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(100) Oriented Poly-Si Film Grown by Ultrahigh Vacuum Chemical Vapor Deposition

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ABSTRACT

Poly-Si films are grown by ultrahigh vacuum chemical vapor deposition (UHV-CVD) with plasma-seeding on SiO_2. The preferred grain orientations are investigated as a function of thickness, source gas flow rate, and growth temperature. The poly-Si films show (100) preferred orientation in a wide range of growth conditions. The (100) orientation increases as thickness and flow rate increases and decreases as temperature increases. UHV-CVD and other deposition methods are compared in order to estimate the role of hydrogen and oxygen as factors controlling the preferred grain orientation.

Poly-Si has become an increasingly important material, because of its potential use in thin film transistors (TFTs), liquid-crystal displays (LCDs), and large-scale integrated circuits (LSIs). Thus, the electrical properties of defects such as grain boundaries, interfaces, and lattice defect in poly-Si films must be clearly understood in order to improve device performance.

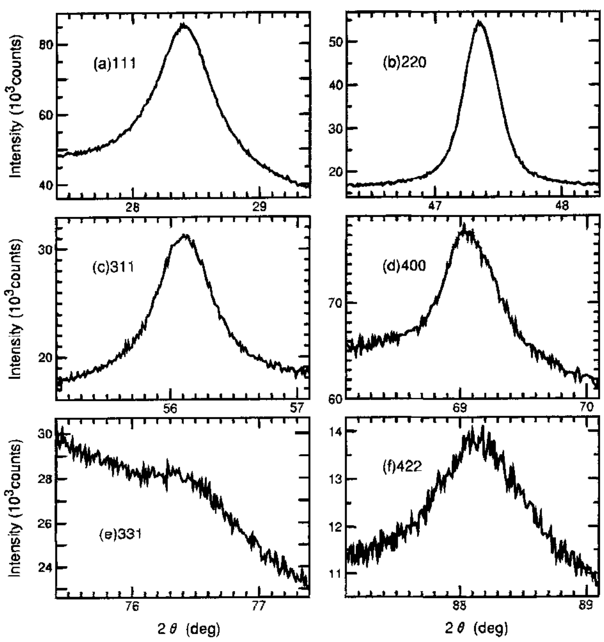


Fig. 1. Typical x-ray diffraction spectra of a poly-Si film. (Substrate temperature: 587°C; flow rate: 20 sccm; thickness: 220 nm.)

Preferred grain orientation is an important characteristic that is related to the electrical properties of poly-Si films. Usually these films have been grown by low-pressure chemical vapor deposition (LPCVD) and have shown (110), (111), and (311) orientation at various growth temperatures.[1,2] Furthermore, these films have shown (100) orientations at 650 to 700°C in limited reports.[3,4] Molecular beam deposited (MBD) poly-Si films in an ultrahigh vacuum (UHV) having (100) preferred orientations have been reported for comparatively thick (>500 nm) films,[5] while 500 nm thick films have shown (110) preferred orientations.[5,6]

Recently, ultrahigh vacuum chemical vapor deposition (UHV-CVD) was studied and applied to Si epitaxial film growth. With UHV-CVD, the growth rates depended on the surface conditions and the crystalline orientations of the substrates. These dependencies varied with growth conditions such as temperature and source gas flow rate.

In this paper, we studied preferred orientations of poly-Si grown by UHV-CVD on SiO_2 films. The poly-Si films showed (100) orientations in a wide range of growth conditions. We also described the dependencies of the preferred orientations of the poly-Si films on growth conditions, *i.e.*, temperature, source gas flow rate, and film thickness. Furthermore, by comparing our data and other reported data, we discussed an issue with factors determining preferred grain orientations of poly-Si.

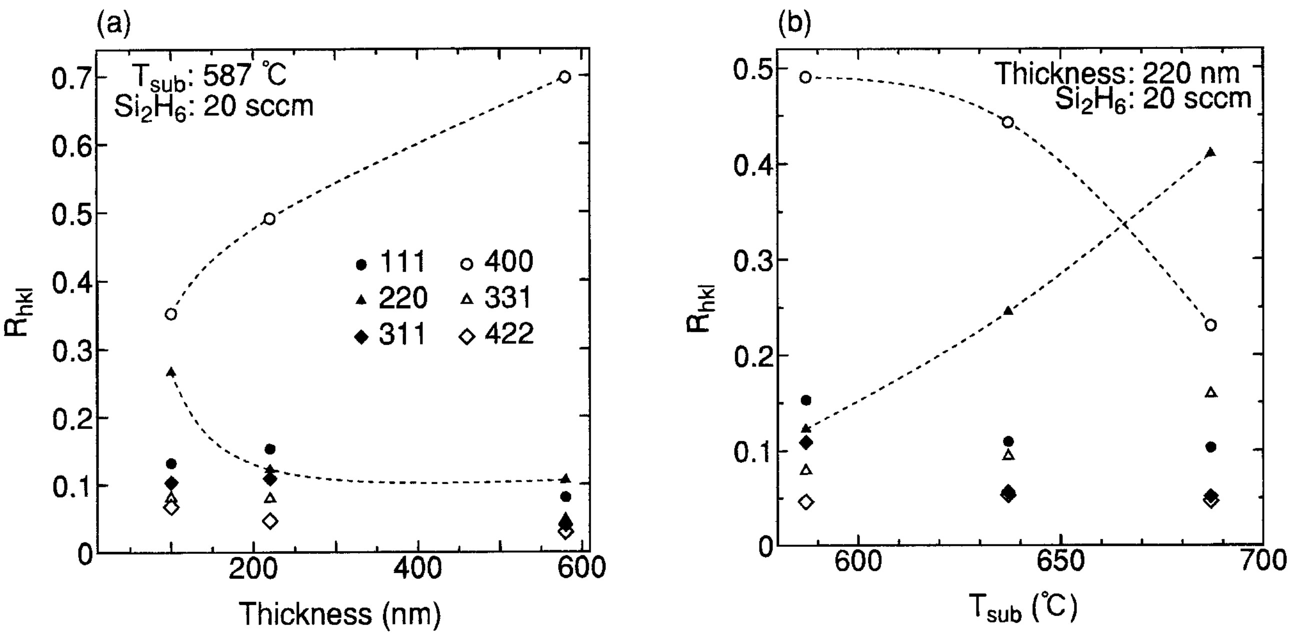
Table I. Numerical values for R_{hkl} calculations.

hkl	2θ (deg)	F	p	L	C_{abs} t = 40 nm	100 nm	220 nm	580 nm	C_{vol}
111	28.443	−59.94	8	4.2732	0.99771	0.99429	0.98750	0.96750	4.0705
220	47.303	−67.51	12	1.6958	0.99858	0.99650	0.99232	0.97993	2.4927
311	56.123	−43.61	24	1.2802	0.99878	0.99701	0.99344	0.98285	2.1258
400	69.131	56.22	6	0.94317	0.99901	0.99752	0.99456	0.98575	1.7626
331	76.377	38.22	24	0.83214	0.99909	0.99771	0.99501	0.98691	1.6175
422	88.032	49.10	24	0.71999	0.99917	0.99797	0.99555	0.98834	1.4391

Experimental

We prepared 4° off (100)Si substrates, *i.e.*, 6 in. wafers, with an SiO_2 layer (500 nm thick) grown by thermal oxidation. All samples were grown in a cold-wall-type UHV-CVD system which has been described elsewhere.[7] The substrate was heated by carbon heaters from the back side. The substrate temperature was always monitored with a thermocouple placed between the substrate and the carbon heaters. The real substrate temperature was directly measured with a pyrometer to calibrate the thermocouple temperature. The calibrated substrate temperature was 113°C lower than the thermocouple temperature, with ±5°C error.

Plasma seeding was then carried out with a nude ion gauge in an Si_2H_6 atmosphere of 10^{-4} to 10^{-3} Torr at a substrate temperature of 587°C. The seeding process was necessary for immediate poly-Si growth on the SiO_2 because Si_2H_6 dissociation rates on SiO_2 surfaces are much lower than on Si surfaces. The Si deposition amount per plasma flash was so small that it was invisible by high-resolution transmission electron microscopy (HRTEM). Poly-Si films were subsequently grown in the same chamber. The sub-



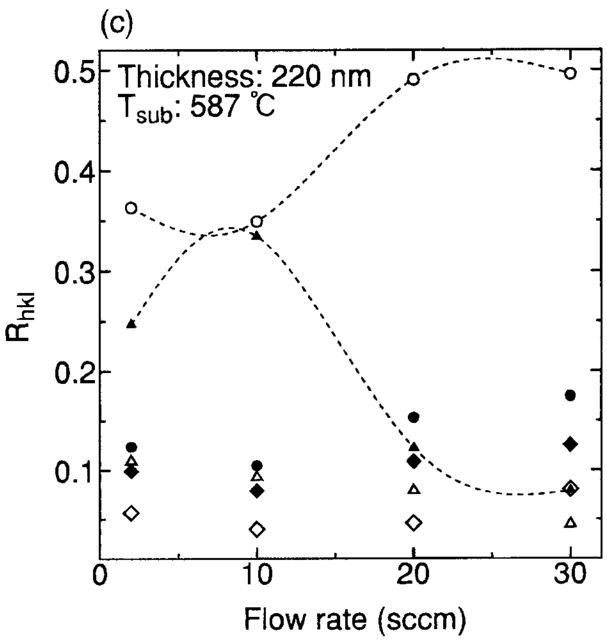


Fig. 2. (a, top left) Film thickness dependence of R_{hkl}; (b, above) T_{sub} dependence of R_{hkl}; (c, left) Si_2H_6 flow rate dependence of R_{hkl}.

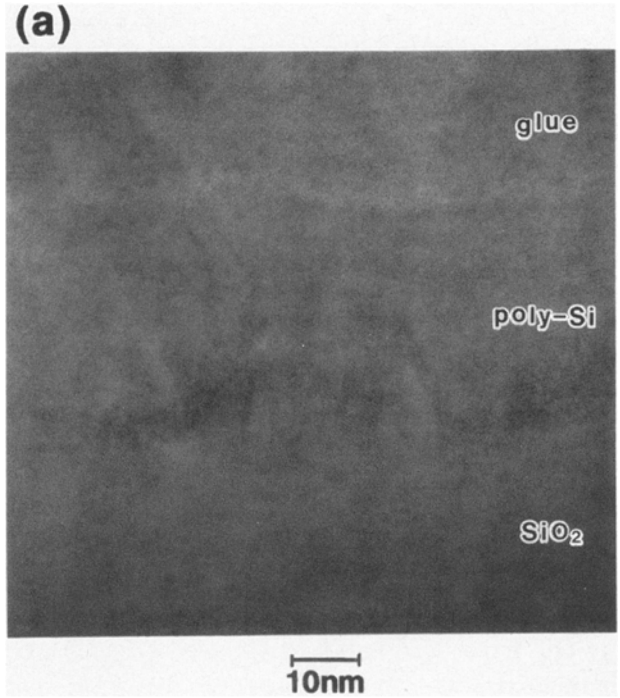
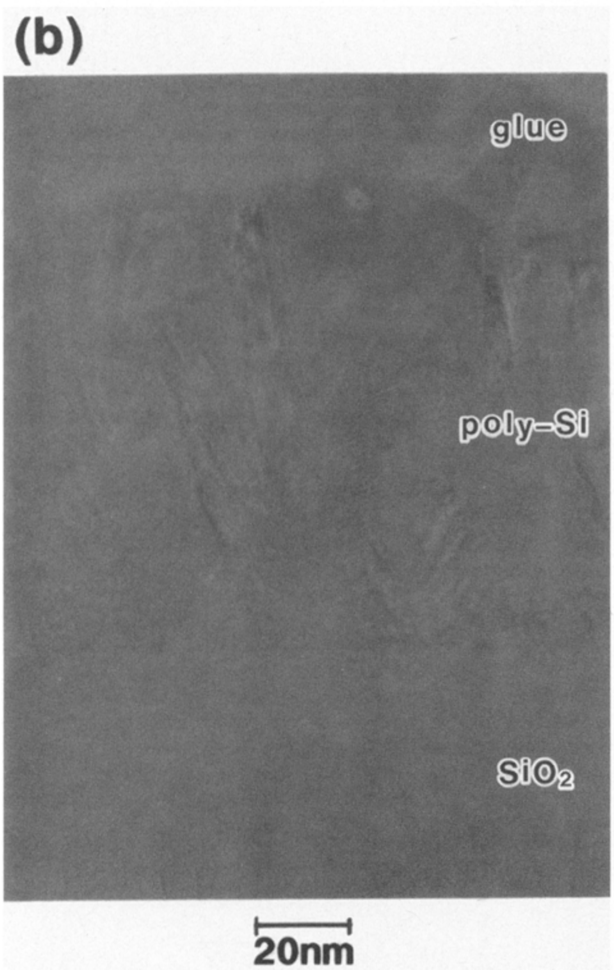
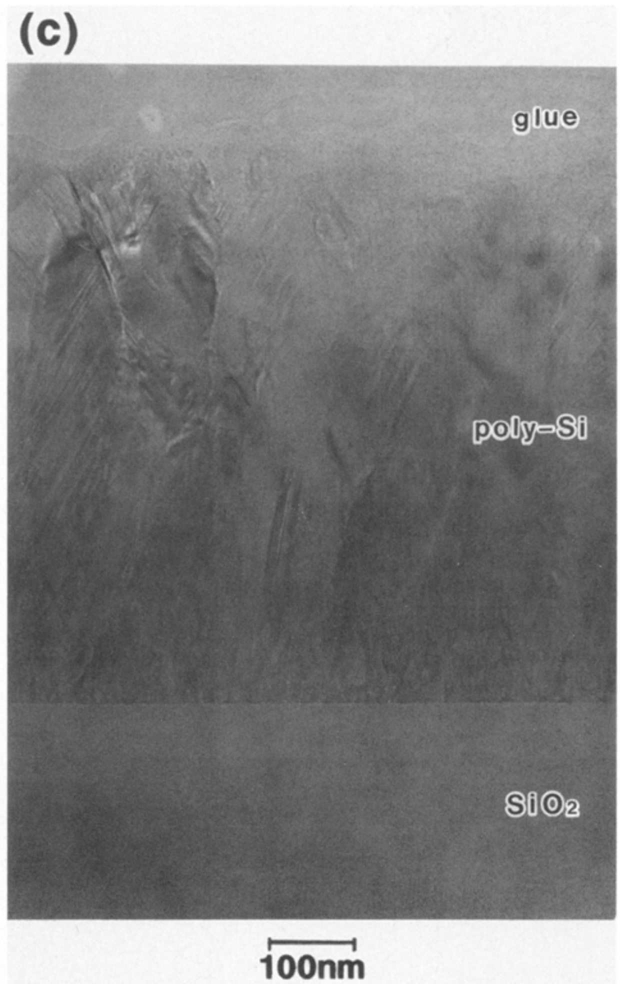


Fig. 3. Cross-sectional TEM images of UHV-CVD-poly-Si films. (a) 40; (b) 100; (c) 580 nm thick.





strate temperature, source gas (Si_2H_6) flow rate, and film thickness were varied independently, from 587 to 687°C, from 2 to 30 sccm, and from 40 to 580 nm, respectively. The typical deposition rates were 11, 36, and 44 nm/min for 587, 637, and 687°C substrate temperatures at 20 sccm flow rate, respectively. The deposition rate was constant (11 nm/min) for 10 to 30 sccm flow rate at 587°C substrate temperature, however the rate became 7 nm/min at 2 sccm flow rate.

The preferred orientations were calculated with spectra, as shown in Fig. 1, measured by counting the diffraction intensity at twice the angle of the incident x-rays[8] (so-called the θ to 2θ scanning) with an x-ray diffractometer

(Cu Kα, 50 kV, 250 mA). The intensities of the (111), (220), (311), (400), (311), and (422) peaks correlate the amounts of (111), (110), (311), (100), (331), and (211) textures in the film, respectively. The fraction of (hkl) texture, *i.e.*, the grains with crystallographic hkl axes oriented normal to the substrate, R_{hkl}, was defined as follows[9]

$$R_{hkl} = \frac{\frac{I_{hkl}}{r_{hkl}}}{\sum \frac{I_{hkl}}{r_{hkl}}} \quad [1]$$

$$r_{hkl} = |F|^2 pLC_{abs}C_{vol}$$

where I_{hkl} is the experimental integral intensity of the diffraction line, r_{hkl} is the estimated integral intensity of the diffraction line for an ideal absolute random oriented polycrystalline film, F is the structure factor,[10] p is the multiple factor, L is the Lorentz factor for polycrystalline substances, C_{abs} is the intensity ratio after absorption of a film, and C_{vol} is the volume ratio determined by the glancing angle of the detector for the hkl diffraction. Summation was carried out for all measured diffraction lines, and then L, C_{abs}, and C_{vol} were calculated, as shown below

$$L = \frac{\cos\theta}{\sin^2 2\theta}$$

$$C_{abs} = \frac{\sin\theta}{2\mu t}\left(1 - e^{-\frac{2\mu t}{\sin\theta}}\right) \quad [2]$$

$$C_{vol} = \frac{1}{\sin\theta}$$

Here, μ is the absorption coefficient (140.73 cm^{-1} for Si with Cu Kα), θ is the incident diffraction angle, and t is the film thickness. The numerical values used are shown in Table I.

Cross-sectional transmission electron microscopy (TEM) was used for observation as the poly-Si film thickness was varied, in order to measure the thickness and to observe the feature of the texture configuration.

Results

The preferred grain orientations were (100) in the thickness range from 100 to 580 nm, at a substrate temperature T_{sub} of 587°C and an Si_2H_6 flow rate of 20 sccm, as shown in Fig. 2a. We deposited a 40 nm thick film. However, the low diffraction intensities of the film causes R_{hkl} errors thus making the preferred orientation difficult to determine. At thicknesses of 100 to 580 nm, R_{400} increased monotonously as the film thickness increased, and was 0.7 for a 580 nm thick film. On the contrary, R_{220} decreased as the film thickness increased.

Figure 2b shows R_{hkl} as a function of T_{sub} at a film thickness of 220 nm and an Si_2H_6 flow rate of 20 sccm. Here, R_{400} decreased as T_{sub} increased. On the other hand, R_{220} increased as T_{sub} increased. The preferred orientation changed from (100) to (110) at about 665°C.

Figure 2c shows R_{hkl} as a function of the Si_2H_6 flow rate at a film thickness of 220 nm and a substrate temperature of 587°C. The preferred orientations were (100) as the flow rate ranged from 2 to 30 sccm. Furthermore, R_{400} increased as the flow rate increased between 10 and 20 sccm and did not show any significant variation between 2 and 10 sccm or between 20 and 30 sccm.

Table II. Comparison of growth atmospheres.

Method	UHV-CVD	UHV-MBD	LPCVD
Base vacuum (Torr)	10^{-10}	10^{-10}	10^{-4}
Vacuum during growth (Torr)	10^{-4}	10^{-8}	1
Effective residual gas	None	None	O_2
Source gas	Si_2H_6	Si (solid)	SiH_4
Atmospheric gas	H_2, Si radical	None	H_2, Si radical

Discussion

The orientation variation with film thickness suggests that (100) grains grew and obstructed the other grains' growth. Cross-sectional TEM observations backed up this speculation. The 40 nm film, although we could not determine its preferred orientation, consisted of column-structured grains, as shown in Fig. 3a. In the 100 nm film, although some grains looked as though they were extending toward the surface, the column-structure still remained, as shown in Fig. 3b. However the 580 nm film consisted of small grains near the poly-Si/SiO_2 interface, with some of the grains extending toward the surface, as shown in Fig. 3c.

In general, a significant issue with poly-Si films has been identifying what factors determine preferred grain orientations. It is well known that the preferred orientations of LPCVD-poly-Si films are growth temperature dependent. The reported preferred orientations of LPCVD-poly-Si films were (110) in the range of growth temperatures in this study.[1,2] Furthermore, (100) preferred orientation of LPCVD-poly-Si film has been reported to be obtained in the relatively narrow range at about 675°C[3] or 700°C.[4] UHV-MBD-poly-Si films having (100) preferred orientations have been reported for films with thicknesses over 500 nm,[5] while 500 nm films have shown (110) preferred orientations.[5,6]

We think the causes of the orientation differences between UHV-CVD grown films and films grown by the other two methods mentioned above may be the source materials in the growth atmospheres, as shown in Table II. We can speculate that the dominant difference between UHV-CVD and MBD is whether hydrogen is present or not. This suggests that hydrogen may play a significant role in enhancing (100) orientations. The dependencies of orientations of UHV-CVD-poly-Si films on growth temperature and Si_2H_6 flow rate also suggests correlations in which a higher concentration of hydrogen causes a stronger (100) orientation. In comparing UHV-CVD and LPCVD, it seems that a slight amount of oxygen may enhance (110) orientations. However, further experiments are necessary to confirm these speculations.

Conclusion

UHV-CVD-poly-Si films showed a preferred (100) orientation for a wide range of growth conditions. The (100) orientation increased as thickness and flow rate increased, and as growth temperature decreased. From these dependencies and from comparison with other deposition methods, hydrogen and oxygen are expected to enhance (100 and (110) orientations, respectively. We believe that further experiments to confirm these speculations will provide clues to a solution of what determines preferred orientations of poly-Si films.

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