Preferred <100> Surface and In-plane Orientations in Self-assembled Poly-Si by Multiple Excimer Laser Irradiation

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Clear preference of <100>- orientation in self-assembled poly-Si is observed for the first time not only in surface, but also in-plane orientations. This textured poly-Si can be used for TFT active channel, expecting a high performance with an excellent uniformity; or can be used as a seed layer for orientation controlling.

Introduction

With µ–Czochraski (grain filter) process, two-dimensional location-controlled single grains can be prepared [1]. Thin film transistors (TFTs) fabricated inside the above single grains have shown excellent performances. a field-effect mobility of 510 cm²/Vs, subthreshold swing of 0.33 V/dec and off-current of 0.04 pA have been reported [2]. It has been found that crystallographic orientation of the grains is random [3]. It is well known that electronic properties of MOSFETs ([4], [5]) have a pronounced dependence on the surface and in-plane crystal orientations with respect to the direction of the current flow due to the anisotropy of the effective mass. The performance of single grain TFTs (SG-Si TFTs) can be improved further if crystallographic orientation of location-controlled single grains can be controlled in some preferred crystal orientation. Furthermore, by this means, the uniformity of TFTs will be improved as well.

In this study, a clearly preferred <100> orientation is observed for both surface and in-plane in square-shaped grains by multiple shots excimer-laser. Laser induced periodic surface structure (LIPSS) is observed and could be the reason for self-assembled square-shaped grains with three-dimensional texture. This textured poly-Si film can be directly used as active material for poly-Si TFT channel or can be used as a seed layer, combined with µ–Czochraski process, to prepare the orientation and location-controlled grains and SG-TFTs.

Experiment details

A 30 nm thick α-Si layer is deposited on thermally oxidized Si wafer (1 µm thick SiO₂) in a conventional horizontal hot-wall LPCVD reactor using pure silane as a source gas at a pressure of 20 Pa and a temperature of 547ºC. Subsequently, the α-Si layer is irradiated with an excimer laser in a vacuum chamber by the XMR 5121 laser system (XeCl laser, λ = 308 nm, FWHM=50 ns) with an energy density varying from 250 to 280 mJ/cm² in 5 mJ/cm² steps. This energy density of the laser is slightly below the...
super-lateral growth (SLG) region [6]. The number of shots varies from 100 to 500, with a pulse repeating frequency of 5 Hz. There is about 3 degree between the incidence light and the normal direction of the surface. No intentional heating of the substrate is applied during the laser irradiation. Within the light path, a tilted quartz attenuator is used to reduce the energy density of the laser and to partly polarize the light.

Results and Discussion

Self-assembly poly-grains:

![SEM images of self-assembly poly-Si grains](image)

Figure 1 SEM images of self-assembly poly-Si grains, crystallized at 260 mJ/cm² after 500 shots: (a) periodic grain boundaries; (b) square-shaped grains.

After the excimer laser crystallization and Secco etching, morphologies of grains are investigated by SEM. Fig. 1 (a) is a SEM image showing the morphology of the poly-Si grains. Parallel, spatially periodic grain boundaries are visible and are well aligned in one direction with a uniform periodicity of about 300 nm. With a high-resolution view [Fig. 1(b)], it is clearly shown that grains are nearly square-shaped, with a grain size of 300 nm, comparatively equal to the wavelength of excimer laser (λ). It is found that the periodicity is independent of the number of shots. These characteristics indicate a very close connection to LIPSS. S. Horita et al. [7] have reported that periodic grain boundaries were created during multiple shots solid-state laser crystallization of an α-Si layer with linearly polarized light. Although excimer-laser light is known to have a minor degree of polarization, in the current experiment settings, the tilted quartz attenuator makes the light partly polarized.

The LIPSS has been confirmed by atomic force microscopy (AFM) analysis. Fig. 2 shows the AFM image of 5 µm by 5 µm area of poly-Si grains. The neighboring grains form a hillock, which represents the grain boundary. The periodic grain boundaries are aligned on one line, with a uniform spacing of about 300 nm. Square-shaped grains are self-assembled, and form a hillock at the each corner of the square.
Figure 2  AFM image of the poly-Si grains, crystallized at 260 mJ/cm² after 500 shots.

Crystallographic orientation:

Figure 3  Texture of poly-Si grains, crystallized at 260 mJ/cm² after 500 shots: (a) SEM image of poly-Si, mapping area is shown inside the rectangle; (b) crystal direction map of the analyzed area, red color indicates <100> crystal orientation in normal direction (ND); (c) pole figure of mapped area and (d) inverse pole figure in ND, rolling direction (RD) and transverse direction (TD).
The texture of the film is analyzed by electron backscatter diffraction (EBSD) with an automatic mapping method. Figure 3 shows the pole figures and inverse pole figure of poly-Si grains in a region as indicated in Fig. 3(a). Fig. 3(a) shows that the square-shaped grains are well-aligned. The clear preference of \( \langle 100 \rangle \) texture is visible not only in the surface orientation [Fig. 3(d)] but also in the in-plane orientation [Fig. 3(c)]. This preferred in-plane orientation is achieved for the first time for lateral growth of Si grains. Furthermore, the preferred in-plane \( \langle 100 \rangle \) orientation is either parallel or perpendicular to the LIPSS direction, i.e., other 4 \( \langle 100 \rangle \) directions are perpendicular to the 4 sides of the square shaped grains.

Figure 4 Texture of poly-Si grains, crystallized at 280 mJ/cm\(^2\) after 500 shots: (a) the selected area for EBSD mapping; (b) crystal direction map of the analyzed area, red color show \( \langle 100 \rangle \) surface orientation (ND); (c) pole figure of poly-Si and (d) inverse pole in ND, rolling direction (RD) and transverse direction (TD).

Figure 4 shows the texture of the poly-Si grains, crystallized at a higher energy. As shown in Fig. 4(a), the periodic grain boundaries are faceted, which means that the periodic grain boundaries, such as LIPSS in Fig. 1 or in Fig. 3 (a) are not well aligned in a
The grain boundaries of square-shaped poly-Si grains are aligned in a zigzagged line. The only difference between Fig.3 and Fig. 4 is the energy density, which indicates that the facet is easily formed at a higher energy density of laser. When the periodic grain boundaries are faceted, there is weak in-plane preferred orientation for these square-shaped grains, shown in Fig.4(c) and Fig.4(d). However, the preferred surface orientation of <100> is still maintained. It should be noted that the poly-Si grains with square shape have the <100> preferred orientation; otherwise the preferred orientation changes to <111> orientation, as indicated in Fig. 4(b).

**Mechanism for preferred orientation**

In liquid phase crystallization, the <100>-texture has been explained by anisotropy of the melting temperature [8]. It is argued that <100>-orientated grains have a higher melting temperature and can coexist in molten Si liquid, as a result of which the new solidified poly-Si grains have <100>-preferred orientation. However, the difference of the melting temperature is negligibly small. For a 0.5 µm thick film, it is about 10^{-2} K. At the melting temperature, the heat conductivity of solid or molten Si is high enough to annihilate the small difference. In this study (Fig.3 and Fig. 4), the <100>-texture can be obtained within a relatively wide energy density window. Furthermore the liquid-solid coexistence is reported to be stable only when the Si contacts with oxide on both sides [9]. Another explanation for the preferred orientation is the anisotropy of surface free energy [9], which is argued for the strong <111>-texture obtained by multiple shots ELC [11]. However, the above anisotropy of the melting temperature is caused by and calculated from the anisotropy of the surface free energy [10]. Thus by the same reason, it could be possible to obtain both <111> and <100>-texture after the multiple shots ELC. In this study, strongly preferred <100> in-plane orientations are successfully obtained as well as the <100> preferred surface orientation in square-shaped poly-grains by multiple shots excimer-laser. LIPSS is observed and could be the reason for self-assembled square-shaped grains with three-dimensional texture.

During the LIPSS formation, the alternate directions of melting and solidification occur on a shot-to-shot basis [12]. Thus melting-solidification cycle requires in-plane 4-fold symmetrical lateral growth direction, the bipolarities of the directions perpendicular and parallel to the LIPSS. It is suggested here that the growth rate, for a given undercooling, is the fastest for <100> direction than other directions. With hundreds of melting-solidification cycles, the preferred in-plane <100> orientation is selected.

This textured poly-Si film can be used as active materials for TFT channels. This textured poly-Si film could be used as seeding layer, combined with μ-Czochraski (grain filter) process, to prepare orientation and location-controlled single grains for TFT fabrication.

**Conclusions**

In summary, strong <100>-texture in self-assembled square-shaped poly-Si grains are observed in both surface and in-plane orientation. This is achieved with for 30 nm α-Si precursor by multiple shots ELC. The strong texture co-exists with the LIPSS and can be obtained in a relatively wide energy density window. It is speculated that the <100>
orientation has fastest growth rate. During the LIPSS formation, in-plane directions of solidification, perpendicular and parallel to the LIPSS, require in-plane 4-fold symmetry and the <100>-orientation is selected and other orientations are occluded. This strong textured film can be used for TFT fabrication or seeds to prepare the orientation controlled grains.

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