gate level. Due to the advantages of ease of formation, low resistivity, and thermal stability, $TiSi_2$ and $TaSi_2$ are particularly promising to silicon device technology.

Silicides are most commonly used in dynamic random access memory (DRAM) and complementary metal oxide semiconductor (CMOS) devices as conducting layers that can withstand high temperature and that have a significantly low sheet resistivity. Besides their role as a stable conductor, silicides have other interesting applications and properties. These include their use as a diffusion source for impurities to generate shallow junctions, or as an alternative to self-aligned silicides. A selective chemical vapor deposition (CVD) process is interesting because it uses no silicon consumption. Implantation into silicide or even an in-situ doped silicide deposition can eliminate implantation damage in silicon and reduce defects.

Among the metal silicides, $TaSi_2$ has high-temperature stability and low contact resistance. The most interesting aspect of $TaSi_2$ is that it can be directly used as a gate material without the need for poly-Si.[1] A large number of studies on $TaSi_2$ have been published in the literature. In this work, direct current (DC)-sputtering methods have been used to

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sputter deposit $TaSi_2$ thin films on silicon substrates. The effects of annealing of the films in inert and steam ambient have been investigated. Sheet resistance and x-ray diffraction (XRD) methods have been used to characterize the films.

EXPERIMENTAL DETAILS

Silicon wafers of orientation (100) type p and n, resistivity 5–10 Ω·cm, 4-in. diameter, and 600-μm thickness have been used as substrate materials. These wafers were cleaned using the standard RCA clean method. A Varian (Peabody, MA) 3125 magnetron DC sputtering system with ultrahigh purity $TaSi_2$ target was used to deposit tantalum silicide thin films. The sputter deposition chamber was pumped to a pressure of better than 8×10^{-7} Torr. Sputtering was performed at an argon pressure of 5–7 mTorr. Tantalum silicide thin films deposited on silicon wafer had thickness values in the range of 100–1000 Å. The films were annealed in N_2 or forming gas or oxygen containing steam at temperatures of 400–900°C for a duration of 0.5–1.5 h.

RESULTS AND DISCUSSION

Four-Point Probe

The sheet resistance of sputter-deposited films before annealing is listed in Table I. As is shown in the table, the sheet resistance decreases with the increase in thickness of $TaSi_2$. The sheet resistance (R_s) of film deposited on p-type wafer is higher than that deposited on n-type wafer for the same thickness. The 1000-Å $TaSi_2$/Si samples were annealed from 400 °C to 900°C for 30 min in N_2 and the sheet resistance of the films was measured for each annealing temperature. These results are presented in Fig.1. From this figure, it may be noted that the sheet resistance of the $TaSi_2$ thin film decreases with increasing annealing temperature. A comparison with the literature[2–5] shows that our results are in agreement with the published data.[2] Figure 2 shows the experimental data of the sheet resistance of $TaSi_2$ films from the literature.[2] $TaSi_2$ is known to have a barrier height of 0.58 eV on n-Si.[1]

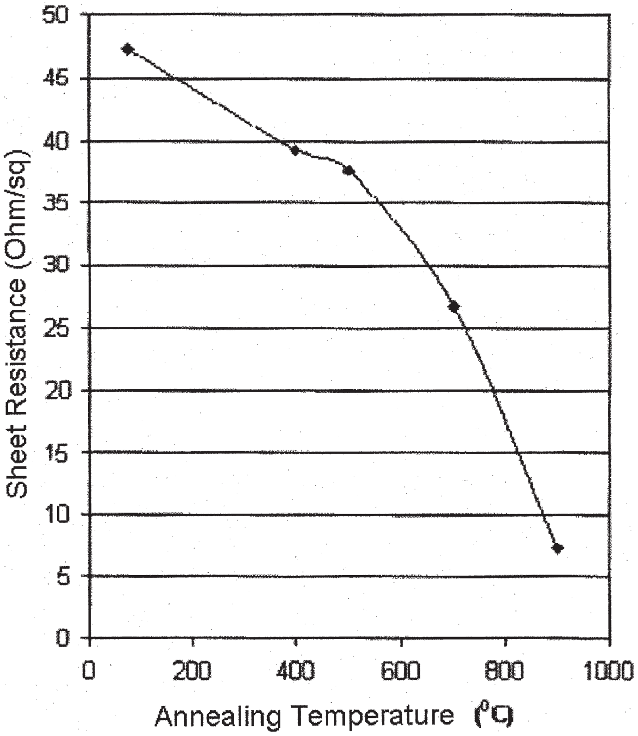

Fig. 1. Sheet resistance of $TaSi_2$ thin films versus annealing temperature. Film thickness = 1000 Å.

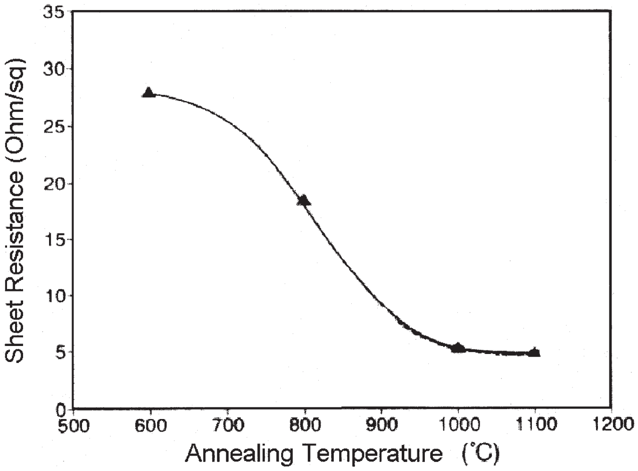

Fig. 2. Cho's experimental data of sheet resistance of $TaSi_2$ thin films.[2]

X-ray Diffraction

$TaSi_2$ thin films annealed in forming gas N_2 or oxygen containing steam ambient at various temperatures were analyzed by XRD. The XRD spectra of as-deposited $TaSi_2$ and films annealed at temperatures in the range of 600°C to 900°C are shown in Figs. 3–5. Four sharp features may be observed in the XRD of as-deposited films in Fig. 3. From the XRD results shown in Fig. 4a and b, annealing in the various ambients did not produce significant differences in their influence on the composition of $TaSi_2$. From these spectra, it is clear that peaks in addition to those of Si are observed. A comparison with the standard XRD data of $TaSi_2$[6] confirms that the peaks obtained are due to $TaSi_2$ (100), (101), (102), (110), (111), (003), (200), and (112) orientations. Other phases such as Ta_2Si and Ta_5Si_3 were absent within the detection limit of the experiment.

Table I. Sheet Resistance of Sputter-Deposited $TaSi_2$/Si

Wafer Type	Film Thickness (Å)	R_s (Ω/Sq)
n	200	66.0
n	600	36.7
n	1000	22.5
p	200	130.1
p	600	46.9
p	1000	27.5

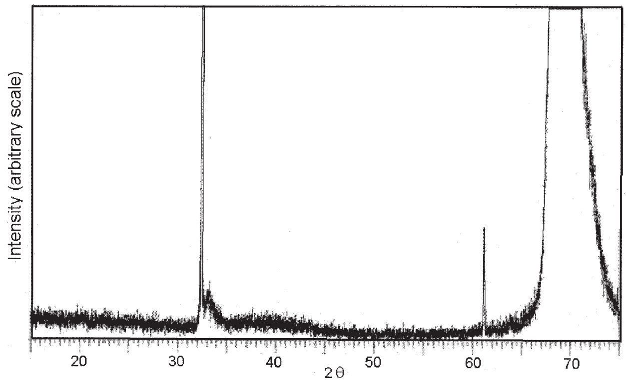

Fig. 3. XRD spectra of as-deposited $TaSi_2$ thin film (1000 Å).

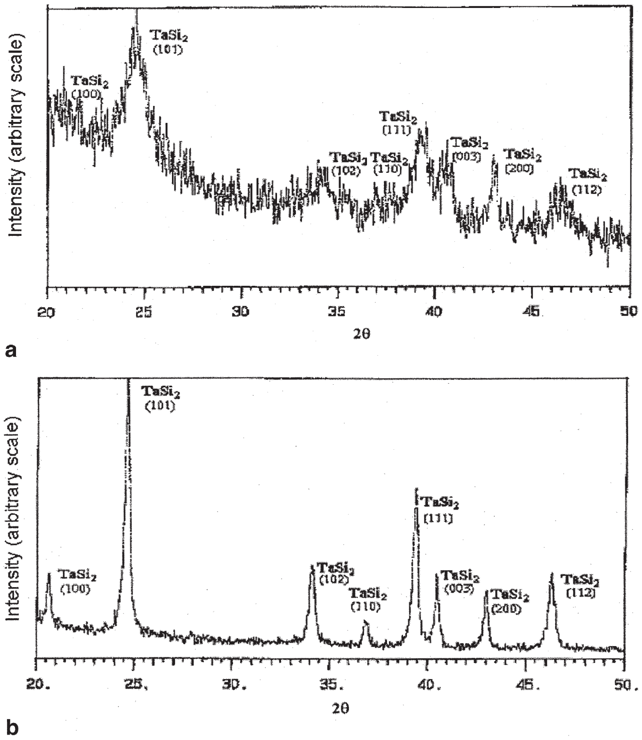

Fig. 4. XRD spectra after oxidation of 1000 $TaSi_2$ thin film on n-Si after annealing: (a) 600°C annealing in N_2 and (b) 900°C annealing in forming gas.

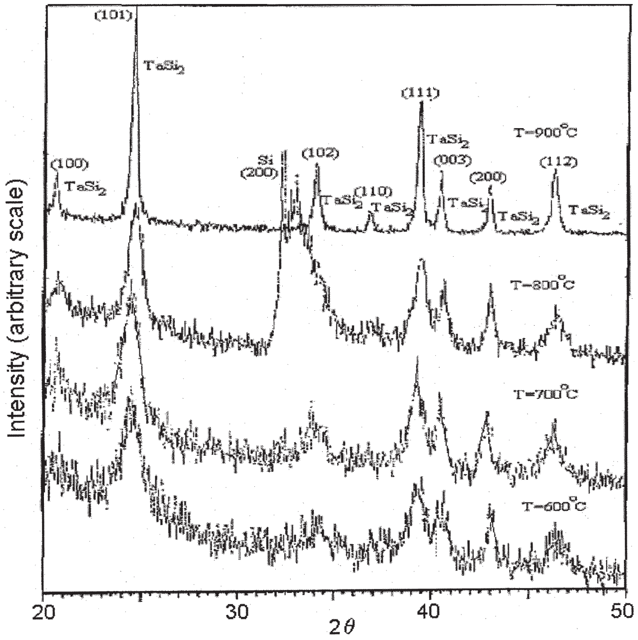

Fig. 5. Comparison of XRD spectra of 1000 Å $TaSi_2$ thin films on n-Si after annealing (from 600°C to 900°C in steam).

This result agrees well with the XRD data published[3,7] in the literature. Comparing the two XRD data, the peaks in Fig. 4a are broader than those in Fig. 4b. This implies that the microstructures of $TaSi_2$ thin film become crystallized after annealing and become more ordered with an increase in annealing temperature. From Fig. 5, it can be seen that as annealing temperature increases, the peaks of $TaSi_2$ thin film become narrower and show an increase in intensity. The data of intensity and full-width half-maximum (FWHM) of the peak (101) are listed in Table II for a quantitative comparison. From this table, it can be seen that between 800°C and 900°C annealing temperatures, the diffraction peak changes abruptly. It can be concluded from this result that the crystallization of $TaSi_2$ occurs mainly between 800°C and 900°C. Results of Cho et al.[3] in Fig. 6 show the occurrence of a continuous phase transformation above 800°C. In the present study, we report the presence of $TaSi_2$ peaks at 600°C. This may be due to various factors such as the integrity of the $TaSi_2$ sputter target, film thickness, and the characteristics of Si substrates.

XRD Measurements on $TaSi_2$ Films after Wet Oxidation

According to the ternary Ta-Si-O phase diagram shown in Fig. 7, it can be predicted that the phase connected by a solid tie-line is stable. Thus, Ta_2O_5 can be produced by the oxidation of $TaSi_2$ at temperatures in the range of 600–1100°C. A comparison of our XRD data with Jiang's[8] of Ta_2O_5 thin films in Fig. 8 shows that there is no Ta_2O_5 phase formation after wet oxidation of $TaSi_2$ thin films. From our XRD data shown in Fig. 9, no visible tantalum oxide peaks are found. All the peaks obtained in this spectrum are peaks that are comparable to the $TaSi_2$ data in Fig. 4. Based on these experimental observations, it can be concluded that there is no oxidation occurring in $TaSi_2$ thin films that are prepared using high-purity $TaSi_2$ sputter targets.

Murarka et. al.[9] have reported their studies on $TaSi_2$ films formed on polysilicon by sintering tantalum thin films on doped polysilicon. They find that these $TaSi_2$ films do not oxidize in dry O_2 and oxidize in steam, giving SiO_2 and a surface layer of mixed Ta-Si oxides. During wet oxidation of $TaSi_2$, the top oxide layers do not act as a diffusion barrier for water molecules. On continued oxidation, SiO_2 is formed, and silicon in the silicon-rich layer is replenished continuously by steady diffusion of silicon from polycrystalline silicon to the silicide-SiO_2 in-

Table II. XRD Data of $TaSi_2$ (101) Peaks for Different Annealing Temperatures

Annealing Temperature (°C)	2-Theta (°)	D-Spacing (Å)	Intensity	FWHM
600	24.60	3.6259	124	2.594
700	24.680	3.6044	135	1.187
800	24.760	3.5929	187	0.836
900	24.640	3.6101	887	0.312

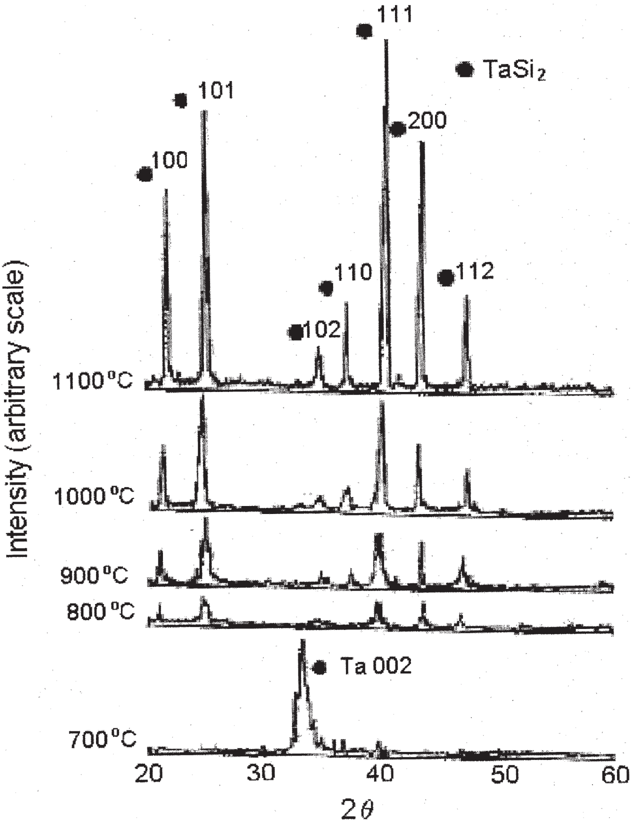

Fig. 6. XRD spectra of $TaSi_2$/Si (Work of Cho[3]).

terface. This steady flow is established during the early stages of oxidation. No further oxidation of tantalum takes place because of the shielding effect of silicon-rich layer. This is schematically shown in Fig. 10. We have also performed XRD measurements on $TaSi_2$ (100 Å and 900 Å) from $2\theta = 30°$ to $60°$. From our XRD data analyses for the 100 Å and 900 Å films, we were not able to observe any phases of Ta_xO_y or SiO_y.

Saraswat et al.[10] have reported that when $TaSi_2$ is deposited by simultaneous sputtering of tantalum and silicon on SiO_2/Si, a mixture of SiO_2 and Ta_2O_5 is formed. However, in the case of $TaSi_2$ films deposited on silicon, only $TaSi_2$ diffraction peaks are observed. The results of their XRD spectra are shown in Fig. 11. The schematic summarizing their results is shown in Fig. 12. In this case, the reaction of $TaSi_2$ with O_2 can be written as

$$TaSi_2 + O_2 = Ta_2O_5 + SiO_2$$

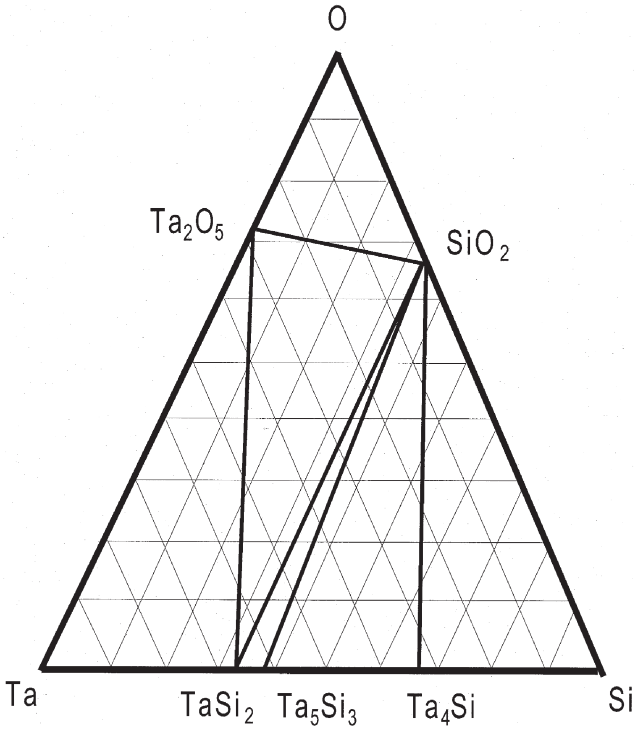

Fig. 7. Ternary Ta-Si-O phase diagram (600–1100°C).[3]

As has been observed in our detailed x-ray analyses, the sputter-deposited $TaSi_2$ films are stable when heated in wet oxygen. This is summarized schematically in Fig. 13.

CONCLUSIONS

$TaSi_2$ thin films were sputter deposited on p-Si and n-Si wafers by using a high-purity $TaSi_2$ target. The thicknesses of $TaSi_2$ thin films were in the range 100 Å to 1000 Å. The wafers were then annealed at temperatures in the range of 400°C to 900°C in nitrogen, forming gas, or oxygen containing steam. Four-point probe results show that the sheet resistance of the $TaSi_2$ thin film decreases with an increase in film thickness and annealing temperature. X-ray diffraction results show that the microstructure of $TaSi_2$ thin film changes from amorphous to crystalline as annealing temperature increases. In the annealing temperature range of 800°C to 900°C, the characteristics of diffraction peaks change considerably. Wet oxidation characteristics of $TaSi_2$ thin films have been investigated in the temperature range of 400–900°C. According

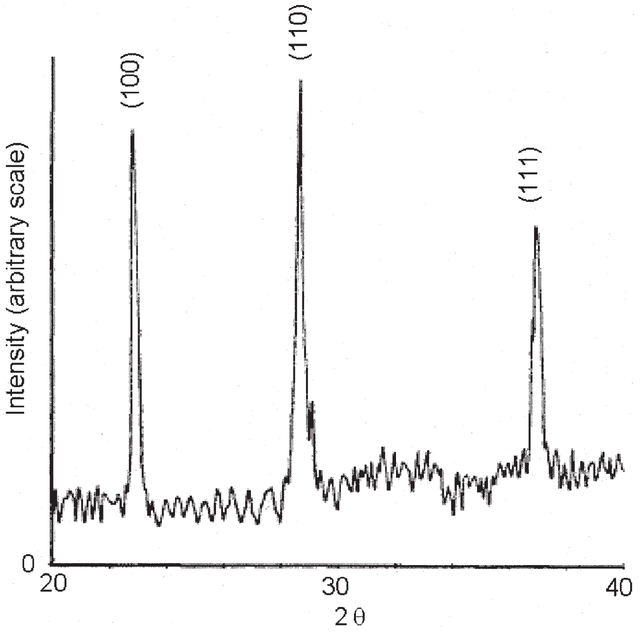

Fig. 8. XRD spectra of Ta_2O_5 thin films.

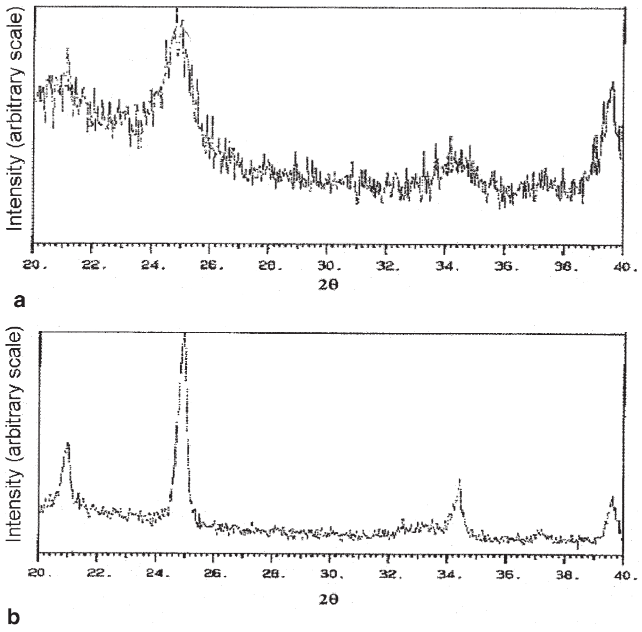

Fig. 9. XRD spectra after wet oxidation of 1000 Å $TaSi_2$ thin film on n-Si: (a) 700°C for 1 h and (b) 900°C for 1.5 h.

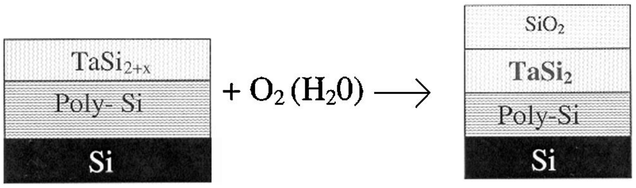

Fig. 10. Schematic of wet oxidation of $TaSi_2$ films formed on polysilicon by sintering tantalum film on doped poly.[9]

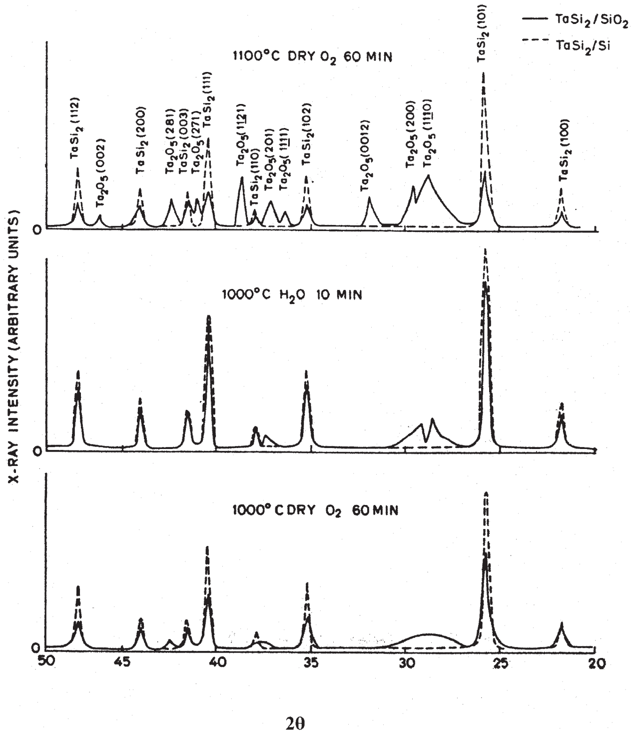

Fig. 11. XRD of oxidation of tantalum silicide films.[10]

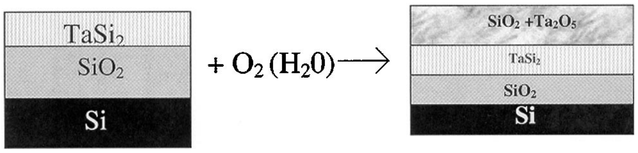

Fig. 12. Schematic showing oxidation of $TaSi_2$ films deposited by simultaneous sputtering of tantalum and silicon. In the case of $TaSi_2$/Si samples, only $TaSi_2$ diffraction peaks are observed, whereas for $TaSi_2/SiO_2$ samples, additional diffraction peaks of Ta_2O_5 are also observed.[10]

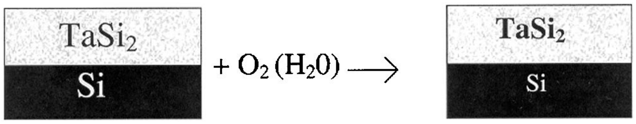

Fig. 13. Schematic showing wet oxidation of sputter-deposited $TaSi_2$ films using ultrapure $TaSi_2$ target.

to our XRD results, there are no detectable Ta_2O_5 peaks in the films.

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