Characterization of crystallographic properties of SMC poly Si using electron backscattered diffraction

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Summary
Crystallographic properties of silicide mediated crystallization (SMC) polycrystalline silicon (poly Si) and excimer laser annealing (ELA) poly Si were studied by electron backscattered diffraction. Large-grain sized poly Si with a large fraction of low-angle grain boundaries was acquired by SMC, and small-grain sized poly Si with high-angle grain boundaries especially around 60° was acquired by ELA. The thin film transistor (TFT) device characteristics were investigated in view of short-range crystallinity (pattern quality) and long-range crystallinity (misorientation distribution) of the specimens. Short-range crystallinity did not significantly affect the TFT device characteristics, and long-range crystallinity considering the low energy level of special boundaries could be better related to the TFT device characteristics of poly Si.

Introduction
Poly Si films on glass are of increasing interest because of their application to large-area electronics such as flat panel display and solar cells. For the fabrication of poly Si thin film, various processes can be applied. Melt and regrowth of amorphous silicon (a-Si) by excimer laser annealing (ELA) is a well-established method for producing large-grained poly Si thin film (Brotherton et al., 1993). It is a suitable method for the low temperature process, and a high quality poly Si thin film can be acquired using the ELA technique below 400 °C. For the non-laser crystallization method, Ni-mediated crystallization of a-Si is one prospective technique to produce high quality poly Si thin film on glass (Hayzelden & Batston, 1993; Jang et al., 1998). It is good for large-scale manufacturing of high performance poly Si TFT.

Until recently, the main technique available to researchers for the characterizations of poly Si thin film was transmission electron microscopy (TEM) and it has been successfully used for the analysis of microstructures and crystalline characteristics in both ELA and silicide mediated crystallization (SMC) poly Si (e.g. Hayzelden & Batston, 1993; Christiansen et al., 2001). High resolution microstructure images and accurate orientation data can be acquired from transmission electron microscopy (TEM) analysis; however, the observed area is limited to the small regions of thin foil, and it is quite time-consuming work to acquire quantitatively reliable orientation data using TEM. Electron backscattered diffraction (EBSD) is another method of analysing the microstructure and orientation information simultaneously. EBSD has an advantage over TEM in that the orientation acquiring procedure is completely automated and data can be acquired from the entire surface of the specimens. Because quantitatively reliable orientation data acquisition from EBSD is easier than from TEM, recently researchers have been applying this technique for analysing the crystalline properties of poly Si thin film (e.g. Nerding et al., 2002). Using high resolution EBSD system on a field emission electron microscopy (FEGSEM), the authors reported the crystalline properties of SMC poly Si by orientation image mapping (Sohn et al., 2003).

In this paper, we describe our use of the EBSD technique to reveal the crystalline properties of poly Si thin films. The information from EBSD is analysed in terms of short-range crystallinity (pattern quality) and long-range crystallinity (grain boundary misorientation distribution), and we discuss which main factors affect the TFT device characteristics.
Experimental methods

Poly Si thin films were fabricated by SMC and ELA. For SMC poly Si film, SiO2 buffer and hydrogenated amorphous Si (a-Si:H) layers were sequentially deposited on the Corning 1737 glass by plasma-enhanced chemical vapour deposition (PECVD). The thickness of SiO2 and a-Si:H layers were 200 and 100 nm, respectively. Ni particles with an area density of \(2.43 \times 10^{14} \text{cm}^{-2}\) were deposited by a low radio frequency (RF) power density in a N2 environment of 0.4 Torr. Heat treatment for the sample was carried out at 500 °C in a vacuum of a rapid thermal annealing (RTA) chamber. For more details of SMC poly Si fabrication methods see Kim et al. (2002) and Sohn et al. (2003). For the ELA poly Si film, a SiO2 buffer layer and a-Si film were deposited by low pressure chemical vapour deposition (LPCVD) at a substrate temperature of 450 °C on the Corning 1737 glass substrate. The thickness of SiO2 and a-Si layers were 500 and 50 nm, respectively, and the polycrystalline Si grains were melt grown from an a-Si layer using XeCl excimer laser pluses with a wavelength of 308 nm and a duration of 30 ns.

Both poly Si films were etched in HF dilute solution (HF: distilled water = 1: 10) for 5 s to remove the SiO2 layer generated during heat treatment for the crystallization, then cleaned in the distilled water and dried.

The crystallographic properties of the poly Si films were examined by the EBSD technique. A JEOL 6500F Schottky type FEG-SEM equipped with Oxford INCA Crystal EBSD system was used for EBSD analysis. EBSD experiments were carried out at 15 kV accelerating voltage and 4 nA probe current. Pseudo-Kikuchi patterns were integrated for 90 ms in each analysis point and the step size for the orientation mapping was varied from 1 μm to 0.1 μm according to the grain size of polycrystalline Si grains.

Results and discussion

General features of poly Si thin film

The typical surface normal direction orientation maps of SMC and ELA poly Si acquired from EBSD are shown in Fig. 1(a) and (b). Each colour indicates the specific crystallographic direction, and it is also shown as a colour triangle in the corner of the maps. Actually a ‘grain’ is defined as a region with the same crystallographic orientations and same phases (Callister, 1991); it is quite reasonable to define the grains from EBSD data that consist of orientation data. The black line in the maps indicates the grain boundaries with more than 5° misorientation angle, and we recognize that the grain size of
SMC poly Si is larger than that of ELA poly Si. The mean grain size of SMC poly Si was 8.5 μm, and that of ELA poly Si was 0.5 μm. Despite the fact that some grains of SMC poly Si were tens of micrometres in size, the orientations inside the grains were fairly identical. However, there were still small orientation variations inside the SMC poly Si grains and it resulted in the low-angle grain boundaries in Fig. 4(a). By contrast, the orientations inside each ELA poly Si grain were almost the same, and there were seldom low-angle misorientation boundaries in ELA poly Si specimens (see Fig. 4b).

In the TFT device characteristics, ELA poly Si showed better characteristics than that of SMC poly Si. Figure 2 shows the Id-Vg characteristics of p-channel in ELA and SMC poly Si TFT. The ELA poly Si TFT exhibits the field effect mobility of 68.0 cm² V⁻¹ s⁻¹, threshold voltage of -1.4 V and a subthreshold slope of 0.37 V dec⁻¹. In case of the SMC poly Si TFT, the corresponding values are 51.37 cm² V⁻¹ s⁻¹, -3.2 V, and 0.57 V dec⁻¹, respectively.

It is well known that the grain size is proportional to the TFT device characteristics (Sasaki et al., 2000). With thin films with large grains, we can make TFT devices without large energy barriers such as grain boundary within itself. However, in our study, although the SMC poly Si had a grain size 17 times bigger, ELA poly Si showed better TFT device characteristics. It was an incomprehensible result, and we analysed the crystalline properties of both poly Si films by EBSD.

**Short-range crystallinity analysis (pattern quality analysis)**

Pattern quality value acquired from EBSD is an integer value in the range 0 (black) to 255 (white). A pseudo-Kikuchi pattern from EBSD consists of several bands diffracted from each crystalline plane. In the normal algorithm of automatic pattern analysis by computer, the lines of diffracted bands are transformed to spots by Hough transformation because the spots can be more easily distinguished than lines from the undiffracted background (Jessen, 1996). If the crystal structure within the interaction volume of the incident electron beam is well arranged and diffracted strongly, the pattern will consist of sharp bright bands. Then the spot pattern, transformed by Hough transformation, will also consist of distinct bright spots. Then the brightness difference between the brightest point and darkest background in the Hough transformed spot pattern can be converted to an integer number between 0 (black) to 255 (white), ‘pattern quality’. Pattern quality indicates the crystalline properties within the incident electron beam, and we adapted it as the criterion for short-range crystallinity of Si thin film.

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Figure 1(c) and (d) are the pattern quality maps of SMC and ELA poly Si. The grey levels of the two maps were quite similar and it can be seen clearly in the pattern quality histogram graph (Fig. 3). The fully crystallized SMC poly Si had a similar and slightly higher pattern quality than ELA poly Si. The maximum frequency appeared near 50 – a slightly lower value than 200 for the Si single grain wafer. Pattern quality values of SMC poly Si films were increased as the crystallization fraction increased. Pattern quality is also strongly related to the stored energy within the diffracted area, and it can be applied to the presupposition of the recrystallization behaviour by laser annealing in the SMC poly Si. The SMC poly Si films with a lower pattern quality than the ELA specimen recrystallized after laser annealing, but those with a similar pattern quality to the ELA specimen did not change after the same annealing process.

It seems that short-range crystallinity does not affect significantly the TFT device characteristics of poly Si, and another
analysis technique such as long-range crystallinity analysis is needed.

Long-range crystallinity analysis (misorientation distribution)

Through EBSD analysis, a full orientation data set can be acquired at each measuring point, and it is easy to calculate the misorientation between each measured point. In orientation image mapping, the misorientation distribution of the specimen indicates the crystal orientation stability, that is the criterion for the long-range crystallinity in comparison to pattern quality.

Figure 4(a) and (b) are pattern quality maps with boundaries disoriented more than 3° superimposed for SMC poly Si and ELA poly Si. The green lines indicate the low-angle misorientation boundaries (disoriented under 10°, and other lines indicate high-angle grain boundaries (cyan: 10–20, red: 20–30, magenta: 30–40, yellow: 40–50, white: > 50). As stated before, SMC poly Si had a large grain size and a high fraction of low-angle grain boundaries, and ELA poly Si had a small grain size and a high fraction of high-angle grain boundaries.

Figure 5 shows the misorientation histogram of SMC poly Si and ELA poly Si. It is well known that the random boundaries of cubic materials, which do not have any texture or any special boundary relationship, show a typical misorientation...
Fig. 6. Schematic description of relationship between grain boundary energy and grain misorientation in Cu: (a) Σ 7 boundary, (b) Σ 5 boundary, (c) Σ 3 boundary.

distribution known as the Mackenzie profile. It is the profile that increases until 45° according to misorientation angle increase, and then decreases until 63° (Hutchinson et al., 1996). In comparison to the random boundary distribution, the misorientation distribution of SMC poly Si had a large fraction of low-angle boundaries, and that of ELA poly Si had a small fraction of high-angle grain boundaries around 45° and a large fraction of high-angle grain boundaries around 60°. By special boundary analysis of the specimens, it was revealed that the high fraction of high-angle grain boundaries around 60° in ELA poly Si was due to the existence of Σ 3 special boundaries 60° misorientation around <111> axis). As shown in Fig. 4(c) and (d), ELA poly Si thin film had a large fraction of special boundaries such as Σ 3, 5, 7, 9, and SMC poly Si thin film had scarcely any special boundaries (yellow: Σ 3, magenta: Σ 5, red: Σ 7, cyan: Σ 9).

Grain boundary structures can be simplified to the mixture of several sets of edge and screw dislocations (Porter & Easterling, 1992). The grain boundary energy of low-angle grain boundaries is simply proportional to the density of dislocations in the boundary, and it is proportional to the misorientation angle. However, the grain boundary energy of high-angle grain boundaries is saturated independent to the misorientation angle, because the dislocations above critical density can be cancelled out easily. Figure 6 shows the typical relationship between misorientation angle and grain boundary energy in Cu, and it can be simplified to the linearly increased up to 15° and then saturated function, which presented as a thick line. Surface energy of Cu was adapted to estimate the boundary energy of Si thin film. Both materials have cubic symmetry and have the same misorientation/axis relationship for the CSL boundaries. If we apply it to the misorientation distribution of Fig. 4, we can estimate the mean grain boundary energy of poly Si thin films, and it can also imply the energy barriers against the electron movement.

Additionally, there is one more considerable factor in the boundary energy estimation of poly Si films. If grain boundary is the special boundary with low Σ-value, the portion of coincidence site lattice is quite high and the grain boundary energy is low. It is also presented in Fig. 6: the a, b, c labels stand for the Σ 7 boundary, Σ 5 boundary and Σ 3 boundary, respectively. By applying both the simplified grain boundary energy function and the low energy value of low Σ special boundaries to the results of Fig. 4, we obtained the mean grain boundary energy of 0.051 J m⁻² in ELA poly Si, and 0.085 J m⁻² in SMC poly Si as shown in Fig. 7. Although the total fraction of high-angle grain boundary in ELA poly Si is larger than that in SMC poly Si, boundary energy considering the special boundary energy level in ELA poly Si is smaller than the boundary energy in SMC poly Si. This coincides with the TFT device characteristics of poly Si thin films.

The long-range crystallinity considering the low energy level of special boundaries could be better related to the TFT device characteristics of poly Si than the short-range crystallinity.

Conclusions

1. Large-grain sized poly Si with large fraction of low-angle grain boundaries was acquired by SMC, and small-grain sized poly Si with high-angle grain boundaries especially around 60° was acquired by ELA.
2. Short-range crystallinity did not significantly affect the TFT device characteristics. That is strongly related to the stored energy within the diffracted area, and it can be applied to the presupposition of the recrystallization behaviour by laser annealing in the SMC poly Si.
3. TFT device characteristics of poly Si could be explained by the long-range crystallinity analysis considering the low energy level of special boundaries.
References


