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ScienceDirect
Physica B 401–402 (2007) 597–599
PHYSICA B
www.elsevier.com/locate/physb

Simultaneous observation of the behavior of impurities and silicon atoms in silicon isotope superlattices

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Abstract

The behavior of impurity (arsenic or boron) and silicon host atoms during ion implantation was investigated using silicon isotope superlattices. The depth profiles of silicon isotopes in the ^{28}Si/^{30}Si isotope superlattices before and after ion implantation were obtained by secondary ion mass spectrometry. The experimentally determined profiles were reproduced very well by a theoretical model to yield the average displacement of silicon atoms as a function of the depth. The critical displacement of silicon to induce the amorphous layer was determined together with cross-sectional transmission electron microscopy.

Keywords: Impurities; Defects; Diffusion; Isotopes

1. Introduction

Ion implantation of impurities, especially arsenic (As) and boron (B), is extensively employed for the formation of shallow junctions in silicon (Si) technology. Since the size of complementary metal-oxide-semiconductor (CMOS) devices reaches the nano-meter scale, understanding of the atomic behavior of the impurities and Si in the CMOS device fabrication becomes crucial for the development of reliable process and device simulators. For example, solid understanding of the behavior of As and B atoms in Si during ion implantation and post-annealing is required to reproduce accurately the impurity profiles in the fabrication process. Moreover, quantitative evaluation of diffusion and chemical reaction in non-equilibrium conditions is needed. Such task is becoming especially challenging in the present era of nano-CMOS. While the behavior of As and B in crystalline Si has been studied extensively in the transient and non-equilibrium conditions [1–3], the behavior of Si host atoms along with those impurities must also be understood to precisely control the distribution, concentration, and activation of the dopants. In this work, we present a direct observation of the behavior of Si host atoms in Si during the ion implantation utilizing Si isotopes as depth markers. Naturally available Si (^{nat}Si) is composed of the three stable isotopes in the fixed abundances: ^{28}Si (92.2%), ^{29}Si (4.7%), and ^{30}Si (3.1%). Recently, isotopically controlled Si heterostructures were employed to investigate diffusion of foreign atoms in Si in the thermal equilibrium conditions [4,5]. In this study, we employed short-period Si isotope superlattices with the periodic stacking of the isotope layers controlled precisely by solid-source molecular beam epitaxy [6,7]. It allows us to understand how amorphization correlates with the distance of the displacement of Si atoms induced by the As implantation by comparison with the cross-sectional transmission electron microscopy (XTEM).

2. Experiment

We prepared a Si isotope superlattice that composed of alternating layers of isotopically pure ^{28}Si (99.92%) and ^{30}Si (99.3%), which referred to as the ^{28}Si/^{30}Si isotope superlattice where the thickness of each layer is 2.7 nm [6,7]. A buffer layer (~100 nm) was firstly grown on a 2 in., floating-zone ^{nat}Si(0 0 1) substrate prior to the growth of the isotope superlattices. In order to investigate the length of the Si atomic displacement induced by As implantation,

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doi:10.1016/j.physb.2007.09.030

we prepared the superlattice implanted with $^{75}\mathrm{As}^+$ ions at the energy of 25 or 60 keV with doses in the range 1×10^{13} to $1\times10^{15}\,\mathrm{cm}^{-2}$ at room temperature. For the B implantation study, we implanted $^{11}\mathrm{B}^+$ ions at 7 keV with 1×10^{15} or $1\times10^{16}\,\mathrm{cm}^{-2}$. The depth profiles of ^{28}Si, ^{30}Si, and impurities (^{75}As and ^{11}B) were obtained by secondary ion mass spectrometry (SIMS).

3. Results and discussion

Fig. 1 shows the depth profiles of ^{28}Si and ^{30}Si in the unimplanted ^{28}Si (2.7 nm)/^{30}Si (2.7 nm) isotope superlattice. Note that the actual intermixed interfaces ^{28}Si/^{30}Si in the superlattices is abrupt. The degree of mixing was only two atomic layers and the smearing of the SIMS profile is due to the artifact [6,7]. A constant amplitude of SIMS intensities (^{28}Si and ^{30}Si) in the sample before implantation was confirmed. Fig. 2(a) shows the depth profiles of ^{28}Si, ^{30}Si, and ^{75}As in the Si isotope superlattice implanted with $^{75}\mathrm{As}^+$ at 25 keV with $1\times10^{14}\,\mathrm{cm}^{-2}$ corresponding to the projective range ~20 nm and the peak of As concentration $\sim5\times10^{19}\,\mathrm{cm}^{-3}$. However, in the region 0–30 nm, the Si isotope intensities are slightly perturbed by the As implantation, while such perturbation was not observed at same energy but with the dose of $1\times10^{13}\,\mathrm{cm}^{-2}$ [8]. We introduce the following model based on the convolution integral to obtain quantitatively the average length of Si atomic displacement as a function of the depth.

$$C_{\text{after-impla}}(x) = \int C_{\text{before-impla}}(x')\,g(x-x')\,\mathrm{d}x' \tag{1}$$

$$g(x) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{x^2}{2\sigma^2}\right). \tag{2}$$

Here $C_{\text{before-impla}}$ and $C_{\text{after-impla}}$ represent the concentrations of ^{28}Si and ^{30}Si in the Si isotope superlattice before and after implantations, respectively. $g(x)$ is a Gaussian function. This function includes σ which we defined as the distance of the displacement as a function of the depth [8]. Fig. 2(b) shows the length of Si displacement (σ) as a function of the depth induced by the As implantation. The maximum displacement of ~0.6 nm was induced by the implantation at 13 nm from the surface, which is much shallower than the peak position of As concentration as shown in Fig. 2(a). Fig. 2(c) shows the XTEM image after the same implantation condition. Note that single crystalline remains in the region 0–4 nm even after the implantation while amorphization occurs in the region 4–23 nm. By comparing the XTEM image with the Si displacement distribution in Fig. 2(b), we obtained only ~0.5 nm of the critical displacement at the amorphous/crystalline interface. The same value was also obtained for the conditions of much higher As implantation dose ($1\times10^{15}\,\mathrm{cm}^{-2}$) and higher energy (60 keV) [8,9]. Thus, obtained σ provides quantitative estimation of the degree of disorder in the

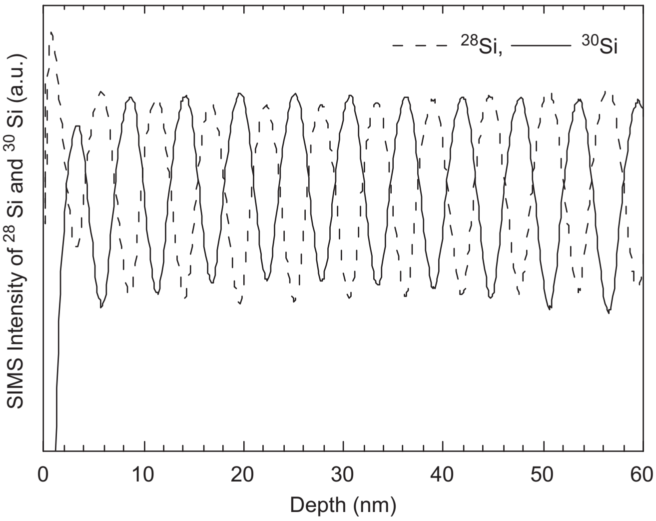

Fig. 1. Depth profiles of ^{28}Si (broken line) and ^{30}Si (solid line) in the ^{28}Si (2.7 nm)/^{30}Si (2.7 nm) isotope superlattice.

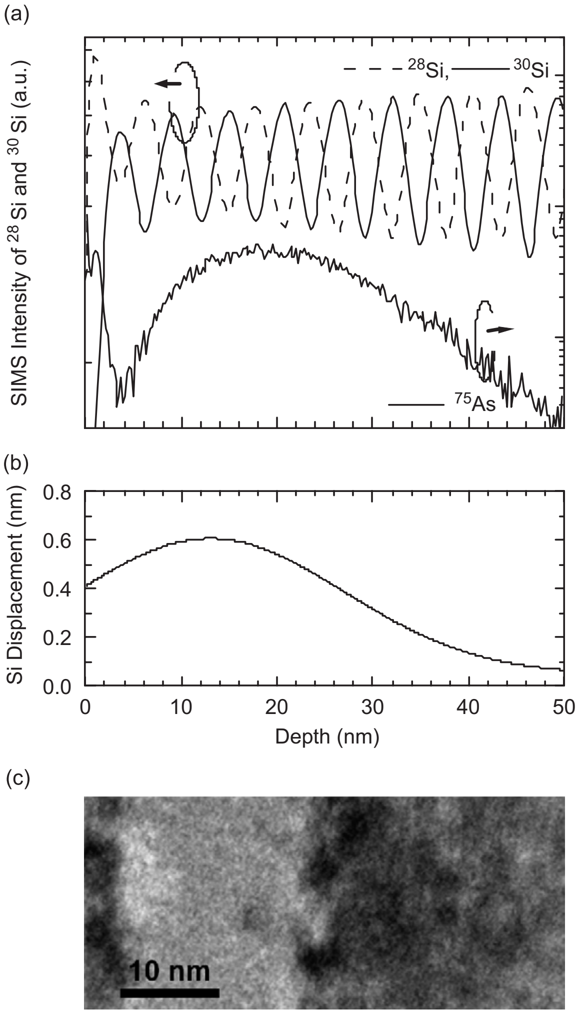

Fig. 2. (a) Depth profiles of ^{28}Si (broken line), ^{30}Si (upper solid line), and ^{75}As (lower solid line) in the ^{28}Si (2.7 nm)/^{30}Si (2.7 nm) isotope superlattice implanted with As ions at 25 keV with the dose of $1\times10^{14}\,\mathrm{cm}^{-2}$. (b) The depth dependence of the Si displacement induced by the As implantation. (c) XTEM image of the sample implanted with the same implantation condition with the depth scale same as (a) and (b).

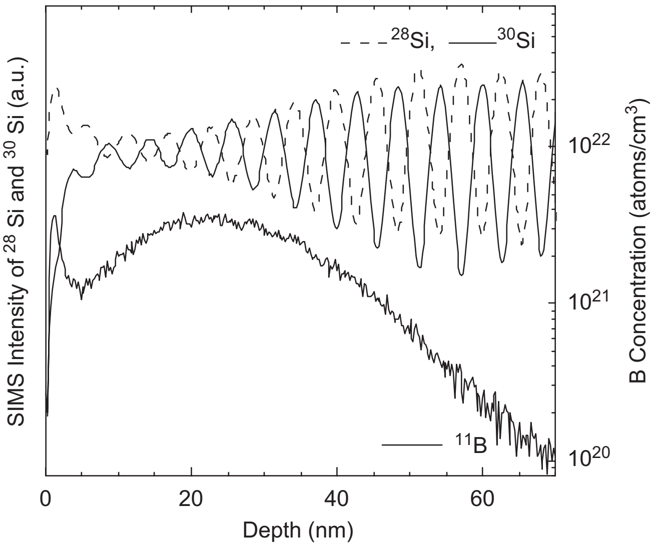

Fig. 3. Depth profiles of ^{28}Si (broken line), ^{30}Si (upper solid line), and ^{11}B (lower solid line) in the ^{28}Si (2.7 nm)/^{30}Si (2.7 nm) isotope superlattice implanted with B ions at 7 keV with the dose of $1 \times 10^{16}\,\mathrm{cm}^{-2}$.

implanted layer. Likewise, Fig. 3 shows the depth profiles of ^{28}Si, ^{30}Si, and ^{11}B in the Si isotope superlattice implanted with ^{11}B^{+} at 7 keV with $1 \times 10^{16}\,\mathrm{cm}^{-2}$ corresponding to the near projected range with the previous As implantation condition. We did not observe the perturbed profiles of Si isotopes in the superlattice after the B implantation even with the dose of $1 \times 10^{15}\,\mathrm{cm}^{-2}$ due to the mass difference between As and B.

4. Summary

The behavior of Si host atoms in Si during As and B implantation was investigated using Si isotope superlattices. We have successfully developed a model based on the convolution integral to simulate the depth profile of mixed ^{28}Si and ^{30}Si to obtain quantitatively the characteristic length of Si displacements as a function of the depth. Comparing with XTEM to measure the thickness of the surface amorphous layer created by implantation allows us to determine how amorphization correlates with the length of the Si displacements.

Acknowledgments

We acknowledge Dr. T. Okui and Prof. Y. Shiraki (Musashi Institute of Technology) for the ion implantations and H. Oshikawa (Keio University) for the TEM observations. This work has been supported in part by the Research Program on Collaborative Development of Innovative Seeds by JST and in part by the Special Coordination Funds for Promoting Science and Technology for INQIE.

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