Behavior of Si Atoms, Ge Atoms and Vacancies for Flash Lamp Annealing

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Abstract
Effects of vacancies on the crystallization of Si and Ge films were investigated for flash lamp annealing (FLA). The crystallization mechanism (crystal orientation) differed between solid- and liquid-phase crystallization due to different vacancy densities. The shape of crystal grain for Si and Ge films differed, and this related with the difference in self-diffusion and vacancy density. From the estimation of vacancy formation energy, the Ge film is easy to crystallize and generate crystal defects (vacancies) in comparison with the Si film. The controlling technique of vacancy during FLA crystallization can be applied to the formation of high-quality polycrystalline Ge films.

1. Introduction
Low-temperature crystallization of amorphous germanium (a-Ge) films is important for realizing high-quality thin-film transistors and solar cells. In general, the crystallized Ge films have high-carrier density due to many crystal defects. Recently, it is reported that junction-less Ge metal-oxide-semiconductor field effect transistors using flash lamp annealing (FLA) have high mobility and high on/off ratio [1]. On the other hand, we have investigated the behavior of Si atom and vacancy in excimer laser annealing [2-4].

In this study, to clarify the crystallization mechanism of Si and Ge films, the difference in behavior of Si and Ge atoms for FLA crystallization was investigated in term of vacancy density.

2. Experimental
Amorphous Si (a-Si) and a-Ge films were deposited on glass or quartz substrate by plasma enhanced chemical vapor deposition and electron beam evaporation, respectively. The thickness of a-Si and a-Ge films were 50 and 100 nm, respectively. After surface cleaning by HF solution, the FLA was carried out at sample-holder temperatures of RT, 200 and 400 °C for various lamp voltages. The shot number of FLA was 1. To compare with a thermal crystallization, the a-Si and a-Ge films were annealed at 1000 or 800 °C for 30 min in a furnace. The structural properties of the polycrystalline Si (polys-Si) and polycrystalline Ge (poly-Ge) were evaluated by Raman scattering spectroscopy, X-ray diffraction (XRD) measurements and scanning electron microscopy (SEM) observation.

3. Results and discussion
The crystalline fraction and full width at half maximum (FWHM) estimated from Raman spectra of the poly-Si and poly-Ge films are shown in Figs. 1 (a) and (b), respectively. The FWHM of the crystallized Si film by FLA was small in comparison with that by the thermal annealing. It is considered that the defect density in the crystal grain or at the grain boundary for the FLA poly-Si films was low, and high-quality poly-Si films can be obtained by FLA. As the lamp voltage increased, the crystalline fraction and FWHM increased for Si films. On the other hand, the FWHM of Ge films was increased by increasing the lamp voltage in spite of constant crystalline fraction. These results show that the vacancy was frozen during liquid-phase crystallization (LPS) and the vacancies in the Ge films was easy to remain compared with Si films.

The XRD patterns of the poly-Si and poly-Ge films prepared by FLA are shown in Figs. 2 (a) and (b), respectively. In the Si films, as the lamp voltage increased from 3400 to 3800 V, the (111) preferential orientation changed to the random orientation. On the other hand, the Ge films had the random orientation. From the previous work, it was found that solid-phase crystallization (SPC) and LPC occurred at 3400 and 3800 V for Si films, respectively. It implies that the random orientation produced under LPS condition [3, 5].

The SEM images of the poly-Si and poly-Ge films subjected to secco etching are shown in Figs. 3 (a) and (b), respectively. The average grain sizes of Si and Ge films was 210 and 70nm, respectively. In the case of Si film, the laterally crystal growth was observed. For the Ge film, circular grains were observed. It is considered that the difference in grain shape is caused by the difference in the self-diffusion of Si and Ge atoms and the vacancy densities between Si and Ge films.

Next, we discuss the crystallization mechanism of Ge film from the difference in behavior of atoms and vacancies between Si and Ge films. The atomic diffusion is produced by site exchange with vacancy. Therefore, as the vacancy density increased, the atomic diffusion is enhanced. The frequency of diffusion for the Ge atoms was larger than that for the Si atoms because the vacancy density of Ge films was higher than Si films (Fig. 4 (a)). In general, the vacancy density for LPC is higher than that for SPC (Fig. 4 (b)). Therefore, the crystalline fraction and FWHM were influenced by the difference in LPC and SPC. In addition, it implies that the divacancies can be generated in the Ge...
films and these divacancies effect the difference of crystallization mechanism between Si and Ge films. This is under consideration. On the other hand, it is considered that the vacancy is generated proportional to equilibrium state for SPC. The formation energy of vacancy relates the binding energy and the coordination number. These energies of Si and Ge were estimated to 4.49 and 3.65 eV, respectively. It is shown that the vacancy density is one of the key points for formation of high-quality poly-Ge films.

4. Conclusions
1) The difference in atomic self-diffusion for SPC and LPC is caused by the difference in vacancy density. This difference affects the crystallization mechanism (crystal orientation).

2) The activation energy of self-diffusion of Ge atoms is smaller than that of Si atoms. The formation energy of vacancy in Ge film was smaller than that in Si film. Therefore, the Ge film is easy to crystallize and generate vacancy in comparison with the Si film.

3) To obtain high-quality poly-Ge film, it is necessary to control both crystallization process and vacancy formation.

References