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Hoshino, Y. / Yachida, G. / Nakata, J.

(出版者 / Publisher)法政大学イオンビーム工学研究所

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### THE EPITAXIAL GROWTH OF AMORPHOUS SI LAYER DEPOSITED ON HYDROGEN-TERMINATED SURFACES USING ION BEAM INDUCED EPITAXIAL CRYSTALLIZATION WITH ION BEAM MIXING

G. Yachida, Y. Hoshino, and J. Nakata<sup>#</sup> Graduate school of science, Kanagawa University, 2946, Tsuchiya, Hiratsuka, Kanagawa 259-1293, Japan

#### Abstract

We have investigated the crystallization process of an amorphous Si (a-Si) layer deposited on hydrogen-terminated Si(001) surfaces by ion beam induced epitaxial crystallization (IBIEC) combined with ion beam mixing (IBMX) aiming at the clarification of the substitutional IBMX effect on the crystallization process. We firstly deposited a-Si layer on two kinds of hydrogen-terminated Si(001) surfaces of dihydride (DH) and monohydride (MH), and then carried out the IBMX by 10-keV Si<sup>+</sup> ion irradiation with a fluence of  $1 \times 10^{15}$  ions cm<sup>-2</sup> at room temperature near the amorphous/crystalline interface followed by the IBIEC treatment by 180-keV Ar<sup>+</sup> ion irradiation with a fluence of  $1 \times 10^{16}$  ions cm<sup>-2</sup> at 300 and 500°C. The crystallization rate of a-Si layer was analyzed by Rutherford backscattering spectrometry with 2.56 MeV  $^{10}B^{2+}$  projectiles under the [001]-aligned geometry. As a result, the a-Si formed on the hydride surfaces with IBMX treatment was crystallized by IBIEC at 500°C, regardless of the amount of interfacial hydrogen. Consequently, we suggest that the IBIEC combined with IBMX treatment makes it possible to epitaxial crystallize at significantly low temperature for amorphous layer on hardly crystallized structure.

#### I. Introduction

Solid phase epitaxial growth (SPEG) of amorphous layer is one of the crucial techniques in semiconductor fabrication. It is widely known that the amorphous/crystalline (a/c)interface should be atomically controlled to achieve the high-quality epitaxial growth of amorphous layer. Furthermore, the amorphous Si (a-Si) layer deposited on a clean Si surface can be easily crystallized via the SPEG at the temperatures as low as 200°C under ultrahigh vacuum (UHV). However, high temperature annealing more than 800°C (typically flashing above 1200°C) in UHV condition is necessary to obtain and keep a clean surface. To remove contaminations and inactivate the surface, H-termination of Si surface using a diluted hydro-fluoric (HF) acid treatment is effective. However, the epitaxial growth of a-Si formed on the hydride surfaces is more difficult than that on the clean Si surface. In order to epitaxially crystallize the a-Si layer formed on the H-terminated Si surface, we propose the special method of ion-beam induced epitaxial crystallization (IBIEC) combined with ion beam mixing (IBMX). In previous studies, Ferla et al. and Nakata individually performed the epitaxial crystallization of a-Si layer deposited on the Si substrate covered with thin native oxide layer by IBMX followed by IBIEC process.<sup>1, 2)</sup> However, they deposited a-Si layer on native oxide layer formed on crystalline Si surface. In general, native oxide layer is not well defined and existing various kinds of contaminations. Moreover, they irradiated As or P ions in the IBMX process, which is

<sup>&</sup>lt;sup>#</sup> e-mail: nakatj01@kanagawa-u.ac.jp

known to significantly enhance the crystallization rate. Several studies have been reported on the epitaxial crystallization of a-Si layer using IBMX process, but the essential IBMX effect is not known yet. In this study, we clarified the essential IBMX effect on the crystallization process.

#### **II. Experimental**

We prepared two kinds of hydrogen-terminated (H-terminated) Si(001) surfaces with dihydride (DH) and monohydride (MH) structure. The DH surface was obtained by conventional RCA method finished by dipping in diluted hydro-fluoric acid solution.<sup>3)</sup> The MH surface was obtained by thermal annealing of the DH sample at 350°C for 30 min in UHV ambient. Gupta *et al.* reported that one of the H atoms on the DH surface was desorbed by the above treatment, and then the DH surface changes into the MH surface.<sup>4)</sup> Next, a-Si layer was deposited on the H-terminated Si surfaces with 10-15 nm by electron bombardment evaporator at room temperature (RT). The deposition rate was calibrated by Rutherford backscattering spectrometry (RBS) in advance, and was estimated to be 0.3 nm min<sup>-1</sup>. These samples were performed by IBMX preparation by 10-keV Si<sup>+</sup> ion irradiation with an ion fluence of  $1 \times 10^{15}$  ions cm<sup>-2</sup> at RT near the amorphous/crystalline (a/c) interface followed by IBIEC treatment, the dose rate was kept to  $1 \times 10^{15}$  ions cm<sup>-2</sup> at 300 and 500°C. In IBIEC treatment, the dose rate was kept to  $1 \times 10^{11}$  ions cm<sup>-2</sup> sec<sup>-1</sup>, because the crystallization rate significantly depends on ion flux in the process. The thickness of crystallized layer was analyzed by RBS-channeling method at the [001]-aligned incidence by 2.56 MeV <sup>10</sup>B<sup>2+</sup> ions.

#### **III. Results and Discussion**

Figure 1 shows the RBS-channeling spectra observed for the Si-deposited samples with ~15 nm thick on the DH surfaces before (open circles) and after IBIEC treatment by 180-keV Ar<sup>+</sup> ions with an ion fluence of  $5 \times 10^{15}$  ions cm<sup>-2</sup> at 300 (gray curve), and 500°C (black curve). Triangles indicate the pristine Si (001) substrate spectrum for reference. It is clearly seen that the a-Si layer deposited on DH surfaces was not crystallized at these temperatures.



Fig. 1. The RBS-channeling spectra observed for the Si-deposited samples with ~15 nm thick on the DH surfaces before (open circles) and after IBIEC treatment by 180-keV Ar<sup>+</sup> ions with an ion fluence of  $5 \times 10^{15}$  ions cm<sup>-2</sup> at 300 (gray curve), and 500°C (black curve). For reference, the spectrum for a pristine Si(001) substrate is depicted by triangles.

Figure 2 shows the RBS-channeling spectra observed for the Si-deposited samples with ~10 nm thick on the DH (a) and MH (b) surfaces before (open circles) and after IBMX treatment (black circles) by 10-keV Si<sup>+</sup> ions with an ion fluence of  $1 \times 10^{15}$  ions cm<sup>-2</sup> at RT, and then IBIEC treatment by 180-keV Ar<sup>+</sup> ions with an ion fluence of  $5 \times 10^{15}$  ions cm<sup>-2</sup> at 300 (gray curve) and 500°C (black curve). The a-Si layer deposited on the DH surfaces was

not crystallized by only IBIEC treatment; whereas that was crystallized by IBMX followed by IBIEC at 500°C. It can be suggested that the IBIEC combined with IBMX treatment is effective method for epitaxial crystallization of amorphous layer on obstructive surface, regardless of the amount of interfacial contaminations.



Fig. 2. The RBS-channeling spectra observed for the Si-deposited samples with ~10 nm thick on the DH (a) and MH (b) surfaces before (open circles) and after IBMX treatment (black circles) by 10-keV Si<sup>+</sup> ions with an ion fluence of  $1 \times 10^{15}$  ions cm<sup>-2</sup> at RT. Gray and black curves indicate the spectra after the IBIEC treatment by 180-keV Ar<sup>+</sup> ions irradiation with an ion fluence of  $1 \times 10^{16}$  ions cm<sup>-2</sup> at 300 and 500°C, respectively.

In order to validate the irradiation effect, we also carried out thermal annealing without IBIEC for the IBMX treated samples under the same condition of temperature, duration and pressure in the IBIEC treatment. Figure 3 shows the RBS-channeling spectra observed for the Si-deposited samples with ~10 nm thick on the DH and MH surfaces before and after IBMX treatment by 10-keV Si<sup>+</sup> ions with an ion fluence of  $1 \times 10^{15}$  ions cm<sup>-2</sup> at RT, and then thermal annealing at 500°C for 350 min in vacuum ( $\leq 10^{-4}$  Pa). As shown in Fig. 3, the a-Si layer formed on H-terminated Si surfaces was not crystallized by thermal annealing at 500°C even by IBMX treated samples. This fact shows that the IBIEC combined with IBMX treatment is effective to induce epitaxial crystallization for the a-Si grown on H-terminated Si surfaces.



Fig. 3. The RBS-channeling spectra observed for the Si-deposited samples with ~10 nm thick on the DH and MH surfaces before and after IBMX treatment by 10-keV Si<sup>+</sup> ions with an ion fluence of  $1 \times 10^{15}$  ions cm<sup>-2</sup> at RT and then thermal anneal at 500°C for 350 min in high vacuum ( $\leq 10^{-4}$  Pa).

We discuss the crystallization process of a-Si layer deposited on the DH surface by IBIEC with or without IBMX treatments. In the deposited process, the deposited Si atoms cannot chemically contact with crystalline Si atoms due to fully occupied H atoms adsorbed on the dangling bonds. In the IBIEC process without IBMX preparation, the energy deposition from projectiles of 180-keV  $Ar^+$  ions was not enough to promote the dissociation and/or diffusion of H atoms. As a result, the a-Si layer formed on the DH surface was not crystallized by the IBIEC at 500°C due to the residual H atoms at interface prevent the epitaxial crystallization. On the other hand, in the IBIEC combined with IBMX treatment case, the Si-H bonds were effectively broken or weaken by Si<sup>+</sup> irradiation near the a/c interface. As a result, even the deposited a-Si on the DH surface was crystallized by the same IBIEC condition.

#### **IV. Conclusions**

We have investigated the crystallization process of a-Si layer deposited on the Hterminated Si(001) surfaces by IBIEC with IBMX treatments. In this study, to clarify the essential IBMX effect, we prepared well-ordered H-terminated Si(001) surface and then performed the IBMX by 10-keV Si<sup>+</sup> ions irradiation at RT around the a/c interface followed by the IBIEC treatment by 180-keV Ar<sup>+</sup> ions irradiation at elevated temperatures. The deposited a-Si layer on the DH surface was not crystallized by the IBIEC treatment without IBMX, whereas that was crystallized by the IBMX followed by the IBIEC treatment at 500°C beyond the initial interface. Furthermore, the deposited a-Si layer was not crystallized by thermal anneal at 500°C with IBMX preparation. This fact shows that the epitaxial crystallization of deposited a-Si region was effectively induced by the IBIEC with IBMX treatment. It can be suggested that the IBIEC combined with IBMX treatment makes it possible to epitaxial crystallize at significantly low temperature for amorphous layer formed on hardly crystallized structure.

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