Quantification of Dimer (Al_2^+, Ga_2^+) SIMS Depth Profiles of a GaAs/AlAs Multilayer Structure using the MRI-model.

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Abstract

Depth profiles of a GaAs/AlAs multilayer structure were obtained by sputter depth profiling with both SIMS and AES using almost identical sputtering conditions. Quantification of the signal intensity in terms of the layer structure was performed by means of the MRI (Mixing-Roughness-Information depth)-model. For quantification of the SIMS results with the dimer ions Al_2^+ and Ga_2^+ a simple empirical formula (concentration $\propto$ intensity$^{0.62}$) was found and applied. The final results based on SIMS and AES data show reasonable agreement in the MRI parameters.

1. Introduction

The MRI-model (named after the three fundamental parameters atomic Mixing, surface Roughness and Information depth) [1] has been shown to be applicable for the reconstruction of the in- depth compositional distribution from both AES and SIMS depth profiles [2]. Indeed, ion bombardment induced atomic mixing and surface roughness are the same under identical sputtering conditions. However, there are basic differences in the analysis signal: (i) the AES signal intensity is, in general, little influenced by matrix effects and therefore it is fairly well proportional to the elemental concentration, (ii) the dynamic range is practically limited to 2 orders of magnitude and, (iii) the information depth in AES depends on the Auger electron kinetic energy. In contrast, in SIMS, (i) the intensity of the secondary ions is strongly matrix dependent and therefore frequently shows a non linear dependence on the elemental concentrations, (ii) the dynamic range is high, covering typically 6 orders of magnitude, and (iii) the information depth is given by the origin of the secondary ions emitted from the first 1-2 atomic monolayers. When cluster ions (dimers, trimers, etc.) of the sample atoms are used as an analysis signal, some nonlinearity is expected, and it appears very difficult to quantify the obtained depth profile. However, by using AES with the same sputtering parameters, we get a kind of reference profile. Furthermore, when both data are quantified by means of the MRI-model, the results should be identical.

2. Experimental

The investigations were performed with GaAs/AlAs multilayer samples with structure, in ML:

40GaAs/1.5AlAs/44GaAs/36AlAs/
/GaAs(bulk)

The depth profiles of the sample were obtained with SIMS (CAMECA 4f) and AES (Microlab 310F) instruments under almost the same sputtering conditions: Ar^+ primary ions with 3 keV energy and 52 (58) deg. incidence angle from the sample normal for SIMS (AES). The experiments were carried out with sample rotation.

In the SIMS experiments, the following secondary ions were measured as a function of the sputtering time: Al^{++}, O^+, AlO^+, Al_2^+, As^+, GaO^+, and Ga_2^+. The data for the Al^+, Ga^+, and As^+ were not available, because the currents of these ions were too high. The intensities of the oxygen containing ions were too low and noisy for quantification. In this paper we only used the data for Al_2^+ and Ga_2^+ ions.

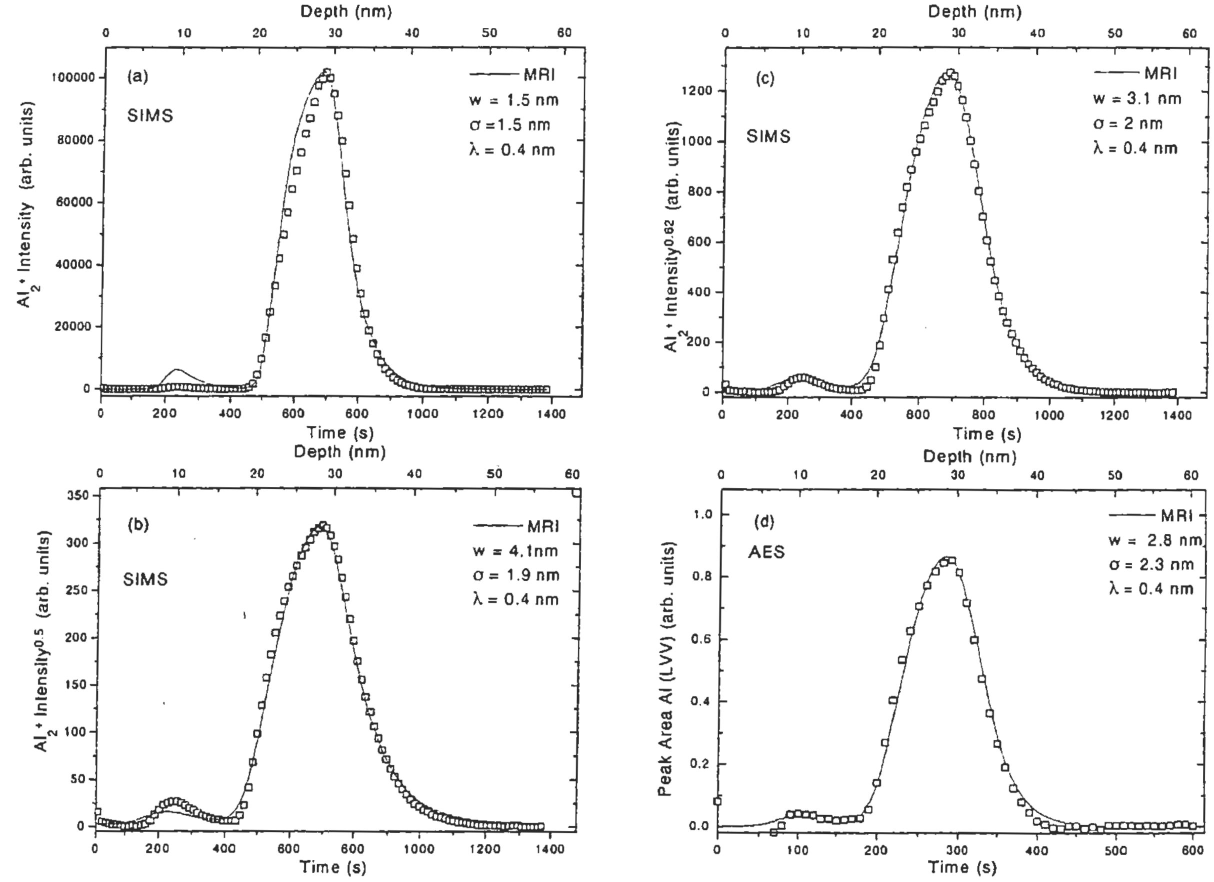

Fig 1. SIMS (a-c) and AES (d) depth profiles obtained with Ar^+ ions with 3 keV energy at 52 (58) deg incidence angle, using the Al LVV peak (68 eV) for AES profiling. The MRI fitting curve (full drawn) of the results, with the MRI-Parameters w, σ, λ, given in the inset. The sputtering time dependence of the Al_2^+ signal intensity was taken from the original plot (a), as a square root of the signal intensity (b) and by plotting this intensity with an exponent of 0.62 (c).

In AES depth profiling the Ga LMM and Al LVV signal intensities were measured. The emission angle for the Auger electrons was 40 deg from the surface normal, which gives the electron escape depth (used here as information depth parameter) 1.58 nm for Ga LMM and 0.4 nm for Al LVV based on the attenuation length values taken from refs. [3, 4].

The results were fitted with MRI model as previously described [1, 5]. The model uses the following 3 physically well defined parameters which describe the depth resolution function: length of the mixing zone (w), surface roughness (σ) and information depth (λ), and calculates their influence in sputter profiles of an assumed layer structure. The calculation result is directly compared with the measured profile, and the optimum fit enables a quantitative reconstruction of the elemental in-depth distribution of composition. Because the latter is known for reference samples of the type used here, the MRI parameters for quantification can be determined [6].

3. Results and Discussion.

For SIMS, the dependence of the Al_2^+ signal intensity on the sputtering time is shown in Fig 1(a) together with the MRI fitting curve. The MRI model results in a bad fit, an unreasonable low mixing length for 3 keV Ar^+ [8] of w = 1.5 nm and in a much too high signal intensity of the first AlAs layer (1.5 ML) as compared to that of the second layer (36 ML). This is not unexpected, because dimer ions in particular are known to show a nonlinear behavior with concentration [7].

The situation is considerably improved by the reasonable assumption that the Al concentration [Al] is proportional to the square root of the intensity, $[Al] \propto (Al_2^+)^{1/2}$ (Fig. 1 b). This corresponds to the case of randomly distributed Al atoms, and to matrix independence of both sputtering rate and ionization probability. It is seen that now the model calculates a too low signal intensity for the first layer, but the fit for the second AlAs layer is much better.

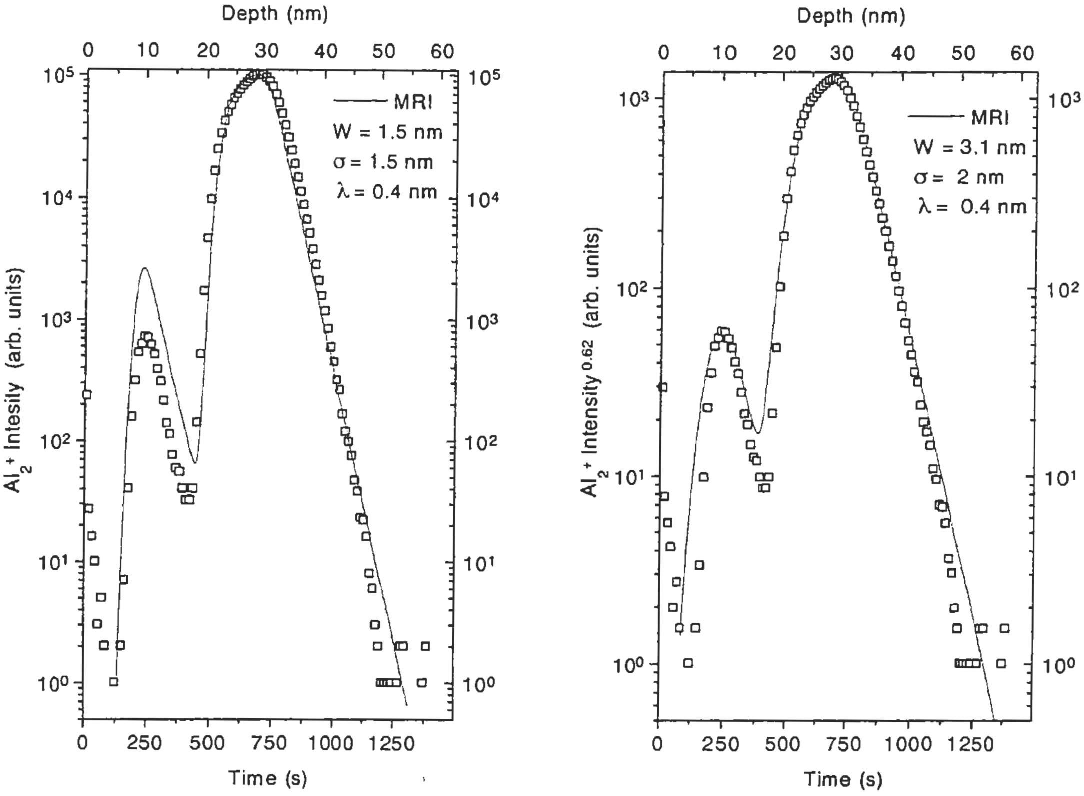

Fig. 2. The SIMS results in Figs.1(a) (original plot) and 1(c) (Al_2^+ intensity replotted with exponent 0.62) are shown on a logarithmic intensity scale together with the MRI-fit. Note the much better fit in c) over more than 1 order of magnitude.

Therefore the correct way to data quantification must be between the former two approaches (linear and square root dependence). Only one free parameter, the power of the experimental signal, was selected for data transformation to yield an optimum MRI fit. The optimum exponent value of 0.62 was found from the measured ratio of the signal intensities from the first and second layer.

The best MRI fitting result obtained for $[Al] \propto (Al_2^+)^{0.62}$ is shown in Fig. 1 c. The reasonable MRI parameters w = 3.1nm, σ= 2 nm were found in this case. The information depth for SIMS was taken as λ=0.4 nm [7]. This value is much lower then the other parameters, and its uncertainty has almost no influence on the experimental results.

To test the validity of the way of SIMS data quantification presented above, AES depth profiling was carried out under the same experimental conditions, with MRI fitting, as usual in AES, on a linear intensity scale. The results are shown in Fig 1(d). The MRI parameters are close to those found for SIMS data (Fig. 1(c)). (Note that the value of λ=0.4 nm accidentally happens to be the same as in SIMS, because of the low energy (68 eV) Al peak used here). For clarity, the SIMS results shown in Figs. 1 (a) and 1 (c) were replotted in Figs. 2 (a) and 2 (b) with more fai logarithmic intensity scale. Note that a good fit with the MRI model was obtained over more than one order of magnitude.

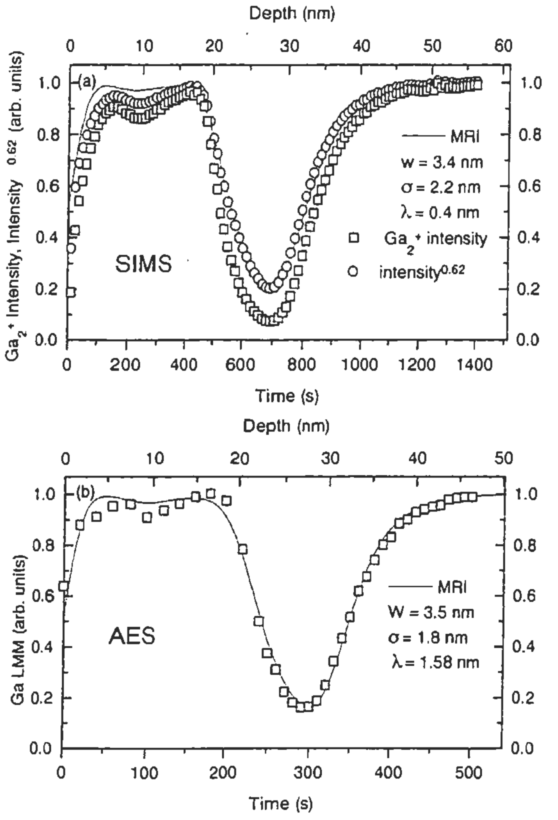

Fig 3. (a) SIMS depth profiling result with the Ga_2^+ signal intensity. The sputtering time dependence of the intensity is shown as received (squares) and plotted with an exponent of 0.62 (circles). The solid line shows the MRI fitting of the latter results.
(b) AES sputtering depth profile with the Ga LMM signal (1065 eV) and the MRI fitting curve of the results.

To further test its validity, the same power law with exponent of 0.62 was applied for the Ga_2^+ signal intensity obtained in SIMS. This is shown in Fig. 3 (a) together with the original Ga_2^+ signal intensity and together with the MRI fitting of the quantified profiling data. The MRI parameters were found to be 3.4 nm and 2.2 nm for mixing length and surface roughness, respectively. This is also close to the parameters found for MRI fitting of the AES depth profiling, 3.5 nm and 1.8 nm (Fig 3(b)) and obviously supports our way of intensity data quantification.

At present, the physical causes of this "0.62 power law" are difficult to explain. Qualitatively, we may assume a combination of a linear low, simple random distribution law, which yields the exponent 0.5, and a change of the ionization probability with concentration. Certainly, more experiments are needed for further clarification.

4. Conclusions

Depth profiles of a GaAs/AlAs multilayer structure were obtained by ion sputtering and SIMS as well as AES.

A simple empirical formula for (concentration ~ intensity $^{0.62}$) was proposed for quantification of the SIMS depth profiles obtained from the dimer secondary ions Al_2^+ and Ga_2^+. Comparison of the SIMS results with the MRI fitting and with quantified AES profile data showed that the MRI parameters mixing length and roughness are almost equal in both cases. Although at present we do not have a consistent physical model for the empirical law, the comparison between SIMS and AES profiles supports the SIMS quantification employed here.

References

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Discussion

Dr. K. Kajiwara (Sony Corp.)

This is a quite interesting manuscript on quantification of Dimer SIMS Depth Profiles based on the MRI-model which has nicely been developed by S. Hofmann.

Dr. T. Hoshi (ULVAC-PHI)

This paper represents the challenging approach for quantification in SIMS.

(a) The results are very complicated, because the author chooses dimer secondary ions for quantification. The choice of single atomic secondary ions will make more simple conversion from the intensity of secondary ions to concentration, if the suppression of the intensities of Al^+ and Ga^+ is succeeded by using ' Energy Offset' during SIMS experiments.

b) It seems that the optimum exponent value of 0.62 will change by the sputtering rate and vacuum conditions in analytical chamber, because the ionization probability is affected by the surface concentration of oxygen.

Authors

(a) We agree to the referee's opinion and we will test and compare the dimer quantification presented here with the monomer quantification in a paper which is now in progress. In addition, we will try to look for the trimers also.

(b) The vacuum in the analysis chamber is in the range of 10^{-10} torr range and the sputtering rate is about 0.1nm/s. Therefore there is little chance that he surface oxygen content be affected by the residual gases and the sputtering rate. However, if the SIMS analysis is done in a poor vacuum and with slow sputtering rate, the optimum exponent value could change. For most of the dedicated dynamic SIMS instruments, we do not have to worry about the poor vacuum and the sputtering rate.