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Positive secondary Ion emission from $Si_{1-x}Ge_x$ bombarded by O_2^+

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Abstract

The positive secondary ion yields of B⁺ (dopant), Si⁺ and Ge⁺ were measured for Si_{1-x}Ge_x ($0 \le x \le 1$) sputtered by 5.5 keV ¹⁶O₂⁺ and ¹⁸O₂⁺. It is found that the useful yields of Ge⁺ and B⁺ suddenly drop by one order of magnitude by varying the elemental composition *x* from 0.9 to 1 (pure Ge). In order to clarify the role of oxygen located near surface regions, we determined the depth profiles of ¹⁸O by nuclear resonant reaction analysis (NRA: ¹⁸O(p,\alpha)¹⁵N) and medium energy ion scattering (MEIS) spectrometry. Based on the useful yields of B⁺, Si⁺ and Ge⁺ dependent on *x* together with the elemental depth profiles determined by NRA and MEIS, we propose a probable surface structure formed by 5.5 keV O₂⁺ irradiation.

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1. Introduction

 $Si_{1-x}Ge_x$ films with an appropriate dopant are widely used in field-effect transistors and hetero-junction bipolar transistors as a material with high electron mobility [1] and in solar cells due to their narrow-band-gap [2,3]. The techniques of chemical vapor deposition (CVD) and molecular beam epitaxy can be used to fabricate $Si_{1-x}Ge_x$ films with a desirable composition. The dangling bond of $Si_{1-x}Ge_x$ is stabilized by introducing hydrogen. In a previous study, we analyzed the hydrogen content by elastic recoil detection using MeV He⁺ ions [4].

Depth profiling of dopants in $Si_{1-x}Ge_x$ is usually performed using secondary ion mass spectrometry (SIMS) [5]. SIMS enables highly sensitive detection of impurities in solid materials using reactive primary ions such as O_2^+ and Cs^+ , which enhance the ionization probability of positive and negative secondary ions, respectively. For example, oxygen bombardment and detection of B⁺ provide one of the most sensitive ways of depth profiling of boron doped in $Si_{1-x}Ge_x$. Such an enhancement of detection sensitivity is called the

oxygen effect. The ionization probabilities of some kinds of atoms strongly depend on the elemental composition, known as the matrix effect [6]. In fact, the detection sensitivity for B^+ varies along with the Ge composition x of $Si_{1-x}Ge_x$. In the case of O_2^+ bombardment, the oxygen concentration of an topmost layer plays an important role in positive secondary ions yields [7], since almost of all secondary ions emerging from a surface originate from the topmost surface region [8]. Of course, the oxygen atoms are introduced by the primary O_2^+ irradiation. The oxygen concentrations at surfaces depend on the elemental compositions of samples. It was also reported that preferential oxidation of Si and oxidation induced atomic movements during thermal treatments affected the elemental composition of the topmost layer of $Si_{1-x}Ge_x$ [9]. Collision cascades induced by ion bombardment may also promote atomic movement.

In this study, we measure the secondary ion yields of B⁺, Si⁺ and Ge⁺ emitted from Si_{1-x}Ge_x by varying the composition x. The depth profiles of oxygen are determined by high-resolution medium energy ion scattering (MEIS) [10] and by the nuclear resonance reaction (NRA) of ¹⁸O(p, α)¹⁵N at 1.762 MeV [11]. In the latter analysis, the Si_{1-x}Ge_x samples were bombarded by ¹⁸O₂⁺. The present result clarifies quantitatively what takes place near the surface region of Si_{1-x}Ge_x (0 ≤ x ≤ 1) by O₂⁺

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bombardment and what enhances the positive secondary ions yields.

2. Experiments

Eight amorphous $Si_{1-x}Ge_x$ (a- $Si_{1-x}Ge_x$; $0 \le x \le 1$) samples were prepared for the measurement of secondary ions yields in SIMS using 5.5 keV ${}^{16}O_2^+$ and ${}^{18}O_2^+$ beams. Total oxygen amounts were evaluated by NRA ($^{18}O(p,\alpha)^{15}N$ at 1.762 MeV) for $a-Si_{1-x}Ge_x$ (0.68 < x < 1) using a 1.5 MV tandem accelerator at Nara-Women's University. We grew the a- $Si_{1-x}Ge_x$ films on glass substrates by plasma CVD and then implanted 40 kV B⁺ ions into the films with a dose of 1×10^{14} (ions/cm²). The accuracy of the dose values is estimated to be better than a few percent. High-resolution MEIS was used to determined the depth profiles of 18 O for Si(0 0 1) and Ge(0 0 1) single crystals using 120 keV He⁺ ions. The present NRA and MEIS measurements were performed ex situ. However, we can distinguish clearly ¹⁸O in MEIS and NRA from ¹⁶O, which may be adsorbed on the sample surface when exposed to the atmosphere. Here, it must be noted that the isotopic abundance of 18 O is only 0.2%.

2.1. Secondary ion mass spectrometry (SIMS)

We employed CAMECA IMS-4F [12] for SIMS measurements. A 5.5 keV O_2^+ beam impinged on a sample surface at an angle of 42° scaled from surface normal. The primary ion beam was scanned over an area 125 μ m² at a current of 50 nA. The secondary ion yields of ¹¹B⁺, ³⁰Si⁺ and ⁷⁰Ge⁺ were measured for the surfaces sputtered by ${}^{16}O_2^+$ and ${}^{18}O_2^+$ sputtered surfaces were supplied for NRA and MEIS.

2.2. ${}^{18}O(p,\alpha){}^{15}N$ nuclear reaction analysis

The nuclear resonance reaction of ${}^{18}O(p,\alpha){}^{15}N$ at a resonance energy $E_{\rm R}$ = 1.762 MeV was used to detect ¹⁸O. In this reaction, the emitted α particles have energy around 4 MeV, which depends slightly on emission angle. Thus, the emitted α particle spectra were basically free from the background of elastic scattering components. The α particles and backscattered proton were detected by a solid-state detector (SSD).

The reaction cross sections at an emission angle of 170° were determined using a standard sample of Si¹⁸O₂/Si(1 1 1) prepared by thermal oxidation with exposure to ${}^{18}O_2$ gas. The absolute amount of 18 O was determined in advance to be 5.1×10^{15} (atoms/cm²) by high-resolution MEIS. Fig. 1 shows the cross sections dependent on incident proton energy at α emission angle of 170°. It is seen that the maximum cross section is 1.13×10^{-25} cm² at $E_{\rm R} = 1762$ keV with a full-width at a half maximum (FWHM) of 7 keV. The incident proton energy was calibrated using narrow resonant reactions of 27 Al(p, γ)²⁸Si at 991.8 keV and of 16 O(He,He)¹⁶O at 2484 and 3034 keV. Here, the magnetic fields of a bending magnet were measured precisely by proton nuclear magnetic resonance. For the $Si_{1-x}Ge_x$ (0.68 < x < 1) samples, an Au layer with thickness about 10 nm was deposited on the surface to suppress

Nuclear Reaction Cross Section (×10⁻²⁶ cm²) 2 1700 1710 1720 1730 1740 1750 1760 1770 1780 Incident H⁺ Energy (keV)

Fig. 1. The ¹⁸O(p,α)¹⁵N reaction cross sections as a function of incident proton energy at an emission angle of 170°. Au(10 nm)/Si¹⁸O₂(1.6 nm)/Si(1 1 1) was used as a target.

a charging-up during 5.5 keV ¹⁸O₂⁺ bombardment in SIMS as well as during proton irradiation. The elemental compositions xtogether with hydrogen content were determined in advance by Rutherford backscattering (RBS) and elastic recoil detection analysis using 2.0 MeV He⁺ ions [4].

2.3. Medium energy ion scattering (MEIS)

MEIS analysis was carried out at Ritsumeikan SR Center (SORIS beamline) for Si(001) and Ge(001) single crystals sputtered by ¹⁸O₂⁺. Well-collimated 120 keV He⁺ ions were incident on a sample and scattered He⁺ ions were energyanalyzed by a toroidal electrostatic analyzer with an excellent energy resolution of $\Delta E/E = 1 \times 10^{-3}$. The resultant depth resolution is estimated to be a few Ångstroms [13]. Taking a double-alignment geometry ([1 1 0]-incidence and $[2 0 \overline{1}]$ emergence) suppressed the scattering yields from Si and Ge and thus allowed precise depth profiling of ¹⁸O in Si and Ge crystals. As will be shown later, the ¹⁸O atoms introduced into Si and Ge during ${}^{18}\text{O}_2^+$ bombardment were selectively seen in MEIS spectra from the ¹⁶O atoms adsorbed on the surface.

3. Results and discussion

The secondary ions yields of Si⁺ and Ge⁺ dependent on the elemental composition (x) of a-Si_{1-x}Ge_x are shown in Fig. 2 for 5.5 keV ${}^{16}O_2^+$ bombardment. Here, the yields of ${}^{30}Si^+$ and ⁷⁰Ge⁺ are divided by the isotopic abundance and normalized by the Si⁺ yield at x = 0. The total yield indicated in Fig. 2 corresponds to the sum of the Si⁺ and Ge⁺ yields. In fact, the yields of other secondary ions emitted simultaneously, such as SiO⁺, GeO⁺, Si₂⁺, Ge₂⁺ and B⁺, are sufficiently low.



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