The MRI- model in COMPRO 5: A New Data Processing Software for the Quantitative Evaluation of Sputter Depth Profiles

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Quantitative evaluation of high resolution sputter depth profiles can be achieved by the so called MRI-model for the description of an appropriate depth resolution function. The MRI-model is based on the three fundamental physical parameter in sputter profiling given by atomic mixing (M), surface roughness (R) and information depth (I). After development and testing of a user friendly Visual Basic version, the program was improved and implemented in the common data processing software COMPRO Ver. 5 of the Surface Analysis Society of Japan. It is now available on the internet for memebers of the Society. A brief introduction on the basic capabilities of the MRI model is outlined and some examples are shown of the actual work with it on the computer screen. The depth profile of a known reference sample can be used to find the mixing, roughness and information depth parameters by fitting the calculation result to the measured profile. After that, similarly sputtered layer structures can be disclosed using the set of parameters for the depth resolution function.

I. INTRODUCTION

Sputter depth profiling by ion bombardment is a destructive method [1]. Actually, only a minor part of the energy transferred to the sample by ion bombardment ends up in surface erosion. Most of the energy is used for radiation damage, that is creation of defects replacement of atoms and temperature increase, leading to some degree of destruction of the original sample structure and composition in the analyzed surface layer. Therefore, the result of a profiling experiment shows a somewhat blurred image of the "true" in-depth distribution of the elemental composition [1]. The relation between the latter and the measured depth profile is described by the depth resolution function (DRF) [2,3]. Knowledge of the depth resolution function can be used to deconvolve the measured profile and to reconstruct the original in-depth distribution. the standard deviation σ (depth resolution $\Delta z = 2\sigma$) were found adequate. The reason is that above about $\Delta z = 5$ nm the dominant contribution to the depth resolution is surface roughness with an rms value of σ of the corresponding Gaussian function type depth resolution function [1].

The depth resolution function can be experimentally determined using appropriate reference samples or it can be theoretically estimated by more or less complicated calculation codes[3]. A major progress in quantitative evaluation of sputter depth profiles was achieved by introduction of the so called MRI-model for the calculation of measured profiles by convolution of a reconstructed in depth distribution of composition with an appropriate depth resolution function (DRF) based on the three fundamental physical parameters: atomic mixing (M), surface roughness (R) and information depth (I) [2]. After development and testing of a user friendly Visual Basic version [5], the program was improved and implemented in the common data processing software COMPRO Ver. 5 of the Surface Analysis Society of Japan. It is now available on the internet for members of the Society.

In this paper, the basic capabilities of the MRI model are outlined and some examples are shown of the actual work with the model on the computer screen.

II. Outline of the MRI model

The MRI-model takes into account the three fundamental effects in sputter depth profiling

[1-5]: (a) Atomic mixing (in sputtering equilibrium) in the approximation of complete mixing, characterized by a mixing length, w, (b) surface roughness is represented by a Gaussian term with a standard deviation σ, and (c) the information depth is represented by an exponential term with λ, the characteristic escape depth of the analytical information. The elements of the DRF of the MRI model, which is described in detail in ref. [2], are therefore the following three basic functions:

atomic mixing:

$$g(w) = \exp[-(z - z_0 + w)/w] \quad (1)$$

information depth:

$$g(\lambda) = \exp[-(z - z_0)/\lambda] \quad (2)$$

surface roughness:

$$g(\sigma) = \frac{1}{(2\pi\sigma)^{1/2}} \cdot \exp\left[\frac{-(z - z_0)^2}{2\sigma^2}\right] \quad (3)$$

The fixed depth coordinate is given by z_0, whereas z is the average location of the sputtering depth. These basic relations have already found useful applications in practical work [6,7, 8].

III. Working with the MRI- Model in Compro .5

At first, we have to use a reference sample of known structure and composition to set up the depth resolution function for a specific set of experimental parameters (e.g. ion species, energy, incidence angle, ion current density, analysis signal, constituents of the sample). Such a test sample is a buried delta layer of monolayer thickness (preferably in SIMS) or an atomically flat interface (preferably in AES). For example, the following GaAs/AlAs multilayer structure containing both features was used: (in atomic MLs): 41-GaAs/1-AlAs/43-GaAs/36- AlAs/GaAs.../Si(111), or in nanometers (1ML=0.28 nm): 11.5/0.28/12.1/10.1/... This structure was checked by high resolution cross section transmission electron microscopy and then depth profiled in a Fisons Microlab 310 F instrument using 0.5 keV Ar^+ ions at a 68° incidence angle, and recording the high energy Al Auger peak-to-peak-heights. AES parameters were a primary beam energy of 10 keV, a beam current of 10 nA and a beam diameter of about 30 nm, rastered over an area of about 10x10 μm^2 and normally incident to the rotating sample surface.

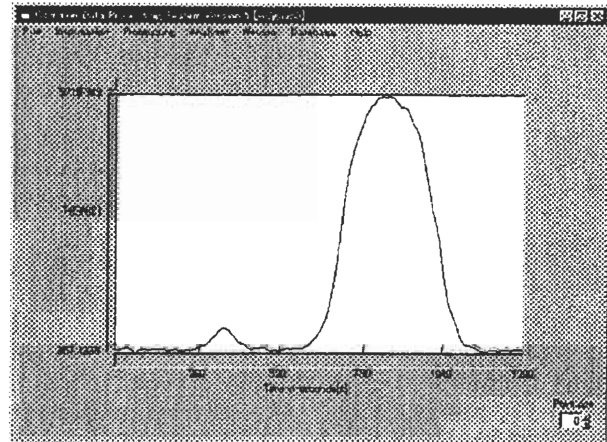

Fig. 1: Visual Basic Surface with the experimental. AES depth profile of a multilayer structure consisting of one monolayer and 36 monolayers AlAs in a matrix of GaAs [5]. See text for details.

The experimental result, in which the 1396 eV Al Auger peak-to-peak-height (APPH) is plotted as a function of the sputtered depth, was stored as an ASCII file in the file named Al2GaAs3. This file can be opened after going to the Common Data Processing –depth profile – MRI and is shown in Fig.1. For the transformation of the sputtering time in a depth scale, we must first type in the correct sputtering rate (see template). It is straightforward in our case, because the layer structure is known (the first monolayer is at 11.5 nm depth). We select 0.032 nm/s and click "fix". (see VB surface in Figs 2a,b). To only display the monolayer in Fig. 1, we click "Zoom" and adjust the two bars to select a useful range and click ("set"). The selected range is zoomed and the maximum value is automatically adjusted to the full scale of the screen.

By clicking the value "1" on the intensity scale, we can choose between "normalized", "absolute", or "arbitrary". The last choice means to give a suitable value on the ordinate for display. By clicking in the

left margin of the ordinate, we can have a zero line to be adjusted to the experimental value.

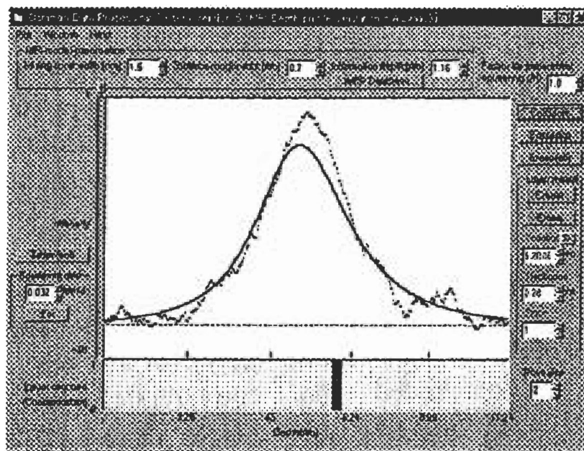

Fig. 2a

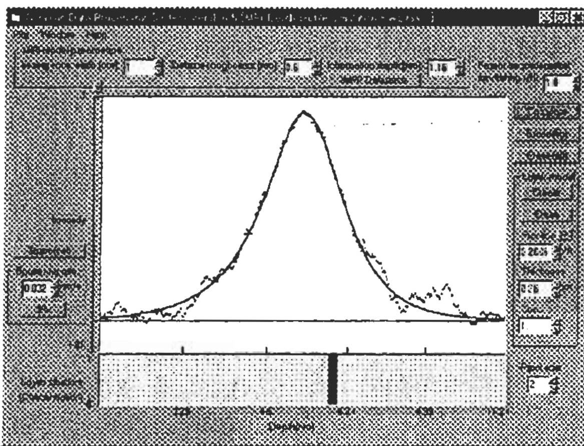

Fig. 2b

Fig. 2: First monolayer from Fig.1 displayed and compared with the curve of the MRI calculation (for detailed explanations see text):
(a): wrong MRI fit parameters
(b): optimum fit with correct MRI parameters

Now we prepare for the MRI calculation. The first parameter, most reliably estimated, is the information depth, which we can take from electron inelastic mean free paths (imfp) databases or from refs. [6, 7], and multiply with the cosine of the emission angle (AES and XPS).(For SIMS we use the first monolayer, 0.3-0.4 nm). Here it is about 1.16 nm [5]. The mixing parameter is roughly of the order of 1-2 nm per keV energy of argon ions, but depends on the angle. Let us first assume 1.5 nm for the mixing zone width. This leaves the roughness parameter, which we can only guess, e.g. 0.7 nm. Now we "Create" (click) the monolayer and draw the appearing yellow "block" in the "Layer structure" compartment by adjusting the position to 6.2 nm, the layer thickness to 0.28 nm, and the concentration to 1.

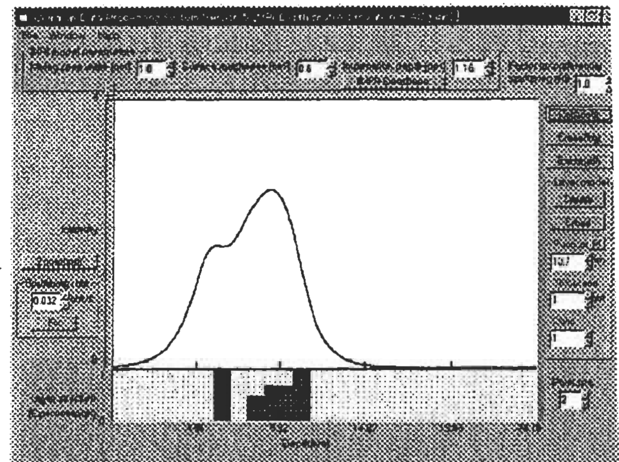

Fig. 3a

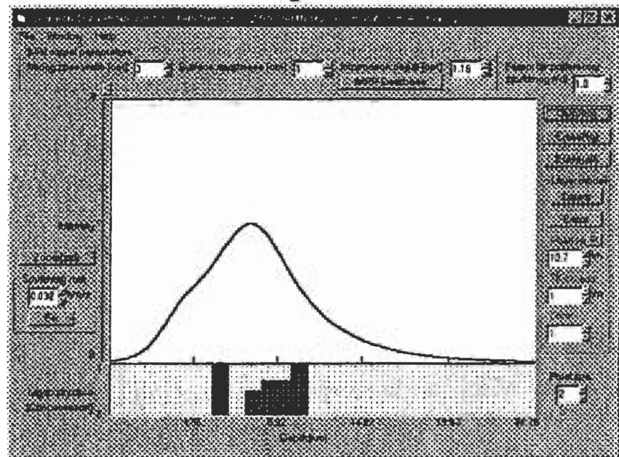

Fig. 3b

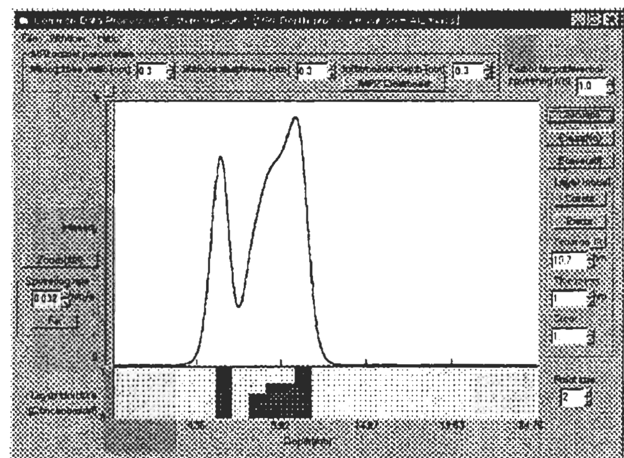

Fig. 3c

Fig. 3: A given layer structure and the expected measured profiles for three different resolution functions with the following MRI parameters:
(a): $w = 1.0$ nm, $\sigma = 0.6$ nm, $\lambda = 1.16$ nm (as in Fig. 2 a)
(b): $w = 3.0$ nm, $\sigma = 1.0$ nm, $\lambda = 1.16$ nm
(c): $w = 0.3$ nm, $\sigma = 0.3$ nm, $\lambda = 0.3$ nm (theor. limit [8])

After setting "set" we click "calculate" and we get a curve shown in Fig 2a, which resembles the measured curve but deviates remarkably. To obtain a better fit, we have to change the MRI parameters. The too broad top indicates that the roughness was assumed too high, and the mixing length should be increased to meet the decay on the right hand side. After shift of the position and about 3-5 iterations, we get the rather good fit shown in Fig. 2b, where the information depth parameter was kept constant but mixing length and roughness were changed to 1.0 and 0.6 nm, respectively.

Figure 3 demonstrates the expected profile measurement of the layer structure given for the data of the depth resolution function retrieved from Fig. 2b(Fig.3a)), that with a rather bad resolution function (high mixing length, e.g. for 3 keV Ar+ sputtering, (Fig3b)), and with an earlier proposed depth resolution function at the theoretical limit (about 1 ML, i. e. 0.3 nm for each MRI Parameter) (Fig.3c)[4,5].

IV Conclusions and Outlook

The MRI model in its present setup for COMPRO Ver. 5 offers a user friendly algorithm for the quantitative evaluation of sputter depth profiles in AES, XPS and SIMS. Its essential, present limitations are: (1) it assumes a compositionally homogenous mixing zone, (2) it neglects preferential sputtering and the associated nonlinear change of the sputtering rate (this will be implemented in the future), (3) it assumes linearity of signal intensity with concentration, and (4) it neglects other nonlinear effects like segregation and radiation enhanced diffusion. (Again, some corrections will be implemented in the future). However, many systems, such as GaAs/AlAs and SiO2/Ta2O5 multilayers [1] show a behavior which can already be successfully evaluated with an accuracy in the monolayer region.

Note: The authors regret that the presented illustrations of the VB surface are too small for reading the numbers given in the text. It is recommended that the reader is using COMPRO 5 on his/her computer while reading through the paper.

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