Effects of implantation energy and annealing temperature on the structural evolution of Ge\(^{+}\)-implanted amorphous Si

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Abstract

High-resolution transmission electron microscopy in conjunction with autocorrelation function analysis have been applied to investigate the evolution of structural order in Ge\(^{+}\)-preamorphized silicon layers. (0 0 1)Si wafers were preamorphized with 5 and 10 keV Ge\(^{+}\) to a dose of \(5 \times 10^{15}\) ions/cm\(^2\). A higher density of embedded nanocrystallites was found to be present in as-implanted amorphous Si layer for 10 keV Ge\(^{+}\) than that for 5 keV Ge\(^{+}\). The densities of embedded nanocrystallites in Ge\(^{+}\)-preamorphized Si layer with 5 and 10 keV Ge\(^{+}\) were found to diminish with annealing temperature first then increase. The effects of ion-implantation energy and annealing temperature on the structural evolution in Ge\(^{+}\)-implanted amorphous Si are discussed in terms of ion-beam induced annealing and free energy change of the system. The depth dependence on the density of embedded nanocrystallites is attributed to the nonuniform distribution of Ge atoms.

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1. Introduction

Ion implantation has been a major method for shallow junction formation in ultra large scale integrated circuits (ULSI) fabrication [1]. Ion implantation induced disorder is of great interest for both basic understanding and industrial application since ion implantation is the most widely used and the best controlled technique for forming p–n source/drain junction. Ge\(^{+}\) preamorphization (PAI) has been used extensively to alleviate dopant channeling during subsequent implantation, especially for the light ions such as B\(^{+}\). The depth of B\(^{+}\) penetration is reduced because PAI limits ion channeling, which can distort the implanted...
dopant profile [2]. It is therefore important to understand the structural evolution in PAI samples [3–5]. Although the structures of amorphous materials have been extensively investigated, a definitive structure of amorphous semiconductor thin films remains to be clarified [6–13]. The continuous random network (CRN) model has been widely used to describe the structure and other features of amorphous materials for many years [6,7,14,15]. However, recent studies using variable coherence microscopy method elucidated medium-range ordering structures, which are not included in the CRN model, in as-deposited amorphous semiconductors. Although diffraction studies are powerful for measuring short-range order in amorphous materials [11–13], the atom pair-correlation function is insensitive beyond short range [16]. Slight difference was found in short-range order between the as-implanted and annealed amorphous samples [11]. On the other hand, the medium range order was found to diminish upon annealing [3,9,10]. Variable coherence microscopy method controlled by the hollow-cone dark-field image speckle imposes several fundamental limitations. In addition, efficient and accurate image acquisition capabilities and powerful image-processing software are required [10,17].

Auto-correlation function (ACF) analysis is a statistical analysis of the scanned high-resolution transmission electron microscope (HRTEM) images in real space. In previous studies, the ACF analysis has been applied to determine the formation of embedded nanocrystalline silicides in the amorphous interlayer of the metal/Si systems [18–20]. The ACF function is equivalent to a two-dimensional form of Patterson function, well known in X-ray crystallography for obtaining a map of interatomic vectors [21,22]. In addition, the ACF analysis has also been successfully used to discuss the effects of dose and the annealing temperature on the structural evolution in Ge⁺-preamorphized Si [4,5].

In an effort to clarify the structure of low energy Ge⁺ implantation amorphous Si (a-Si) on (0 0 1)Si, an investigation on the structural evolution in Ge⁺ implantation a-Si on the dependence of the implantation energy and annealing temperature by using HRTEM in conjunction with ACF analysis has been carried out.

2. Experimental procedures

Commercially available single crystal, 8 in. (0 0 1)Si p-type wafers were used in the present study. A high current implanter of model GSDIII/LED manufactured by Axcelis corp. was used to implant Ge⁺ ions. Following a standard cleaning procedure, Ge-ion implantation was carried out at a fixed dose of 5 × 10¹⁵ ions/cm² and with ion energies of 5 keV (projected range (Rp5) = 8 nm, straggling (ΔRp5) = 2.8 nm) and 10 keV (Rp10 = 12.5 nm, ΔRp10 = 4.5 nm). The tilt/twist angles for all implants were kept to be zero. After implantation, the samples were annealed for 2 min in high purity N₂ ambient at temperatures between 300 and 500 °C. Previous studies showed that the diffusion of Ge atoms in silicon wafers annealed at 500 °C or lower temperature is not significant [4,23].

To minimize the artifacts induced by heating, the samples for HRTEM observation were prepared by mechanical grinding and without any ion milling. Specimens were examined using a JEOL 4000EX TEM operating at 400 kV with a point-to-point resolution of 0.18 nm. The cross-sectional TEM (XTEM) micrographs were all taken along the [1 1 0] zone axis of single-crystal Si. The ACF analysis was conducted on templates of 1 × 1 nm² in size from the scanned HRTEM images. In order to obtain more accurate data, the templates selected to carry out ACF analysis were shifted horizontally, vertically and diagonally by 0.5 nm, respectively. The different sampling areas of HRTEM images were found to yield similar number of nanocrystallites. The number of nanocrystallites was obtained from sum of all discrete nanocrystallites. The detailed diagrams and descriptions for the ACF analysis are shown in the previous study [5]. Image simulation based on multi-slice methods was executed with a software “MacTempas” to determine unambiguously the thickness of XTEM specimens [21]. The average thickness of XTEM specimens was determined to be about 25 nm.
3. Results and discussion

As the dose is increased and the damages from individual tracks overlap, a continuous amorphous layer (a-layer) can be formed. The thickness of an a-layer increases with higher accelerated ion bombardment. From cross-sectional HRTEM observation, 14-nm-thick and 20-nm-thick a-Si layer were found to form at the surface of the as-implantated samples, which were implanted by 5 keV and 10 keV Ge\(^+\) to a dose of $5 \times 10^{15}$ cm\(^{-2}\). No crystallites were directly observed in the amorphous surface layers of the as-implanted samples from cross-sectional HRTEM images. However, from ACF analysis, a high density of periodic structure was observed in the ACF images of outlined regions in the HRTEM micrographs for both as-implanted samples. More accurate distribution of embedded nanocrystallites would be found by ACF analysis with the shifting of templates [5]. Fig. 1(a) shows the typical schematic diagrams for the ACF analysis and Fig. 1(b) shows cross-sectional HRTEM image of an as-implanted sample, which was implanted with 5 keV Ge\(^+\). No crystallites were directly detected. However, periodic structures were observed in the ACF images of outlined regions in the HRTEM images. As a result, the distribution of embedded nanocrystallites in amorphous region was found, as shown in Fig. 1(b). The result provides direct evidence that the as-implanted or annealed amorphous regions consist of a high density of nanocrystallites.

Fig. 2 shows the density of nanocrystallites versus annealing temperature curves for both 5 keV and 10 keV implantations. For the as-implanted samples with 5 and 10 keV Ge\(^+\) implantations, it appears that the density of embedded nanocrystallites in the as-implanted samples with 10 keV Ge\(^+\) implantation is higher than those with 5 keV Ge\(^+\) implantation. Ion-implantation-induced amorphization has generally been recognized to be generated by the displacement cascades. A fair amount of implantation damage was introduced for all chosen implantation energies. With increasing implantation energies the radiation-damaged regions become amorphous, grow wider and are eventually submerged below an essentially crystalline layer.

Fig. 1. (a) Schematic diagrams for the ACF analysis and (b) HRTEM images of as-implanted sample. The black, double white, white and dotted white outlines denote the original, shifted horizontally, vertically and diagonally templates for embedded nanocrystallites, respectively.

Fig. 2. The density of embedded nanocrystallites versus annealing temperature curves.
However, the effect of ion-implantation energy on the structures of ion-implantation-induced a-Si layers still remains to be clarified. From previous studies, it was found that the a-layer widens with increasing implantation energy and that above a critical threshold energy the ion-implantation-induced amorphous regions near the surface become a crystalline region by using differential reflectometry and XTEM [25]. An apparent structural change from amorphous states to crystalline states at the surface would occur above a critical threshold implantation energy. However, while the implantation energy is varied to a constant implantation dose, the XTEM analysis and differential reflectometry only reveal the changes from the a-layers to the damaged crystalline layers at the surface (i.e. the movement of a/c interface) rather than clarifying the structural changes of amorphous states in a-layers.

It has been shown that pre-existing damages may be partially annealed out by ion bombardment. This has been observed at room temperature [26] and even at 30 K [27]. As dynamic annealing is effective, structural state of amorphous implanted layer will be changed. As a result, although continuous a-layers at the surface were formed by both 5 keV and 10 keV Ge\(^+\) implantations in the present study, it is thought that 10 keV Ge\(^+\) implantation would form a-layer with higher ordered state than that with 5 keV implantation. The present HRTEM in conjunction with ACF analysis indeed shows that the density of embedded nanocrystallites in the as-implanted samples with 10 keV Ge\(^+\) is higher than those with 5 keV Ge\(^+\). For the samples with 5 keV and 10 keV Ge\(^+\) implantation, the change of the density of nanocrystallites with the annealing temperature show the similar trends. The pronounced diminution in the density of embedded nanocrystallite in 300–350 °C annealed samples is a clear sign of network relaxation to lower energy with respect to the as-implanted samples. After above 400 °C annealing,

![Graphs showing the density of embedded nanocrystallites (NCs) with depth from front and rear regions in as-implanted a-Si layer for (a) 5 keV Ge\(^+\)- and (b) 10 keV Ge\(^+\)-implanted samples. Distributions of Ge atoms in as-implanted samples were calculated with the TRIM code for (c) 5 keV and (d) 10 keV Ge\(^+\)-implanted Si(0 0 1) with a dose of \(5 \times 10^{15} \text{ cm}^{-2}\).](image)
the density of nanocrystallites increases. It is attributed to the supply of sufficient thermal energy for the nucleation of nanocrystallites. Detailed mechanism has been discussed previously [4,5]. Nonuniform distribution of the density of embedded nanocrystallites in an a-layer was observed in as-implanted samples, as shown in Fig. 3(a) and (b). For both as-implanted samples with 5 keV and 10 keV Ge⁺ implantation, higher densities of embedded nanocrystallites in the upper half part were formed than that in the rear half part of a-layers. The structure of as-Si⁺-implanted a-Si layer at a depth of approximately 500 nm has been recognized to be much closer to the continuous random network, compared to the structure near the surface in previous studies by a variable coherence microscopy [10]. Vacancy redistributions during implantation allowing annealing of the paracrystalline state and the proximity of the surface were thought to play important roles in introducing nanostructural seeds on which paracrystalline material forms. In addition, since the Ge atoms are known to be larger in diameter the Si atoms by about 4%, enormous compressive stress is expected to be present in heavily damaged regions. A previous study also indicated that the growth of the Ge⁺-implanted a-Si layer could be attributed to randomization of heavily damaged regions in order to lower the free energy of the system [28]. Fig. 3(c) and (d) show the calculated Ge distribution with the depth. For 5 keV Ge⁺-implanted samples, lower density of nanocrystallites is present in the rear half part of a-layers, as seen in Fig. 3(a), which corresponds to the Ge-rich region, as shown in Fig. 3(c). For the samples with 10 keV Ge⁺ implantation, the change of the density of nanocrystallites with the depth of a-layer and distribution of Ge atoms shows the similar trend, as seen in Fig. 3(b) and (d). With lower free energy, the structure of Ge-rich regions resembles more like a random network with uniformly distributed strain energy. As a result, the lower densities of embedded nanocrystallite found in the rear half part of Ge⁺-implanted a-Si layers than that in the front half part can be attributed to the presence of nonuniform distribution of Ge atoms in a-Si layers.

4. Conclusions

The density of embedded nanocrystallites in Ge⁺ implantation a-Si layer was found to diminish with annealing temperature first and then increase. The effects of ion-implantation energy on the structural evolution in Ge⁺-implanted a-Si layer are discussed in terms of ion-beam induced annealing. The depth dependence on the density of embedded nanocrystallites may also be caused by the nonuniform distribution of Ge concentration. The clarification of the effect of implantation energy on the structural state of low energy Ge⁺ implantation a-Si and the relationship between the distribution of Ge atoms and nature of the a-Si structure provides critical insights for the possible minimization of transient enhanced diffusion in shallow junction formation.

References