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Film thickness determining method of the silicon isotope superlattices by SIMS

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ABSTRACT

It is becoming important to evaluate silicon self-diffusion with progress of a silicon semiconductor industry. In order to evaluate the self-diffusion of silicon, silicon isotope superlattices (SLs) is the only marker. For this reason, it is important to correctly evaluate a film thickness and a depth distribution of isotope SLs by secondary ion mass spectrometry (SIMS). As for film thickness, it is difficult to estimate the thicknesses correctly if the cycles of SLs are short. In this work, first, we report the determination of the film thickness for short-period SLs using mixing roughness-information (MRI) analysis to SIMS profile. Next, the uncertainty of the conventional method to determine the film thicknesses of SLs is determined. It was found that the conventional methods cannot correctly determine film thickness of short-period-isotope SLs where film thickness differs for every layer.

1. Introduction

Diffusion of dopants, oxygen and metals, etc. in silicon has been evaluated in the silicon semiconductor field [1]. It is becoming important to evaluate silicon self-diffusion with the progress of a silicon semiconductor industry. In order to evaluate the self-diffusion of silicon, silicon isotope superlattices (SLs) is the only marker. On the other hand, only secondary ion mass spectrometry (SIMS) and Raman spectroscopy can measure the film thickness of SLs, and only SIMS can further evaluate the depth distribution of SLs. However, because SIMS profile depth resolution is limited by atomic mixing, etc., it has been difficult to correctly determine the film thickness of the short-period SLs.

In this work, first, we report the determination of the film thicknesses for short-period SLs. SLs which has alternating layers of isotopically enriched ^{28}Si and ^{30}Si were grown periodically by molecular beam epitaxy (MBE) growth [2]. In order to determine the film thicknesses, we analyzed the SIMS depth profile of the SLs using mixing-roughness information depth model (MRI) [3,4]. SIMS depth profile was fitted with MRI simulated profile. The determined film thicknesses values by MRI analysis were almost the same as those calculated by the planar bond-charge model [1,2] applied to Raman spectra.

Moreover, we evaluated the error of the conventional methods to determine the film thicknesses of SLs. Fig. 1 shows a schematic diagram of ^{28}Si and ^{30}Si profiles. Conventionally, ^{28}Si thickness (T_{28}) has been determined by follow equations from the SIMS profile.

$$T_{28} = L \times \frac{I_{28}}{I_{28} + I_{30}} \text{ or } T_{28} = L \times \frac{S_{28}}{S_{28} + S_{30}},$$

where L is the wavelength, I_{28} is the peak intensity of ^{28}Si, I_{30} is that of ^{30}Si, S_{28} is the peak area of ^{28}Si and S_{30} is that of ^{30}Si. In this paper, the former is called "the peak intensity method", and the latter is called "the peak area method". By these methods, when cycles are constant, there is no problem in calculating the film thickness. However, when there was one wider layer between the regular cycles, the peak intensity and the peak area of the surrounding layers would change by the wider layer. This causes an error of film thickness. We report the error of the film thickness caused by this effect.

2. Evaluation of the film thickness by MRI

2.1. Experimental

SLs used has (^{nat}Si/^{30}Si)$_{50}$ on the Si (1 0 0) substrate, films were grown with MBE. The cycle of the SLs was grown regularly so that the film thickness could be determined using planer bond-charge model to Raman spectra. The film thickness of each ^{nat}Si was 16 ± 2 ML corresponding to 2.18 ± 0.27 nm, and the film thickness of each

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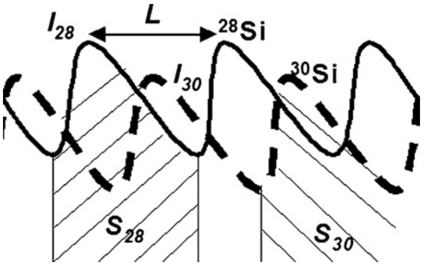


Fig. 1. Schematic diagram of the ^{28}Si and ^{30}Si profile.

^{30}Si was 10 ± 2 ML corresponding to 1.36 ± 0.27 nm. SIMS depth profiling of specimens was performed with Cs^{+}, 1 keV, 45° and negative ion detection using ATOMIKA SIMS 4000. Secondary ion optics was set up in order to avoid detector saturation.

2.2. Results and discussion

Fig. 2(a) shows the SIMS depth profile of ^{28}Si obtained on the SLs sample and MRI fitted data. Fig. 2(b) shows the SIMS depth profile of ^{30}Si and MRI fitted data. A mixing parameter of fitting was determined from the gradient at the superlattice/substrate interface, and the roughness parameter and film thickness were determined by fitting over the superlattice layers. The information depth was set to 0 in this work, because most secondary ion is emitted from the top layer, and this depth is much smaller than the mixing layer. The MRI fitting profiles of ^{28}Si and ^{30}Si reproduce SIMS profiles well. The film thickness of ^{nat}Si determined by MRI calculation to SIMS profile was 2.1 ± 0.05 nm, and the film thickness of ^{30}Si determined by MRI was 1.35 ± 0.05 nm. These values are consistent with the thickness values determined by Raman. It follows from this that film thickness of short-period SLs can be determined by MRI calculation on SIMS profile. Because the thermal diffusion and ion-induced diffusion between Si and Si are very small in SLs, MRI model, which was considered only with the mixing model by atomic collision, can be applied.

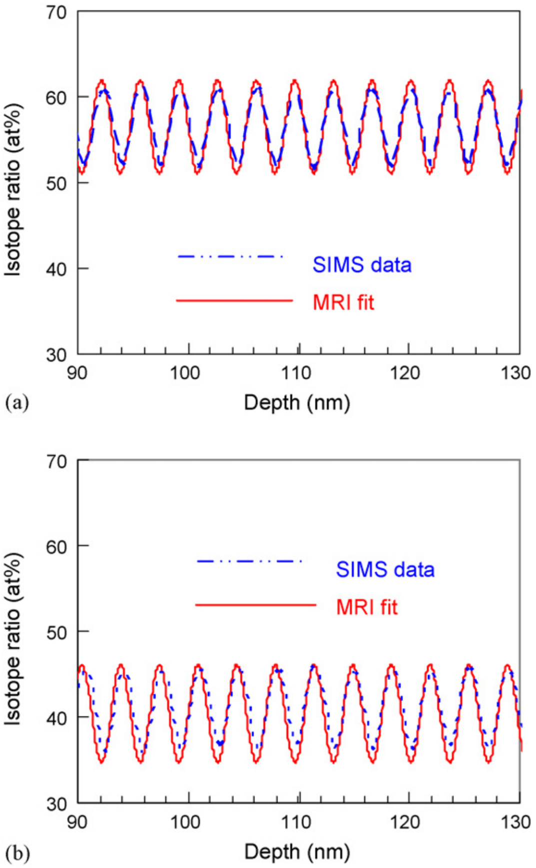


Fig. 2. Depth profiles of SLs measured by SIMS with 1-keV Cs^{+} at 45° and MRI fitted profiles of SLs. (a) SIMS profile and MRI fitted data of ^{28}Si and (b) SIMS profile and MRI fitted data of ^{30}Si.

3. Evaluation of the film thickness determined by conventional methods when each film thickness being differs

Generally, when each layer cannot be clearly distinguished by SIMS profile, each film thickness of SLs was determined by the peak intensity method or the peak area method. By these methods, if the film thickness differs for every layer, it is expected that the correct film thickness cannot be given, because each layer will be influenced by the film thickness of the adjoining layer. It was already shown that MRI analysis can reproduce the SIMS profile of SLs. In this chapter, the SIMS profiles for SLs with different film thickness are simulated by MRI. We estimated the error of the film thickness obtained with the peak intensity method or the peak area method to the simulated profile. The simulated SLs structure was (^{28}Si (13 nm)/^{30}Si (13 nm))$_{10}$/^{28}Si (30 nm)/(^{30}Si (13 nm)/^{28}Si (13 nm))$_{40}$. A mixing parameter of 2.5 nm and a roughness parameter of 0.7 nm were used.

Fig. 3(a) shows the MRI simulated profile of ^{28}Si, and Fig. 3(b) shows MRI simulated profile of ^{30}Si, for the structure given above. The simulation is affected by the wider ^{28}Si layer, ^{28}Si intensity near it is high, and ^{30}Si intensity near it is low.

Fig. 4(a) shows the layer thicknesses of ^{28}Si layers determined by the peak intensity method and the peak area method as a

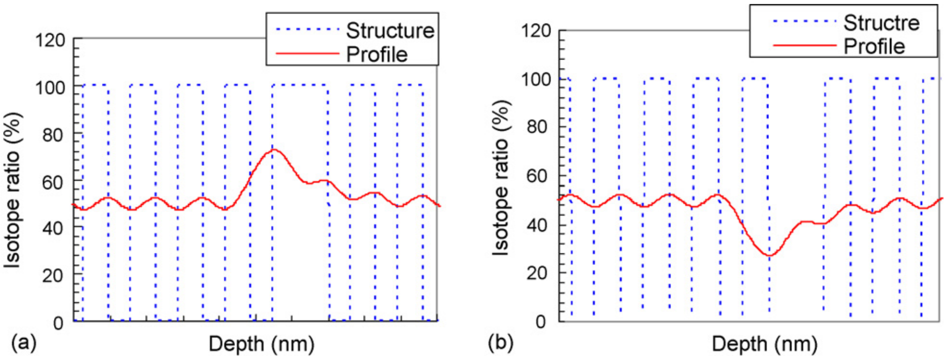
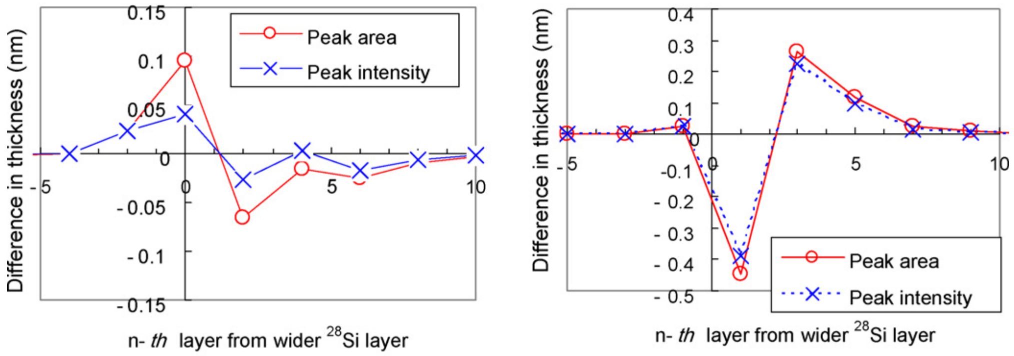


Fig. 3. MRI simulated profile and SL layer structure used for MRI calculation. SL structure was (^{28}Si (13 nm)/^{30}Si (13 nm))$_{10}$/^{28}Si (30 nm)/(^{30}Si (13 nm)/^{28}Si (13 nm)$_{40}$. The mixing parameter was 2.5 nm and the roughness parameter was 0.7 nm. (a) ^{28}Si and (b) ^{30}Si.



(a) ^{28}Si

(b) ^{30}Si

Fig. 4. Dependence of difference between calculated thickness and layer thickness on the layer number from wider ^{28}Si layer. Calculations used were the peak intensity method and the peak area method.

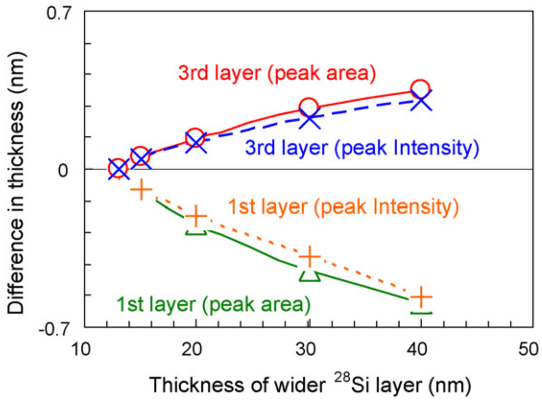


Fig. 5. Difference between calculated thickness and layer thickness of 1st ^{30}Si layer and 3rd ^{30}Si layer as a function of the wider ^{28}Si layer thickness. Calculations used were the peak intensity method and the peak area method.

function of the layer number from the wider ^{28}Si (30 nm) layer, in the same way Fig. 4(b) shows the layer thickness of ^{30}Si. In calculating, it was considered one cycle to be the combination of ^{28}Si/^{30}Si, and the position of wider ^{28}Si (30 nm) layer is defined as the 0th layer. Setting the thickness of the wide layer to 15, 20, 30 and 40 nm, we calculated the film thickness in the same way. Fig. 5 shows the 1st ^{30}Si layer thickness and 3rd ^{30}Si layer thickness as a function of the thickness of the wider ^{28}Si layer. The thickness of 1st ^{30}Si layer was calculated narrower, and the thickness of 3rd ^{30}Si layer was calculated wider. And the error on the thickness becomes larger as the wider ^{28}Si layer's thickness becomes larger. Incidentally, when the wide layer thickness was set to 50 nm, 1st ^{30}Si layer could not be recognized, and its thickness was not able to be calculated. It is clear that the conventional methods cannot determine correctly film thickness for short-period SLs if film thickness differs for every layer.

4. Conclusions

By these methods, if the film thickness differs for every layer, it is expected that the correct film thickness cannot be given, because each layer will be influenced by the film thickness of the adjoining layer. It was already shown that MRI analysis can reproduce the SIMS profile.

The film thickness of the short period isotope SLs can be determined using MRI calculation to SIMS depth profile. The conventional methods cannot determine correctly the film thickness of the short-period-isotope SLs if the film thickness differs for every layer.

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