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Formation of periodic grain boundary in an Si thin film crystallized by a linearly polarized Nd:YAG pulse laser with an ultra sonic oscillator

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ABSTRACT

In order to obtain a large silicon (Si) grain and to control the location of its boundary in a Si film melting-crystallized by a pulse laser, we have proposed to use periodic thermal distribution spontaneously induced by irradiation of a linearly polarized laser beam. We estimated the suitable amorphous Si (a-Si) thickness taking account of multiple reflection theoretically and confirmed it experimentally. Also, we proposed a novel technique to reduce the irradiation pulse number to control the grain boundary location stably in the crystallized Si film, in which the elastic wave was generated on the surface of a-Si film prior to melting-crystallization by using an ultra sonic oscillator. Owing to this technique, we can control the grain boundary location periodically with only 1 pulse irradiation in the crystallized Si film.

INTRODUCTION

Low temperature polycrystalline Si (poly-Si) thin film transistors (TFTs) are widely used for various applications such as driver circuits of active matrix liquid crystal displays (AM-LCDs) and active matrix organic light emitting diode displays (AM-OLED). Moreover, system on panel (SOP) displays in which the system circuits of the controller and memory are integrated with the driver circuits on a glass substrate will be the most suitable application for poly-Si TFTs in the near future [1]. The pulse laser annealing (PLA) method is effective to produce a poly-Si film consisted of larger grain with the high carrier mobility on a glass substrate [2-5]. In order to control the location of the Si grain boundary which reduces the mobility, we proposed a PLA method with a linearly polarized laser beam. By this method, periodic temperature distribution on the surface of the irradiated Si film is generated spontaneously and the grain boundary location in the crystallized Si film is controlled without additional processes and components [6-8]. This temperature distribution is caused by a periodic beam intensity profile modified due to interference between the incident beam and its diffracted beam on the irradiated surface. This periodic spacing $\Lambda$ is formulated by Rayleigh's diffraction conditions as

$$\Lambda = \frac{\lambda}{n_0 (1 \pm \sin \theta)}$$

(1)
for a p-polarized beam, where $\lambda$ is the incident laser wavelength, $\theta$ is the angle from the normal incidence and $n_0$ is the refractive index of the incident medium above the surface [9]. However, using this method, some irradiation pulses are needed to control the grain boundary location stably [8]. Reducing the pulse number is desired from a viewpoint of the mass-production. Guosheng et al. calculated the periodic beam intensity on a surface with small sinusoidal corrugation of a bulk specimen [10]. Their calculation result indicates that the amplitude of the periodic beam intensity is proportional to the height of the corrugation. In fact, we found that the surface height or roughness of the irradiated Si film was an essential factor for the generation of the periodic temperature distribution [8]. Therefore, it can be considered that if the pseudo surface corrugation is generated prior to irradiation by anything, we can reduce the pulse number to produce a periodic beam intensity profile. Previously, according to the above idea, we tried to generate a shockwave on surface of an Si film due to a laser pre-irradiation prior to melting-crystallization [11]. Using this method, we can produce stably the periodic grain boundary with only 2 irradiation pulses. However, with 1 irradiation pulse, any periodic boundary was not formed at all. On the other hand, Guosheng’s calculation model is available for a bulk specimen, not a thin film on the substrate. For the thin film case, the irradiation beam is reflected multiply between the two interfaces of the atmosphere/thin film and thin film/substrate. Since this multiple reflection makes difficult to apply the Guosheng’s theory to bulk state, we should find the suitable a-Si thickness for generation of a periodic beam intensity profile by irradiation of a linearly polarized laser. In this study, we estimated theoretically the suitable a-Si thickness for our laser melting-crystallization method and then we tried a novel technique for reducing irradiation pulse number, in which the surface of a-Si film is vibrated by an ultrasonic oscillator prior to melting-crystallization.

EXPERIMENTAL

An a-Si film was deposited on a Pyrex glass at 350°C in an ultra high vacuum chamber and the sample was moved to another vacuum chamber. Then, it was irradiated by a linearly polarized Nd:YAG pulse laser (wavelength: 532 nm, repetition frequency: 10 Hz, pulse width: 6-7 ns) at room temperature. The laser irradiation conditions were as follows: The a-Si film thickness was 46-78 nm, the laser energy density ($F$) was 110-170 mJ/cm$^2$ and the irradiation pulse number was 1 or 2. In order to reduce the irradiation pulse number, before irradiating the laser beam to an a-Si film, an ultrasonic oscillator was set up beneath the sample and vibrated. The frequency and input power of the ultrasonic oscillator were $36$ kHz and 19 to 23 W, respectively. After crystallization, some samples were Secco-etched in order to reveal the grain boundary. The surface morphology was characterized by scanning electron microscope (SEM) and Nomarski optical microscope.
RESULTS AND DISCUSSION

At first, we estimated theoretically the suitable a-Si thickness for generation of a periodic beam intensity profile due to radiation of a linearly polarized laser beam, taking account of multiple inner reflection in the Si film. Figure 1 shows the calculation model of the sample structure consisted of vacuum/a-Si or crystalline-Si (c-Si)/SiO₂. In this figure, E₀ is the electric field of the incident laser beam. Eᵦ and Eᵣ are the reflected electric fields for the bulk and film cases, respectively. Eᵦ and Eᵣ are the transmitted electric fields for the bulk and film cases, respectively. r and i are reflection and transmission coefficients, respectively, and the subscripts of 1 and 2 mean the interfaces of vacuum/a-Si or c-Si) and (a-Si or c-Si)/SiO₂, respectively. φᵢ is the incident angle, and φᵣ and φ₂ are refractive angles calculated by Snell's law in the medium of (a-Si or c-Si) and SiO₂, respectively. d is the thickness of a-Si or c-Si film. According to the fundamental optical interference theory, the ratio between Eᵣ and Eᵦ can be easily calculated as

$$\frac{Eᵣ}{Eᵦ} = \frac{1}{r} \cdot \frac{1 + r \cdot \exp(-2i\delta)}{1 + r \cdot \exp(-2i\delta)}$$

where δ is the optical phase difference between the surface of the Si film and the interface of the Si film/substrate. Also, the ratio between Eᵦ and Eᵣ can be calculated as

$$\frac{Eᵦ}{Eᵣ} = \frac{1 + r \cdot \exp(-2i\delta)}{1 + r \cdot \exp(-2i\delta)}$$

The imaginary parts of these equations indicate the difference in electric field phase between the bulk and thin film cases. Therefore, when the imaginary parts of these equations equal to zero, we can apply Guosheng’s theory to our thin film case. Figure 2 shows the dependences of the imaginary parts of Eqs. (2) and (3) on the film thickness of the a-Si and c-Si films in the case of

![Figure 1. Schematic model of the sample structure and multiple reflection in the Si film.](image-url)
normal incidence, i.e., \( \phi = \phi_0 = 0 \). From this figure, it is found that the imaginary parts are equal to zero around 30, 60, and 90 nm. This result suggests that the thickness of the as-deposited a-Si film should be set to be around 30, 60 or 90 nm for formation of the periodic grain boundary. In order to check the validity of this calculation experimentally, we investigated whether the periodic grain boundary was formed or not in the crystallized Si film whose thickness decreased from 45 to 78 nm. Figure 3 shows the a-Si film thickness dependence of the periodic boundary area ratio to the total irradiation area of the crystallized Si film, where the pulse number is two and the laser energy density is 110 to 170 mJ/cm². The grain boundaries were observed from the non-etched Si film by Nomarski optical microscope. The ratio of 100% means that the whole observed area (50 x 50 \( \mu \text{m}^2 \)) of the crystallized Si film has the periodic surface roughness or periodic grain boundary [8]. From this figure, we can see clearly that the periodic boundary area ratios are almost 100% around 60 nm and are almost zero around 50 and 70 nm for any laser fluence. From this result, we can conclude that our calculation to take account of multiple reflection is adequate and one of suitable a-Si thicknesses is 60 nm for our laser crystallization method.

Next, we investigated the effect of the ultra sonic oscillator on the formation of the grain boundary. Figure 4 shows the dependence of the periodic boundary area ratio on the input power of the ultra sonic oscillator with 1 pulse irradiation, where the laser energy density is 170 mJ/cm² and the a-Si thickness is 60 nm. From this figure, we can find that the periodic boundary area increases with the input power of the oscillator although it is notting without the vibration. The length of elastic wave on bulk c-Si is roughly estimated to be 30 cm which is much larger than the period of grain boundary of 520 nm at \( \theta = 0 \). However, our sample dimension is 2 x 3 cm² and the sample consists of layer structure is held on the stage of the oscillator with some fittings, which means that the boundary condition of the vibration is much different from the

![Figure 2. Dependence of the imaginary parts of the \( E_\mu/E_\lambda \) and \( E_\mu/E_\lambda \) on the film thickness for the a-Si and c-Si films.](image)

![Figure 3. Dependence of the periodic structure area ratio of the non-etched Si film crystallized at 2 pulses on the a-Si film thickness, where the laser energy density is 110 to 170 mJ/cm².](image)
ideal case of semi-infinite sample. So, it is possible that the oscillator generates an elastic wave with so short length as to satisfy Rayleigh’s diffraction conditions of Eq. (1) on the surface. Since the amplitude of the elastic wave on the a-Si film surface is increased with the input power, the periodic temperature distribution is generated more easily than without oscillator. As a result, the periodic boundary area ratio is increased with the input power.

Further, with SEM, we observed the surface morphology of the Secco-etched Si film crystallized at P = 170 mJ/cm² and 1 pulse irradiation as shown in Figs. 5 (a) and 5 (b), where the input powers of the oscillator were 0 and 23 W, respectively. In this case, the electric field of the laser beam is horizontal direction. From these figures, we can observe that the vertical grain boundaries are generated periodically in the Si film crystallized with oscillator vibration while the random grain boundaries are generated all over the Si film without oscillator vibration. This means that the periodic temperature distribution occurs only at 1 pulse irradiation by means of

![Figure 5](image1.png)  
(a)  
(b)  

**Figure 5.** SEM images of the Secco-etched Si film crystallized at P = 170 mJ/cm² and 1 pulse, where the input power of the ultra sonic oscillator is (a) 0 and (b) 23 W.
using the ultrasonic oscillator. However, the grain size of this film is very small due to random nucleation which is probably resulted from small amplitude of the periodic temperature distribution for the lateral crystallization. So, in order to obtain good crystalline quality, we must enhance the height of the elastic wave on the Si film surface. Also, since the amplitude of periodic temperature distribution increases with the laser fluence, we should find more optimum laser fluence.

CONCLUSIONS

We investigated the suitable a-Si film thickness and the effect of the ultrasonic oscillator on the grain boundary control in the Si film crystallized by a linearly polarized Nd:YAG pulse laser beam. From the analysis to consider the multiple inner reflection in the Si film, we found that the suitable a-Si thicknesses were about 30, 60 and 90 nm. Also, by using the ultrasonic oscillator, we can form the periodic grain boundaries in the Si film crystallized only at 1 pulse irradiation. This is because the oscillator generates the surface elastic wave as a pseudo periodic surface roughness on the a-Si film.

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