STRUCTURAL PROPERTIES OF POLYCRYSTALLINE SILICON FILMS FORMED BY PULSED RAPID THERMAL PROCESSING


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ABSTRACT

A novel pulsed rapid thermal processing (PRTP) method has been used for realizing the solid-phase crystallization of amorphous silicon films prepared by PECVD. The microstructure and surface morphology of the crystallized films are investigated by X-ray diffraction (XRD) and atomic force microscopy (AFM). The results indicate that this PRTP is a suitable post-crystallization technique for fabricating large-area polycrystalline silicon films with good structural qualities such as large grain size, small lattice microstain and smooth surface morphology on low-cost substrate.

INTRODUCTION

Polycrystalline silicon (poly-Si) is a material of great importance in microelectronics, photovoltaics and display technologies [1-5]. In recent years, there is growing interest in developing practical techniques for fabricating larger-area and high-quality poly-Si films on low-cost glass substrate at a low temperature. Generally, post-crystallization of amorphous silicon is thought to be a preferred technique for this purpose [6,7]. Compared to those as-grown, the poly-Si films prepared by post-crystallization have perfect structure and smooth surface morphology that are required for critical applications. Several post-crystallization methods have been reported. Among them, zone melt recrystallization (ZMR) can produce large-grain poly-Si films [8], but the very high process temperature (>1000 °C) makes the use of low-cost substrate actually impossible; Conventional furnace annealing requires several tens of hours at the temperature around 600 °C (softening point of glass) [9,10], which means high thermal budget and low throughput, diseconomic for large-scale production; Rapid thermal processing (RTP) can greatly shorten the process time [11,12], but due to the continuous thermal exposure to high temperature, the damage to the glass substrate is inevitable; Although laser beam annealing can realize the crystallization at lower temperature [13,14], it is very expensive and also needs to take a long time to scan over a large area; Post-crystallization using a metal as seed can also be carried out at the temperature lower than 600°C [15-17], but the contamination of metal impurity to the Si film is induced. So developing a new effective method to prepare poly-Si films on low-cost substrate is still an attractive and challenging target.

Currently, we have presented an improved rapid thermal processing method—pulsed rapid thermal processing (PRTP), which involves a number of cycles of thermal process. In each cycle, a 60-s thermal bias of 550 °C is used for preheating the films to a "critical state" of crystallization, so that the rapid nucleation and grain growth can be triggered by a following 1-s high-temperature thermal pulse of 850 °C. By using this annealing method, solid-phase crystallization in amorphous silicon films can be completed in several minutes, without need for a metal seed. Moreover, the thermal bias temperature of 550 °C is well below the softening point of Corning 7059 glass, and
the samples are exposed to the high temperature pulse of 850°C for a very short time (only 1-s) in each cycle, thus the thermal damage to the glass substrate can be effectively minimized.

Many of the electrical properties of the poly-Si depend upon its structural quality since carrier transport is sensitive to the lattice imperfection. Perfect structure and smooth surface are desirable for device-quality poly-Si films. In this paper, using X-ray diffraction and atomic force microscopy, we investigate the microstructure and surface morphology of the poly-Si films obtained by PRTP. The structural properties of the poly-Si films are characterized in terms of crystalline orientation, grain size, lattice microstrain and surface roughness. The effect of the deposition parameters of the precursor amorphous silicon on the structural qualities of the crystallized films is also discussed.

EXPERIMENT

The precursor amorphous silicon films for post-crystallization were prepared by the plasma enhanced chemical vapor deposition (PECVD) method at different deposition rates by changing the ratio of gas flow (SiH₄/H₂). Typical deposition parameters are summarized in Table 1. The substrates are Corning 7059 glass and fused quartz. The thicknesses of these films are determined by the measurements of the optical transmission spectra, and the deposition rates are calculated by dividing film thicknesses by the deposition time. The crystallization by PRTP was carried out in a KST-2 rapid thermal processor with thirteen tungsten halogen lamps as heat source and N₂/Ar as ambient atmosphere. The heating rate is about 300 °C/s. The samples were placed on a silicon wafer holder, on which a Pt-PtRh thermocouple was set beside the samples, used for measuring and controlling process temperature. The time-temperature pattern of the PRTP was programmed, as shown in Figure 1.

Table 1 Deposition parameters of amorphous silicon films

<table>
<thead>
<tr>
<th>Sample</th>
<th>T_d (°C)</th>
<th>H₂/SiH₄</th>
<th>Time (hour)</th>
<th>Thickness (µm)</th>
<th>r_d (Å/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>s₁</td>
<td>400</td>
<td>10</td>
<td>4</td>
<td>0.932</td>
<td>0.647</td>
</tr>
<tr>
<td>s₂</td>
<td>400</td>
<td>8</td>
<td>4</td>
<td>1.213</td>
<td>0.842</td>
</tr>
<tr>
<td>s₃</td>
<td>400</td>
<td>5</td>
<td>4</td>
<td>1.435</td>
<td>0.995</td>
</tr>
<tr>
<td>s₄</td>
<td>400</td>
<td>3</td>
<td>4</td>
<td>1.773</td>
<td>1.231</td>
</tr>
</tbody>
</table>

Fig. 1. PRTP diagrams (a) programmed pattern and (b) actual pattern.
The X-ray measurements were performed using a Philips Diffractometer. The diffraction profiles were recorded by automatic Savitzky-Golay's scanning with Ni-filtered Cu Kα radiation (1.542 Å). With the accurate measurement and strict analysis of the diffraction peak, it is possible to give a reliable analysis of the lattice microstrain and a reasonable evaluation of the mean grain size which was usually overestimated by averaging the sizes of the maximum grains observed in the TEM images. AFM analyses of both annealed and unannealed films are performed using a Digital Instruments Nonoscopy III Multimode Microscopy, operating in tapping mode.

RESULTS AND DISCUSSION

Figure 2 shows the X-ray diffraction profiles of the sample 4 on glass before and after 1-, 5-, 10- and 20-cycle PRTP, respectively. No obvious diffraction peak is observed before PRTP, which exhibits the unprocessed Si film is X-ray amorphous, while several small peaks appear after 1-cycle PRTP, indicating the initiation of the crystallization. Then the intensity of each peak is enhanced with increasing the processing time and reaches stable values after 10-cycle processing, showing that the post-crystallization can be completed within several minutes, which is 2 orders of magnitude shorter than the time required by the conventional furnace annealing method. We can see the very strong diffraction peak at 28.52° that represents (111) preferred orientation. In general, the crystallite size can be evaluated from the breadth of the X-ray Bragg diffraction peak using the Scherrer formula

\[ D(\text{hkl}) = \frac{kλ}{β(2θ)\cosθ} \]

This formula can give a mean grain size assuming that the peak line broadening only results from the size distribution after subtracting the instrument broadening from the measured FWHM \( β(2θ) \). Actually, with increasing crystallite size the peak broadening due to lattice imperfections such as microstrains becomes considerable. For obtaining reliable values of the crystallite size in this case, we used the Fourier analysis method [18] that was originally used to evaluate the structural quality of cool-worked metals. The method is based on the analysis of the peak profile rather than the
estimation of peak half width. Following the work of Warren and Averbach [19,20], the
diffraction peaks are fitted by a Fourier series after subtracting the background and $k\alpha_2$-
component profile by making the Rachinger correction [21]. Then the mean grain size and root-
mean-square strain can be determined from a plot of the natural logarithm of the Fourier cosine
coefficient vs. the square Miller index sum $(h^2+k^2+l^2)$.

For studying the effect of deposition parameters on the crystallization, the four samples(s1-
s4) deposited at different rates were processed by PRTP for 10 minutes. The crystallization was
then completed and the stable values of grain size and microstrain were obtained by the X-ray
analysis method mentioned as above. Figure 3 shows the grain size and microstress as functions of
deposition rate of the precursor amorphous films. It can be found that higher deposition rates
result in larger grain sizes and smaller microstrains. This can be explained as follows: with
increasing deposition rate, structural disorder of the Si network increases, which usually results in
low nucleation rates [10] during the post-crystallization procedure, thus giving rise to larger grain
sizes and the smaller lattice strains.

Figure 4. shows AFM images of sample 3 before and after 10-cycle PRTP. The image (b)
reveals features on the crystallized film surface which correlate well with the grain sizes evaluated
from X-ray diffraction. Furthermore, the root-mean-square (rms) roughness is calculated from
“raw” 1×1 μm scans, transformed into k-space with the $k_x=0$ and $k_y=0$ lines removed to correct
for AFM artifacts [22]. As a result, the rms roughness of the sample 3 before and after PRTP are
found to be 0.580nm and 0.955nm, respectively. Such a roughness of the crystallized film is far
smaller than that of the as-deposited poly-Si , and beneficial to the device fabrication.

CONCLUSIONS

Using X-ray diffraction and atomic force microscopy, we examined the microstructure and
surface morphology of the polycrystalline silicon films formed by pulsed rapid thermal processing.
The results suggest that this post-crystallization technique has potential for preparing poly-Si films
with large grains and smooth surfaces. Moreover, the mean grain size and microstrain in these
poly-Si films are closely related to the deposition parameters of the precursor amorphous silicon
films. A higher deposition rate results in larger grain sizes and smaller lattice strains in the post-
crystallized films.
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REFERENCES


