Interface Effect in O_2^+-SIMS Depth Profiling of $In_{1-x}Ga_xAs_{1-y}P_y$/InP Multilayer Samples

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The interface effect in depth profiling of $In_{1-x}Ga_xAs_{1-y}P_y$/InP multilayer samples using secondary ion mass spectrometry with an O_2^+ primary ion beam (O_2^+-SIMS) was investigated. By comparing the indium profiles measured by O_2^+-SIMS with those measured by laser-ionization sputtered neutral mass spectrometry (laser SNMS) and reconstructing the profiles by simulation, the distortion in the O_2^+-SIMS indium profiles near the $In_{1-x}Ga_xAs_{1-y}P_y$/InP interfaces was qualitatively explained by the combination of these effects: (1) the change in the sputtering status, including preferential sputtering, and (2) the change in the secondary ion yield caused by the change in the surface oxygen concentration.

1. Introduction

$In_{1-x}Ga_xAs_{1-y}P_y$/InP multilayers are used in heterojunction bipolar transistor devices (HBT) and multiple quantum well (MQW) laser devices. The electronic and optical properties of the devices are controlled by changing the species and concentrations of dopants in each of the layers, so it is important to measure the concentration distribution profiles of the dopants in the multilayer structure in order to check the device fabrication processes.

Secondary ion mass spectrometry (SIMS) is generally used to measure the in-depth concentration profiles of the dopant and the major elements in such devices because of its high sensitivity and good depth resolution. However, depth profiling of $In_{1-x}Ga_xAs_{1-y}P_y$/InP multilayer samples using SIMS with an O_2^+ primary ion beam, which is generally used to enhance the sensitivities of the electropositive elements, often reveals distortion in the measured depth profiles near the $In_{1-x}Ga_xAs_{1-y}P_y$/InP interfaces. The distortion, which is one of the so-called 'interface effects' of SIMS, prevents us from quantitatively interpreting the composition of the matrix elements and the concentration profiles of the dopants near the interfaces.

In this work, we investigated an interface effect, in particular, the distortion in indium profiles, in analyzing $In_{1-x}Ga_xAs_{1-y}P_y$/InP multilayer samples. The change in secondary ion intensities near the interfacial regions may be caused by the combination of changes in the sputtering status and in the secondary ion yield (defined as the fraction of the secondary ions among the whole sputtered species), even when the interfacial regions are thoroughly free of contamination. Besides the O_2^+-SIMS measurements, we used laser-ionization sputtered neutral mass spectrometry (laser SNMS) to analyze the multilayer samples. Laser SNMS with nonresonant multiphoton ionization (NRMPI) detects sputtered neutral atoms whose fraction among the whole sputtered species is large and almost unchanged by the chemical state of the sputtered surface, unlike the secondary ion yield [1], and can provide better quantitative (matrix-effect–free) depth profiling than conventional SIMS [2-6]. By comparing the laser-SNMS results with the O_2^+-SIMS results, we can decouple the change in the secondary ion yield from the interface effects. Furthermore, we tried to explain the O_2^+-SIMS and laser-SNMS profiles using a simple simulation of the changes in the sputtering status and the secondary ion yield.

2. Experiment

The $In_{0.53}Ga_{0.47}As$/InP multilayer samples, (a) InP/[$In_{0.53}Ga_{0.47}As$ (12 nm)/InP (100 nm), 4 pairs]/InP and (b) InP/[$In_{1-x}Ga_xAs_{1-y}P_y$ (122 nm, x~0.47, y~0)/InP (113 nm), 10 pairs]/InP, were prepared by metalorganic vapor phase epitaxy at the NTT Opto-electronics Laboratories.

The O_2^+-SIMS measurements were made with a quadrupole-type dynamic SIMS system (Atomika SIMS 4000). The O_2^+ beam energy was 2 keV and the angle of incidence was 81°. The laser-SNMS measurements using NRMPI were made with a quadrupole-type dynamic SNMS system [7]. A 10-keV Ar^+ continuous ion beam bombarded the sample surface at an incident angle of 77°. The sputtered arsenic and indium atoms were ionized by nonresonant two-photon processes using an intense KrF excimer laser beam, and the phosphorous atoms by nonresonant three-photon processes. The KrF excimer laser system was operated at a laser pulse energy of 100 mJ in the constant energy mode with a repetition rate of 333 Hz.

3. Simulation method

In this work, we suppose that the changes in secondary ion intensities near the $In_{1-x}Ga_xAs_{1-y}P_y$/InP interfaces are caused by the combination of changes in the sputtering status and in the secondary ion yield. The change in the sputtering status includes not only the difference between the sputtering rates of $In_{1-x}Ga_xAs_{1-y}P_y$ and InP but preferential sputtering. A certain element may be more preferentially sputtered out of the sample surface than the other component elements, and this may cause the distortion at the interface that can be seen in the SIMS profile. We used the simple model proposed by Patterson and Shirn [8] for the preferential sputtering. The elements have different constant sputtering yields in both the $In_{1-x}Ga_xAs_{1-y}P_y$ and the InP layers, and these differences in elemental sputtering yields bring about the formation of the surface altered layer whose elemental composition is different from that of the underlying bulk region during sputtering. The sputtering yield of the surface altered layer is given as

$$S = \sum_{j} S_j c_j \qquad (1)$$

where S_j is the sputtering yield and c_j is the concentration of element j in the surface altered layer. The elemental sputtering yields are difficult to accurately determine, however, the most important point in the following simulation is that phosphorus is more preferentially sputtered out than indium. This was already confirmed by the experimental fact that the surface altered layer of InP was rich in indium after sputtering [9]. The difference in sputtering yields between InP and $In_{0.53}Ga_{0.47}As$ in O_2^+-sputtering at several incident angles was reported by Homma and Wittmaack [10]. Referring to these results, we used the following relative S_j values to S_{In}, $S_{In}:S_P:S_{Ga}:S_{As}$ = 1:2:1:1, which are not the exact values but are close enough to qualitatively investigate the elemental profiles. The c_j values at the beginning of sputtering were supposed to be the original elemental concentrations (c_{In} = 50%, c_P = 50%), and the c_j values during sputtering were numerically calculated point by point along the scale of the sputtering time. The total sputtering yield S was also given point by point by equation (1).

The change in secondary ion yield should be mainly caused by the change in oxygen concentration on the sample surface in these experiments. To simplify the calculation, we assumed that the oxygen concentration, c_O, was proportional to $1/(1+S)$ and the secondary ion yield, Y, was enhanced by the n-th power of c_O, that is,

$$Y \propto c_O{}^n \propto \left(\frac{1}{1+S}\right)^n . \qquad (2)$$

Generally speaking, the n value ranges from 2 to 3. We adopted n = 3, following Homma and Wittmaack [10], for simulating the O_2^+-SIMS profiles, and n = 0 for the SNMS profiles because the SNMS measurement is not greatly influenced by the surface oxygen concentration.

The actual measured profiles are of course subject to distortion caused by the limitation of the depth resolution even when the SIMS and laser-SNMS measurements were both done at the grazing angle of incidence of 81° and 77°, respectively. Many workers have studied the resolution functions in depth profiling using SIMS, Auger electron spectroscopy (AES), etc, however, we did not take such resolution functions into account in this simulation because we simply wanted to compare the measured profiles with the calculated ones for the sake of a basic discussion. Bad depth resolution would only make the measured

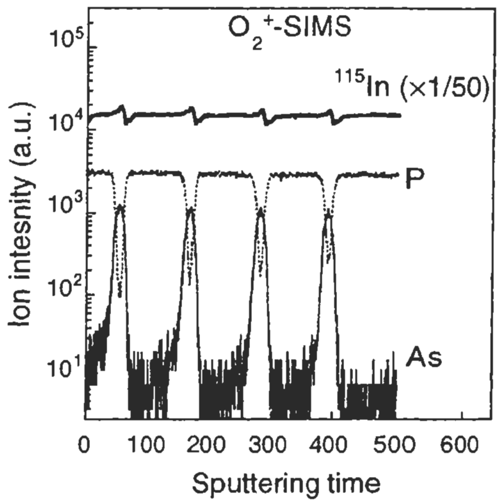

Fig. 1 Measured O_2^+-SIMS profiles of In, P, and As in sample (a).

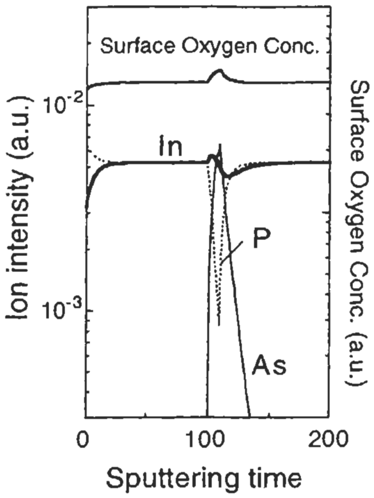

Fig. 3 Calculated O_2^+-SIMS profiles of In, P, and As in sample (a). Calculated surface oxygen concentration is also shown.

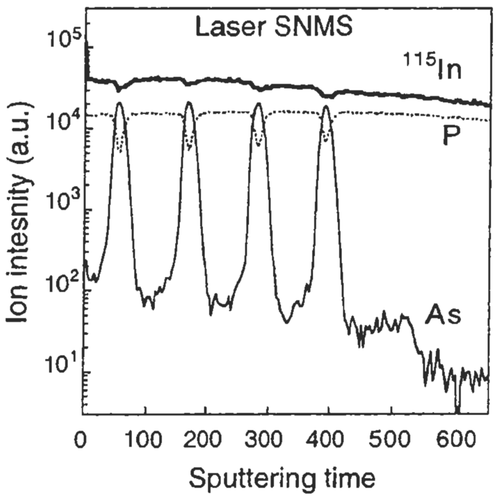

Fig. 2 Measured laser-SNMS profiles of In, P, and As in sample (a).

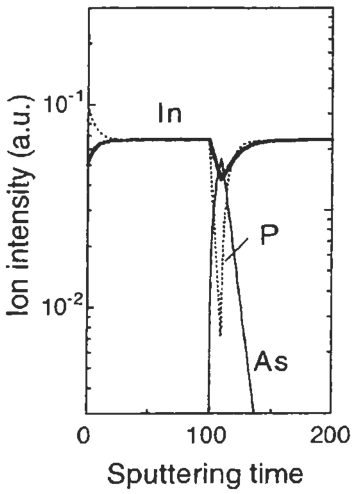

Fig. 4 Calculated laser-SNMS profiles of In, P, and As in sample (a).

profiles dull.

4. Results and discussion

The measured O_2^+-SIMS and laser-SNMS profiles for sample (a) are shown in Figs. 1 and 2. Although the composition ratio of indium in the $In_{0.53}Ga_{0.47}As$ layer is about half that in the InP layer, the indium profile in Fig. 1 showed 'peaks' and 'dips' at the interfaces. On the other hand, the indium profile in Fig. 2 only showed 'dips' in the $In_{0.53}Ga_{0.47}As$ layers, and no 'peaks'.

Figures 3 and 4 show the calculated O_2^+-SIMS (n = 3) and laser-SNMS (n = 0) profiles near the interface by simulation. In Fig. 3, we found that the change in indium secondary ion intensity near the interface in Fig. 1 was qualitatively reproduced by this simulation. The peak and dip were also qualitatively reproduced by another simulation using n = 2. In Fig. 4, the calculated SNMS indium profile showed only 'dips' and also successfully reproduced the measured indium profile seen in Fig. 2. As a result, the 'peaks' and 'dips' in the indium profile in the O_2^+-SIMS measurement can be explained by the combination of the changes in sputtering status and in the secondary ion yield that occurred in the interfacial regions forward and back of the thin $In_{0.53}Ga_{0.47}As$ layer.

Sample (b) involved thicker $In_{1-x}Ga_xAs_{1-y}P_y$ layers than sample (a) and was measured by O_2^+-SIMS. In this sample, the interface effects forward and back of the $In_{1-x}Ga_xAs_{1-y}P_y$ layer can be separately observed and distinguished

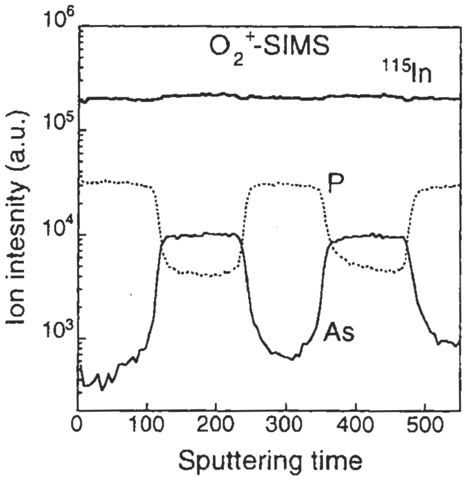

Fig. 5 Measured O_2^+-SIMS profiles of In, P, and As in sample (b).

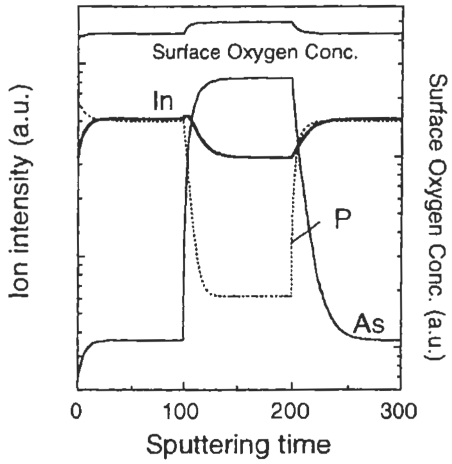

Fig. 6 Calculated O_2^+-SIMS profiles of In, P, and As in sample (b).

from each other. Figures 5 and 6 show the measured and calculated O_2^+-SIMS profiles for a few layers. The change in indium intensity at the interfaces in Fig. 5 seemed to be qualitatively reproduced by simulation in Fig. 6. The deviation of the measured indium profile from the calculated one might have arisen from the degradation in depth resolution due to limitations of measurement and from the difference in the intrinsic matrix effects of the layers.

5. Conclusion

The interface effect in O_2^+-SIMS depth profiling of $In_{1-x}Ga_xAs_{1-y}P_y$/InP multilayer samples was investigated by comparing the measured O_2^+-SIMS and the laser-SNMS profiles and by reconstructing the O_2^+-SIMS profile using simulation. The simulation took into account the effect due to preferential sputtering and that due to changes in the secondary ion yield caused by oxygen concentration on the analyzed surface and successfully made a qualitative reconstruction of both profiles near the $In_{1-x}Ga_xAs_{1-y}P_y$/InP interface. Clarifying the mechanism that causes the interface effects in various samples will be very helpful for finding a way to conduct quantitative depth profiling in interfacial regions using SIMS.

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