Analysis of Auger Depth Profiles by Logistic Function

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We have analyzed the interfaces in Auger depth profiles, for the Ni/Cr multilayer specimen and the GaAs/AlAs superlattice specimen, using curve fitting process by the logistic function. In consequence, the calculated fitted profile curves are in very good agreement with the measured points. Moreover, it has been found that the depth resolution function is expressed by two parameters of the interface-width and the asymmetry. In this report, we recommend that the surface roughening effect and atomic mixing effect are clearly shown using these two parameters. It is shown that the roughening parameter D_0 in the logistic function also well correlate with the roughness parameter in the MRI model.

1. Introduction

An Auger depth profile of a layered system is generally evaluated by an interface width. The interface width[1] is expressed as the distance between 16 and 84% (or 84 and 16%) of the intensity change between plateau regions at an interface. However, this method can not be adopted for the analysis of an asymmetric interface profile.

J. Fine et al. proposed the Auger depth profiling analysis using the logistic function[2], including parameters for the interface width and asymmetry, to evaluate an interface profile. Then, we have analyzed the asymmetric interfaces in Auger depth profiles using the logistic function. We have also compared the results with the MRI model[3].

2. Experimental and Calculation

2.1 The logistic function

The logistic function is expressed as follows:

$$Y = \frac{A + A_s(X - X_0) + A_q(X - X_0)^2}{1 + e^{Z}} + \frac{B + B_s(X - X_0) + B_q(X - X_0)^2}{1 + e^{-Z}} \quad (1\text{-}1)$$

$$D = 2D_0 / [1 + e^{Q(X - X_0)}] \quad (1\text{-}2)$$

$$Z = (X - X_0) / D \quad (1\text{-}3)$$

where Y is the Auger peak intensity, and X is the independent variable, such as time or depth. X_0 is the midpoint of the interface region. The scaling factor D_0 is the interface width and Q is an asymmetry parameter. Pre-interface and post-interface elemental surface concentrations are described by the parameters A and B, respectively. The indices, s and q, correspond to the coefficients of the $(X\text{-}X_0)$ term (slope) and $(X\text{-}X_0)^2$ term (quadratic), respectively. The depth resolution function is obtained as the function differentiated of the logistic function. In this report, when the peak value is negative in the resolution function, it is multiplied by −1, resulting that peak is in positive region.

2.2 Auger depth profiles

The Auger depth profiles investigated in this analysis were actually measured for the Ni/Cr multilayer specimen (NIST SRM 2135b[3]) and the GaAs/AlAs multilayer specimen (NIMC CRM 5201-a[4]). These Auger depth profiles were using the commercial apparatus (PHI 660) with the rastered Ar^+ beam at the energies of 1.0 kV and 3.0 kV. We carried out the curve fitting of the interface profiles using the logistic function. We have also examined the relationship between the interface-width-parameter D_0 and the asymmetry-parameter Q in the function and the depth resolution function.

3 Results and discussion

3.1 Curve fitting by logistic function

It is found that a fitted logistic function curve is generally in very good agreement with the depth profiling measured points. The typical example of the curve fitting at the interface is shown in Fig. 1 for measured Ga *MVV* Auger line.

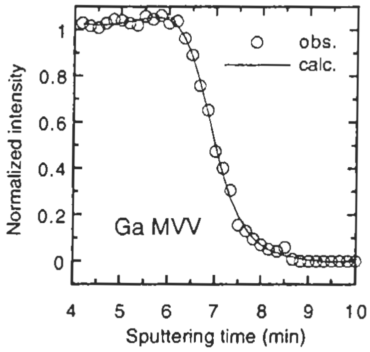

Figure 1. An example of the curve fitting by logistic function for Ga MVV in GaAs/AlAs superlattice specimen.

3.2 The depth resolution function

We carried out the curve fitting of the interface profiles using the logistic function and we have got the depth resolution function derived from the obtained calculation curve. Examples of the depth resolution functions are shown in Fig. 2. The peak shape of the depth resolution functions is asymmetric for the both specimens. Comparing Figs. 2(a) and 2(b), the baseline is flat in the both side of the peak for Ni/Cr, while the decay length is larger in the deeper side of GaAs/AlAs and there is a negative overshoot in the shalower side. We are speculating that this overshoot is caused by the material characteristics. As

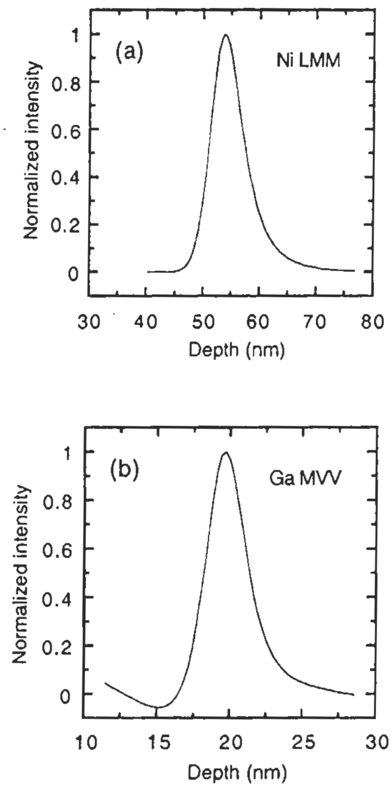

Figure 2. Examples of the depth resolution functions.
(a) obtained from interface profile of Ni LMM Auger line.
(b) obtained from interface profile of Ga MVV Auger line.

results of calculating depth resolution functions for all interface profiles, it is found that it is different between the curve shapes at the odd-number interfaces and those at the even-number interfaces where the number is counted from the surface.

So far, we have reported that the Auger depth resolution of Ni/Cr multilayer specimen increased by surface roughening[5] and that of GaAs/AlAs superlattice specimen increased by atomic mixing[6]. These results were explained from the SEM and the AFM observation. From the results in this work and the previous works, we consider that the surface roughening and the atomic mixing are reflected on the shape of the depth resolution function.

Figure 3 shows the depth resolution functions at the first and the second interfaces from the surface for measured Al *LVV* Auger line in the GaAs/AlAs superlattice specimen. The open circles represent the shape that the values of the D_0 and Q for the second interface are substituted for those of the first

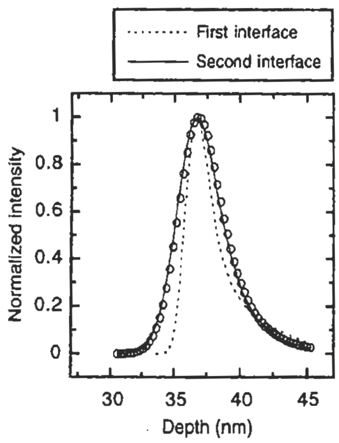

Figure 3. The depth resolution functions obtained from Al LVV Auger line.
The solid and dotted lines represent the depth resolution function of the first interface and that of the second interface, respectively.
The open circles are the values obtained from depth resolution function for the first interface, substituting the values of Do and Q for the second interface.

interface. This figure shows the curve of open circle is in very good agreement with the depth resolution function of the second interface. It clearly means that the same type of the depth resolution function can be commonly adopted for the same element transition in the same specimen, varying the parameter values. Then, we conclude that interfaces in a depth profile can be analyzed by the parameters of the interface-width and asymmetry. We recommend that it is better to estimate the interface sharpness by these parameters than the use of the simple traditional definition of the interface width.

3.3 Analysis of the interface profiles using the parameters D_0 and Q in logistic function

In figure 4 the parameters D_0 and Q are plotted as a function of the depth from the surface for the Ni/Cr multilayer specimen and the GaAs/AlAs superlattice specimen. Figure 5 shows the replotted relationship between the parameters D_0 and Q shown in Fig.4. For the Ni/Cr multilayer specimen the Q values are constant and the D_0 values increase from 2 to 4. The change of D_0 values of 2 to 4 correspond to the depth increasing from 53 to 285 nm, where the ion sputtering was performed at the constant ion energy. On the other hand, the D_0 values of GaAs/AlAs superlattice specimen are almost constant and the Q values scatter in the region from −1.5 to 0.25 where the ion sputtering was performed at the constant ion energy. The Q values do not clearly correspond to the depth from the surface.

It is thought that the change in the parameter D_0 of the Ni/Cr multilayer specimen is caused by the surface roughening

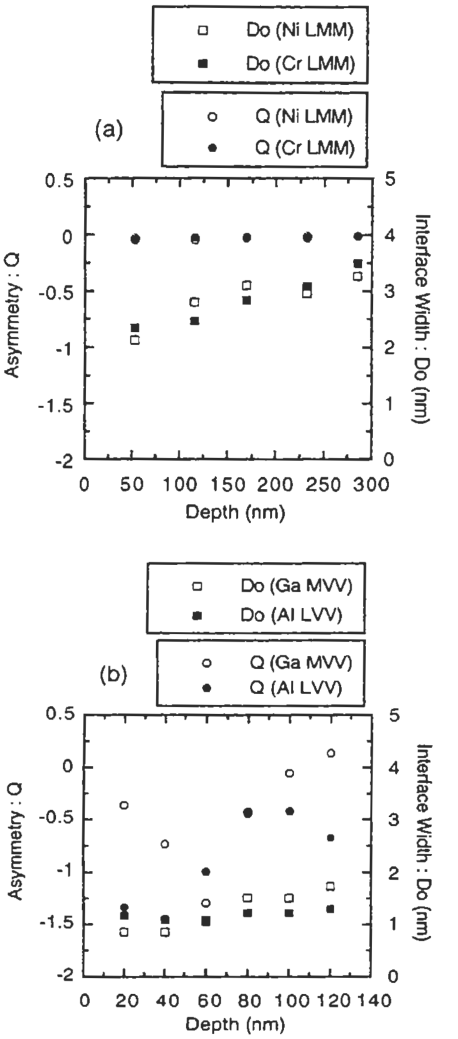

Figure 4. Relationship between the parameters Do, Q and the depth from the surface. The symbols of circle and square correspond to Q, and Do, respectively. Ar ion accelerating voltage was 1kV.

(a) The Ni/Cr multilayer specimen
(b) The GaAs/AlAs superlattice specimen

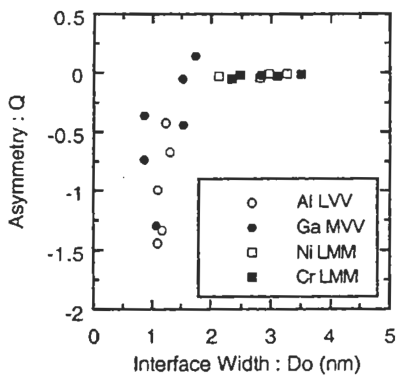

Figure 5. Relationship between the parameters Do and Q

depending on the depth from the surface[5]. On the other hand, the scattering in the parameter Q of GaAs/AlAs superlattice specimen is supposed to be caused by atomic mixing[6]. These results show that it is potentially possible that the parameters, D_0 and Q, in the logistic function quantitatively graspe ion irradiation damages.

3.4 Analysis by MRI model

We have investigated the interface analysis of Auger depth profiles of Ni *LMM* Auger line using the MRI (Mixing-Roughness-Information depth) model[7]. The results obtained from the MRI model are shown in Table 1. When the parameters of M and I are fixed to be 2.8 nm and 1.3 nm, respectivery, and R is varied from 2.5 to 4.9 nm, the calculated resolution function by the method proposed by Hofmann is in good agreement with the measured profile for Ar^+ of 1 kV. When the parameters are fixed at 5.9 nm for M, varied from 3.5 to 9.9 nm for R, and fixed at 1.3 nm for I, the calculated resolution function is also in good agreement with the measured profile for Ar^+ of 3 kV.

Table 1 Results of the curve fitting of the Ni/Cr multilayer specimen by MRI model

	Depth(nm)	53	116	169	232	285	348	401
Ni LMM (1kV)	M (nm)	2.8	2.8	2.8	2.8	2.8	2.8	
	R (nm)	2.5	3.0	3.7	4.2	4.5	4.9	
	I (nm)	1.3	1.3	1.3	1.3	1.3	1.3	
Cr LMM (1kV)	M (nm)	2.8	2.8	2.8	2.8	2.8	2.8	2.8
	R (nm)	2.5	3.0	3.7	4.2	4.5	4.7	4.9
	I (nm)	1.3	1.3	1.3	1.3	1.3	1.3	1.3
Ni LMM (3kV)	M (nm)	5.9	5.9	5.9	5.9	5.9	5.9	
	R (nm)	3.8	5.0	6.9	7.5	8.6	9.4	
	I (nm)	1.3	1.3	1.3	1.3	1.3	1.3	
Cr LMM (3kV)	M (nm)	5.9	5.9	5.9	5.9	5.9	5.9	5.9
	R (nm)	3.5	5.0	6.9	7.5	8.6	9.4	9.9
	I (nm)	1.3	1.3	1.3	1.3	1.3	1.3	1.3

Fig. 6 shows the relationship between the parameter D_0 in logistic function and the parameter R of MRI model for Auger depth profiles of Ni *LMM* and Cr *LMM* measured

Ar^+ of 1 kV. The horizontal axis is shown with $3.32 \times D_0$. In this study, $3.32 \times D_0$ is almost equivalent to the distance between 16 and 84% of the intensity change at an interface. There is a positive correlation between R and $3.32 \times D_0$ as shown in Fig. 6. The result of Fig. 6 is well shown that the depth resolution of the Ni/Cr multilayer specimen increases with the increase of the depth from the surface for the surface roughening.

We will report the comparison of the logistic function analysis with the MRI model analysis for GaAs/AlAs superlattice elsewhere.

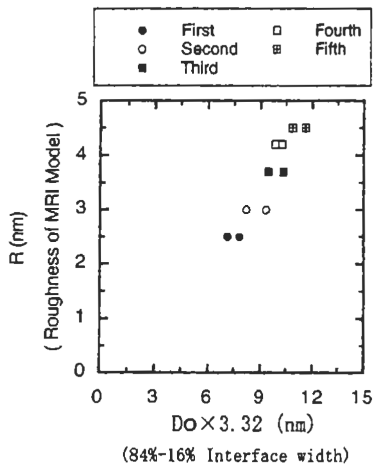

Figure 6. Relationship between the parameter Do in logistic function and the parameter R of MRI model.

4. Summary

We have investigated interface analyses in Auger depth profiles, for the Ni/Cr multilayer specimen and the GaAs/AlAs superlattice specimen, using curve fitting process by the logistic function. It has been found that the depth resolution function is expressed by two parameters of the interface-width and the asymmetry. The surface roughening effect and atomic mixing effect are clearly shown using these two parameters. It is shown that the roughening parameter D_0 in the logistic function also well correlate with the roughness parameter in the MRI model.

5. References

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[2] W. H. Kirchhoff, G. P. Chambers, J. Fine : J. Vac. Sci. Technol., **A4**, 1666 (1986).

[3] NIST SRM 2135-b, Cr/Ni multilayer specimen. Cr: 53 nm x 5 layers / Ni: 63 nm x 4 layers.

[4] NIMC CRM 5201-a, GaAs/AlAs superlattice reference material. GaAs:24 nm / AlAs: 22 nm / GaAs: 23 nm / AlAs: 22 nm / GaAs (substrate).

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