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Improvement of the surface roughness and the electrical resistivity of polycrystalline $Si_{1-x}Ge_x$ films by two step deposition and Ar/H_2 plasma treatment

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Poly-$Si_{1-x}Ge_x$ films were prepared on thermally oxidized Si(100) wafers using two step deposition (550 °C, 400Pa + 600 °C, 400Pa) by rapid thermal chemical vapor deposition. The deposited films were subjected to in-situ annealing and Ar/H_2 plasma treated. The changes to the surface roughness, the grain size, and the electrical resistivity were investigated. The surface roughness was improved greatly by two step deposition whereas the grain size was slightly decreased. By in-situ annealing, the grain size increased up to 170 nm. Both the rms value and the resistivity decreased during Ar/H_2 plasma treatment and were influenced by the surface etching effect of Ar ions and the hydrogenation effect, respectively.

Key words: Poly-$Si_{1-x}Ge_x$, Chemical vapor deposition (CVD), Surface roughness, Atomic force microscope (AFM).

Introduction

Thin films of polycrystalline $Si_{1-x}Ge_x$ with a large grain and smooth surfaces are required to obtain high mobility and high stability thin film transistors [1, 2]. It is, however, very difficult to have the improved properties concurrently because they are contrary to each other. Therefore, a process for both enlarging grain size and decreasing surface roughness of polycrystalline $Si_{1-x}Ge_x$ is needed.

We have recently attempted to analyze the effects of the initial surface state by varying the deposition temperature and pressure on the final film surface roughness and grain size of poly-$Si_{1-x}Ge_x$ [3]. Although a the large grain size (~180 nm) was obtained at higher temperature and lower pressure, the resultant film was very rough. Thus in order to obtain a smooth surface, it is necessary to prepare films through an initial low temperature deposition method to obtain a surface with a large number of nucleation sites. A two-step deposition process has been used to improve the surface roughness of poly-Si, however, the use of this two-step process on the surface roughness of poly-$Si_{1-x}Ge_x$ has not been examined previously.

Furthermore, it has been reported that an Ar plasma treatment, which was mainly used to clean the surface of the substrate prior to thin film deposition, modified the surface roughness of the thin film after deposition due to the surface etching effect of ions [4]. To date, no thorough study of this effect on the modification of poly-$Si_{1-x}Ge_x$ film surfaces has been undertaken.

For this reason, we have attempted to investigate the effect of the two-step deposition process and Ar/H_2 plasma treatment on the surface roughness, the grain size, and the electrical resistivity of the resulting poly-$Si_{1-x}Ge_x$.

Experimental details

Poly-$Si_{1-x}Ge_x$ films were deposited by the rapid thermal chemical vapor deposition (RTCVD) on thermally oxidized Si (100) wafers using SiH_4 (5% SiH_4 in Ar) and GeH_4 (7% GeH_4 in H_2) as the source gases. After a thin buffer Si layer was deposited on SiO_2 at 470 °C for 4 minutes, the poly-$Si_{1-x}Ge_x$ films were deposited using two-step deposition (550 °C, 400Pa + 600 °C, 400Pa) process. The deposition temperature change from low temperature to high temperature occurred rapidly in the same reactor by an increase of lamp power. The samples were then in-situ annealed at 580 °C for 30 minutes. Figure 1 shows a schematic diagram of the two-step deposition process. In addition, a one-step process (600 °C, 400Pa) was conducted in order to compare the results between the two processes.

To investigate the effect of an Ar/H_2 plasma on the surface roughness of poly-$Si_{1-x}Ge_x$ films after two-step deposition and the in-situ annealing process, the plasma treatment was performed in a plasma enhanced chemical vapor deposition reactor using a mixture of Ar and H_2 as the plasma gas and N_2 gas for purging. Reaction parameters were as follows; a substrate temperature of 100 °C, a working pressure of 133Pa, a rf power of 50W, a electrode distance of 25 mm, and a reaction time

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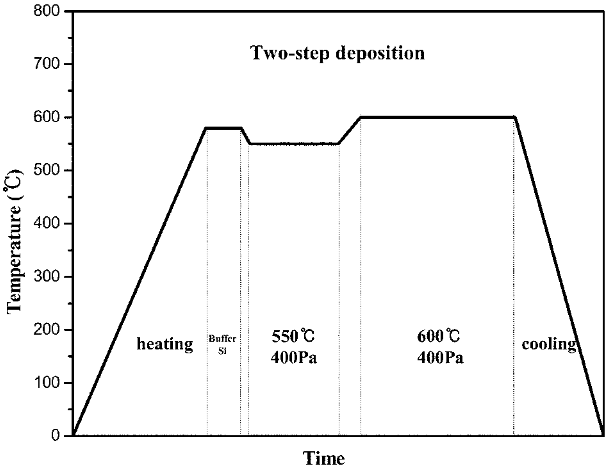

Fig. 1. Schematic diagram of the two-step deposition process.

of 4 minutes. The discharge frequency was 13.56 MHz.

Atomic force microscopy (AFM) and transmission electron microscopy (TEM) were used to examine the surface morphology and the grain size of the poly-$Si_{1-x}Ge_x$ films. Electron spectroscopy for chemical analysis (ESCA) and Fourier transform infrared spectroscopy (FT-IR) were used to analyse the chemical state and the hydrogen bonding of films before and after plasma treatment, respectively. The resistivity was measured by a four-point probe method.

Results and Discussion

Effect of two- step deposition

Figure 2 shows AFM images of a 200-nm-thick $Si_{1-x}Ge_x$ film to demonstrate the effect of the two- step deposition on the surface roughness of the films. Figure 2(a) shows the surface roughness of the film deposited by a one step (600 °C, 400Pa) and Fig. 2(b) is for a film deposited using a two step- (550 °C, 400Pa + 600 °C, 400Pa) deposition. In this figure, the remarkable improvement of the surface roughness achieved by the two-step deposition can be seen and the surface cluster size is smaller in the two-step case than that of the one-step deposition. The calculated rms values and the grain size of the film by the two-step deposition are compared to that of the film deposited by the one-step deposition in Table 1. The rms values of the thin film deposited by two-step and the film deposited by one-step process are 6.1 and 16.3 nm, respectively. This result can be explained as follows; Generally, the nucleation sites act as seed crystallites for the diffusing adatoms and form the initial grains in the polycrystalline film. Therefore, when a lower deposition temperature process is used for the initial stage of film deposition to form many nucleation sites, a smoother surface may be obtained by the faster nucleation rate than the grain growth rate due to the formation of a large number of nuclei before grain growth. Following this, by altering the deposition temperature rapidly to a higher value, it is likely that large grains are obtained because the increased temperature provides enhanced surface mobility and diffusion distances. For this reason, the surface will be considerably smoother after the two-step deposition process although the grain size will be slightly smaller.

Table 1. Surface roughness, grain size, and resistivity of poly-$Si_{1-x}Ge_x$ films deposited by one-step and two-step process

Experimental conditions	Surface roughness (rms) (nm)	Grain size (nm)	Resistivity (Ω·cm)
One-step deposition	16.3	180	4.2
Two-step deposition	6.1	140	5

This result may be due to the difference of the initial cluster state between the single step deposition process with sparse large clusters and the two-step deposition process with fine clusters as shown in Fig. 2.

Effect of in-situ annealing

After the two-step deposition, in order to increase the grain size, the samples were in-situ annealed at 580 °C for 30 minutes. Figure 3 shows plan-view TEM micro-

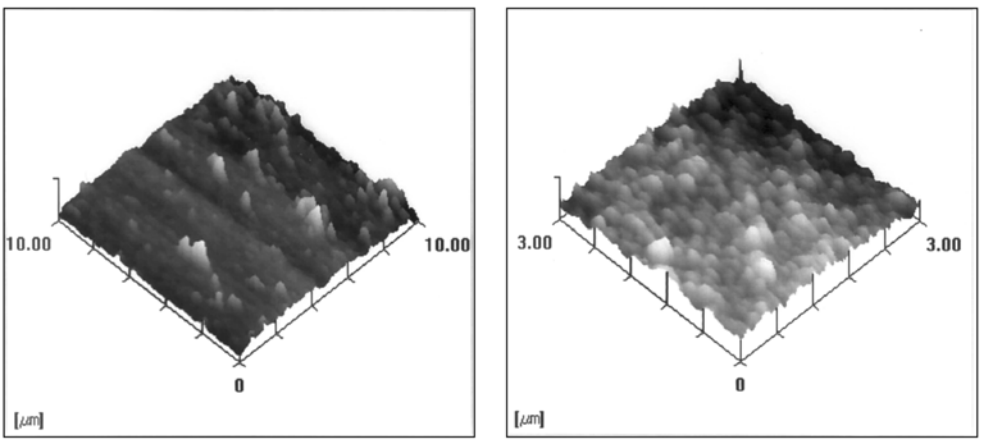

Fig. 2. AFM images of the poly-$Si_{1-x}Ge_x$ films deposited by (a) one-step (600 °C, 400Pa) and (b) two-step (550 °C, 400Pa + 600 °C, 400Pa) process.

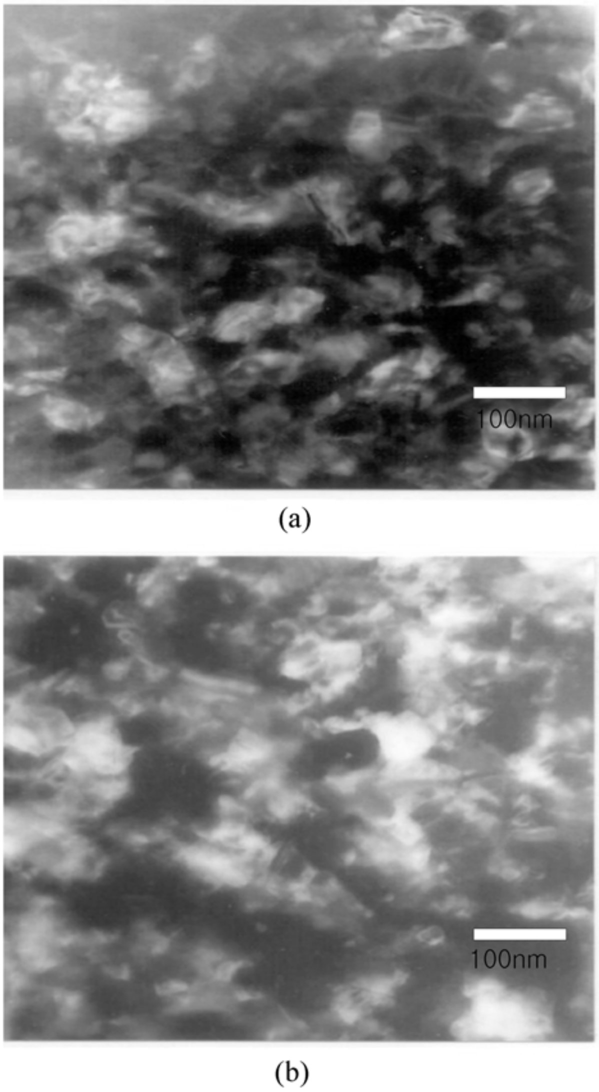

Fig. 3. Plan-view TEM micrographs of the poly-$Si_{1-x}Ge_x$ films after (a) two-step deposition and (b) in-situ annealing.

graphs of $Si_{1-x}Ge_x$ films after two-step deposition (Fig. 3(a)) and after the in-situ annealing process (Fig. 3(b)). The average grain size of the film in-situ annealed is 170 nm, which is shown in Table 2. Although the reason why the grain size is increased by in-situ annealing is not fully explained, it may be caused by the adatoms which attach unstably to existing clusters due to the rapid cooling rate when the lamp is switched off after deposition. These adatoms can achieve sufficient energy to diffuse as annealing progresses. This causes clusters to coalesce, and this leads to a larger grain size.

Table 2. Surface roughness, grain size, and resistivity of poly $Si_{1-x}Ge_x$ films treated by in-situ annealing and Ar/H_2 plasma

Experimental conditions	Surface roughness (rms) (nm)	Grain size (nm)	Resistivity (Ω·cm)
In-situ annealing	3.5	170	2.5
Ar/H_2 plasma treatment	2.4	170	1.2

Comparison of this result with other investigations which studied means to obtain large grain sizes by various processes shows good agreement [5] except for the solid phase crystallization (SPC) process [6, 7] which required very long times. Therefore, it can be concluded that the two-step deposition process with in-situ annealing process is useful to obtain smooth surfaces and a large grain size because it needs a relatively low deposition temperature and short time. On the other hand, the resistivity is decreased from 5 Ω·cm to 2.5 Ω·cm by in-situ annealing, which is discussed later.

Effect of Ar/H_2 plasma treatment

As seen in previous data (Table 1), the resistivity and rms value of $Si_{1-x}Ge_x$ films deposited by the two-step process are still high. In order to decrease the resistivity and modify the surface roughness, a plasma treatment was performed in an Ar/H_2 mixture after the two-step deposition and in-situ annealing processes.

AFM images of an in-situ annealed film and a Ar/H_2 plasma treated film are shown in Fig. 4. The rms values, the grain sizes, and the resistivities are given in Table 2. The rms value decreased from 3.5 nm to 2.4 nm and the resistivity decreased from 2.5 Ω·cm to 1.2 Ω·cm, but there was no change in the grain size. The

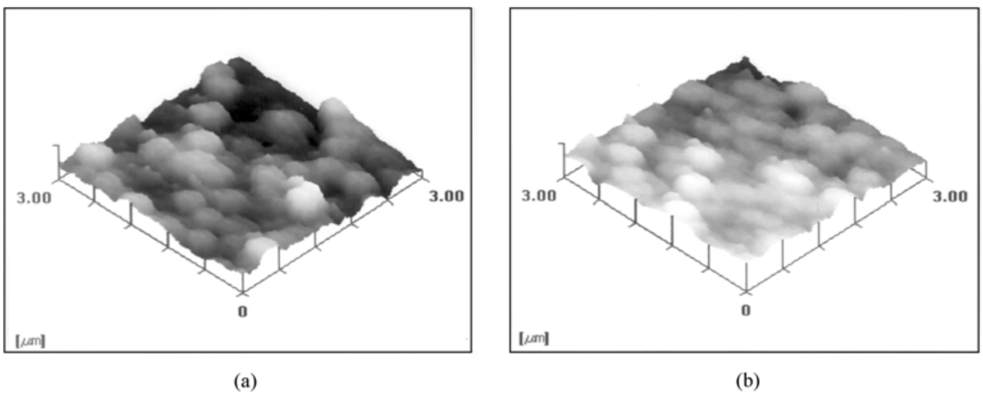

Fig. 4. AFM images of the poly-$Si_{1-x}Ge_x$ films after (a) in-situ annealing and (b) Ar/H_2 plasma treatment.

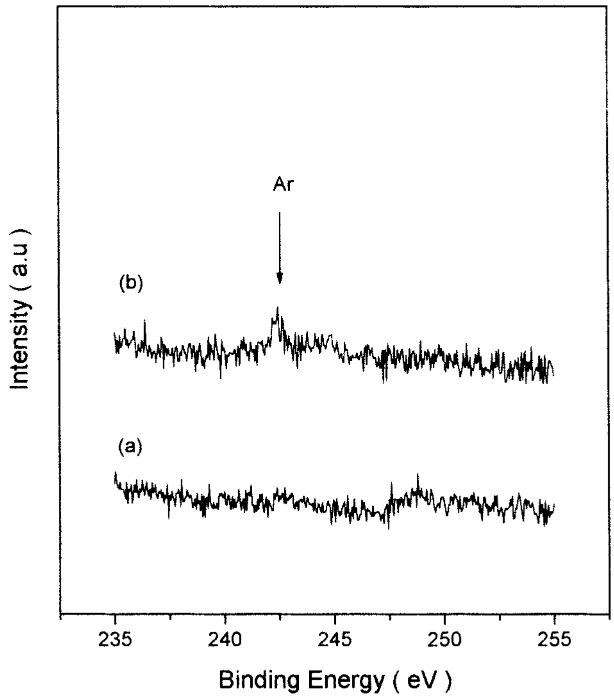

Fig. 5. ESCA spectra of the poly-$Si_{1-x}Ge_x$ films after (a) in-situ annealing and (b) Ar/H_2 plasma treatment.

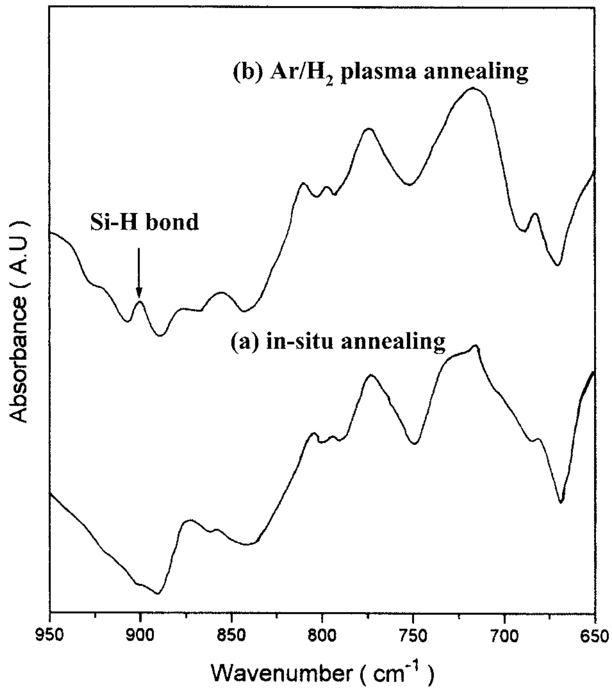

Fig. 6. FTIR spectra of the poly-$Si_{1-x}Ge_x$ films after (a) in-situ annealing and (b) Ar/H_2 plasma treatment.

decrease of surface roughness after the Ar/H_2 plasma treatment can be explained by the surface etching effect due to the increasing surface collision energy of particles in the plasma. This is evidenced by the existence of an Ar peak at a binding energy of 242.5 eV in the case of the Ar/H_2 plasma treated sample as shown in Fig. 5. Since the Ar ion can sputter-etch the surface, the surface roughness is improved a little.

The effect of the Ar/H_2 plasma treatment on the resistivity can be explained as follows; the adsorption of hydrogen onto a solid surface is known to have a strong influence on the electrical properties of semiconducting materials. The hydrogen diffuses into the bulk of the semiconductor and passivates the electrically active defects, especially at grain boundaries. Thus the potential barrier is lowered at the grain boundaries and this leads to a decrease in the resistivity of the material. From the Ar/H_2 plasma treated sample, the hydrogen from the surface of $Si_{1-x}Ge_x$ films favours incorporation into the defect sites, which is confirmed by the Si-H bond peak [8, 9] at a wavenumber of 890 cm^{-1} (Fig. 6). As a result, the Ar/H_2 plasma treated film has a lower resistivity than the in-situ annealed film by this hydrogenation effect.

Conclusion

In this study, we have investigated the effects of a two-step deposition process and an Ar/H_2 plasma treatment on the surface roughness, the grain size, and the electrical resistivity of poly-$Si_{1-x}Ge_x$ films. It was found that a remarkable improvement in the surface roughness of the films was achieved by the two-step deposition process due to the formation of a large number of muclei before grain growth. After the two-step deposition process and in-situ annealing, the grain size was around 170 nm. Upon plasma treating in an Ar/H_2 mixture, the rms value decreased from 3.5 nm to 2.4 nm and the resistivity decreased from 2.5 Ω·cm to 1.2 Ω·cm. These changes were predominantly influenced by the surface etching effect of Ar ions and the hydrogenation effect, respectively.

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