Characterization of a Single Layer of $Si_{0.73}Ge_{0.27}$ and a Quantum-well Structure of $Si_{0.4}Ge_{0.6}$/Ge by Quantitative SIMS Depth Profiling Using the Analytical Depth Resolution Function of the MRI Model

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Abstract. The analytical depth resolution function of the Mixing-Roughness-Information (MRI) model is used to fit the measured SIMS depth profiling data of a single layer of $Si_{0.73}Ge_{0.27}$ and a $Si_{0.4}Ge_{0.6}$/Ge quantum-well structure on Si substrate. The interface roughness and the individual layer thickness and the depth resolution values are determined accordingly. The obtained layer thickness values in $Si_{0.4}Ge_{0.6}$/Ge quantum-well structure are consistent with the ones measured by HR-TEM with a maximum relative error less than 1.2%.

1. Introduction

Quantum-well structures with layer thickness in the range of a few nm or tens of nm have been widely used for micro-electronic devices [1]. The performance of device depends strongly on the quality of the quantum-well structure. In particular, the variations of layer thickness and interface roughness may have a significant influence on the function of device [2]. The layer thickness in a few nm range is conventionally measured by HR-TEM, which involves the complex procedures of sample preparation and measurement. On the other hand, quantitative SIMS depth profiling may provide an alternative way to determine the layered structure with one nm resolution. Recently, with the development of the advanced SIMS instrument, the artifacts that present often in any depth profiling, such as sputtering induced roughness, crater effect and matrix effect, have been significantly minimized and the HR-SIMS depth profile could be simply obtained. In this paper, it will be demonstrated that not only could the quantum-well structure and the depth resolution but also the interface roughness be well determined by fitting the measured SIMS depth profiling data using the analytical depth resolution function of the MRI model.

2. Analytical depth resolution function of the MRI model

The measured depth profiles differ from the true concentration-depth profiles as a result of various interactions of the ion beam bombardment with the measured sample, e.g. ion implantation, cascade mixing, etc. A so-called depth resolution function (DRF) is often used to describe the distortion of

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the measured depth profiles as compared to the true ones, which causes the depth profiles degradation in the physical mechanism. Generally speaking, in sputter depth profiling, the measured and normalized intensity I(z)/Io can be described as the convolution of the true concentration X(z') at the original depth z' in the sample with a DRF g(z-z') as [3]:

$$\frac{I(z)}{I_0}=\int_0^{\infty} X(z')g(z-z')dz' \tag{1}$$

Where z' is the running depth parameter for which the composition is defined and z is the sputtered depth. With the measured and normalized intensity I(z)/Io and a known DRF g(z-z'), the true in-depth distribution of composition can be calculated by Eq. (1). Therefore, the exact knowledge of the DRF is the key to accurate reconstruction of the original depth distribution of the composition from the measured depth profile [4]. In the MRI model, the DRF g(z-z') takes into account the three physically meaningful effects in any sputtering depth profiling: atomic mixing, surface/interface roughness, Information depth, which are described, respectively , by [5]:

Mixing length (w):

$$g_w(z-z')=\frac{1}{w}\exp\left[\frac{-\left(z-z'+w\right)}{w}\right] \tag{2}$$

Roughness (σ):

$$g_\sigma(z-z')=\frac{1}{\sqrt{2\pi}\sigma}\exp\left[\frac{-(z-z')^2}{2\sigma^2}\right] \tag{3}$$

Information depth (λ):

$$g_\lambda(z-z')=\frac{1}{\lambda}\exp\left[\frac{-\left(z-z'\right)}{\lambda}\right] \tag{4}$$

Where w is the atomic mixing length, σ is the surface/interface roughness and λ is the information depth parameter. With the above three partial resolution functions, the DRF g(z-z') can be written as:

$$g(z-z')=g_w(z-z')\otimes g_\sigma(z-z')\otimes g_\lambda(z-z') \tag{5}$$

In general, the quantitative results of the MRI model are obtained by the numerical solution of the convolution integral with combining Eq. (1) and Eq. (5).

With respect to the above-discussed refinements of the DRF in terms of symmetric (Gaussian functions) and asymmetric (non-Gaussian functions) functions, it is necessary to clarify the contribution to the depth resolution △z (16-84%). According to the MRI model, three physically meaningful effects contribute to the depth resolution function. A symmetric contribution to the depth resolution function originates from the intrinsic roughness and the surface roughening by ion sputtering, which both are described by a Gaussian smearing function (see Eq. (3)), characterized by its standard deviation of the surface roughness parameter σ. For the asymmetric broadening functions, the atomic mixing is described by an exponential function (see Eq. (2)), characterized by the atomic mixing length w; the information depth of the Auger electrons (for AES) is also described by an exponential function (see Eq. (4)), characterized by the information depth λ. Hence, on the basis of the three MRI parameters, the total depth resolution can approximately be rewritten as [6]

$$\Delta z=\left[(2\sigma)^2+(1.668w)^2+(1.668\lambda)^2\right]^{1/2} \tag{6}$$

Fitting the experimental depth profile by the MRI model leads to obtain the values of σ, w and λ. Then, the depth resolution Δz can be calculated with Eq. (6).

2.1. Analytical solution for delta layer

For the special case of being an ideal delta function with vanishing thickness, an analytical resolution function can be derived with the result $I(z)/I_0=g_{\Delta MRI}$ by Eq. (1) given by [7]

$$g_{\Delta MRI}(z) = \left\{\frac{1}{2w}\left[1-\exp\left(-\frac{w}{\lambda}\right)\right]\exp\left[\left(\frac{-z-w}{w}\right)+\frac{1}{2}\left(\frac{\sigma}{w}\right)^2\right]\right\}\times\left\{1-erf\left[\frac{1}{\sqrt{2}}\left(\frac{-z-w}{\sigma}\right)+\frac{\sigma}{w}\right]\right\}$$
$$+\left\{\frac{1}{2\lambda}\exp\left[\frac{z}{\lambda}+\frac{1}{2}\left(\frac{\sigma}{\lambda}\right)^2\right]\right\}\times\left[1+erf\,\frac{1}{\sqrt{2}}\left(\frac{-z-w}{\sigma}-\frac{\sigma}{\lambda}\right)\right] \tag{7}$$

For SIMS, assuming that practically all of the detected ions stem from the first atomic layer, the information depth parameter in the MRI model for SIMS can be set to zero. The DRF for MRI-SIMS is given by

$$g_{\Delta(MRI-SIMS)}(z) = \frac{1}{2w}\exp\left[-\frac{z+w}{w}+\frac{1}{2}\left(\frac{\sigma}{w}\right)^2\right]\left[1-erf\left(-\frac{z+w}{\sqrt{2}\sigma}+\frac{\sigma}{\sqrt{2}w}\right)\right] \tag{8}$$

To demonstrate the behavior of the analytical resolution function of the MRI model for different roughness, Figure 1. a shows a plot of Eq. (7) for w = λ = 1nm and σ = 0.01, 0.1, 0.3 and 1.0 nm. The steep rise at z = z(0) -w is caused by the actual onset of complete mixing of the delta layer, with the mixing zone length w governing the decay of the signal for z > z(0) -w. When the roughness increases, this behavior is smoothed out because of the microscopically different spatial onsets of mixing. [9] For increasing roughness, the maximum of the total DRF shifts from z = z(0) -w in the direction of z = z(0), until it coincides with its centroid given by a combination of both exponential functions for w and λ. [8]

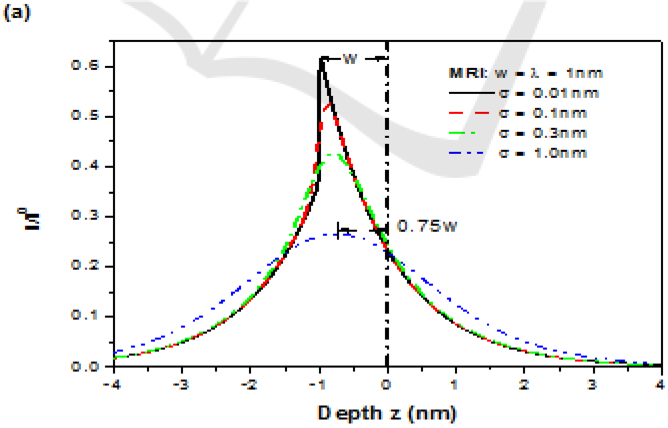

Figure 1. Analytical depth resolution function of the MRI model (Eq. (7)) for w =λ = 1nm and different roughness parameter values, σ = 0.01, 0.1, 0.3 and 1nm. Replotted from Ref [9].

2.2. Analytical solution for thick layer

As already proposed by Zalm [9] and later by Gautier et al.[10], including a term for layer thickness appears to be possible in the analytical DRF. In the MRI model we can introduce a layer thickness d = $z_2 - z_1$, where z_1 denotes the beginning and z_2 the end of the layer. For SIMS (λ→0), the DRF for a layer with thickness of $z_2 - z_1$ is given by [8]

$$\begin{aligned}(I(z)/I_0)_{d-MRI-SIMS} &= \frac{1}{2}\left[erf\left(\frac{z+w-z_1}{\sqrt{2}\sigma}\right)-erf\left(\frac{z+w-z_2}{\sqrt{2}\sigma}\right)\right]\\ &+\frac{1}{2}\exp\left[-\frac{z+w}{w}+\frac{1}{2}\left(\frac{\sigma}{w}\right)^2\right]\\ &\times\left\{\exp\left(\frac{z_2}{w}\right)\left[1+erf\left(\frac{z+w-z_2}{\sqrt{2}\sigma}-\frac{\sigma}{\sqrt{2}w}\right)\right]-\exp\left(\frac{z_1}{w}\right)\left[1+erf\left(\frac{z+w-z_1}{\sqrt{2}\sigma}-\frac{\sigma}{\sqrt{2}w}\right)\right]\right\}\end{aligned} \tag{9}$$

In SIMS, the simple analytical solution of the ideal delta layer is usually applied for monolayers. In reality, however, the thinnest layer is an atomic monolayer, with a thickness of 0.25 ± 0.05 nm in most semiconductors and metals. If we assume a DRF of lower limit, for example for the case of SIMS (Eq. (9)) with $\sigma = w = 1$ ML, the resulting FWHM (full width at half maximum) of the profile for $z_2 - z_1 = 0$ is about 2.9 monolayers or ca.0.8 nm for a delta layer [8]. It shows that the FWHM of the measured profile after Eq. (9) increases slightly with increasing layer thickness until it becomes identical to the latter for a thickness above 8 monolayers [8]. For higher values of the DRF parameters the deviation between an ideal delta layer and a monolayer is reduced.

In summary, analytical DRFs can be applied to the convolution integral of (1) Delta layers, (2) Layers with any finite thickness and constant analyte concentration, (3) Multilayers of type 2). [8]

The main advantage of the analytical solution of the DRF is that the application of it is simple and user friendly because no computer programming is necessary for graphical representation. It is particularly useful for quantifying measured delta layer depth profiles in AES and SIMS [11]. This paper will demonstrate that the layer thickness and the depth resolution values could be obtained by fitting the measured SIMS depth profiles of a multilayer (a quantum-well structure) and a thick layer respectively by applying the analytical solution of the convolution integral. It is customary to assume X(z) and to calculate the intensity $I(z)/I_0$ in a “forward” manner with a known depth resolution function g(z), and compare it with the measured $I/I_0(z)$. This procedure is performed repeatedly by trial and error until an optimum fit of both is obtained. This is done by a computational program that varies the X(z) distribution until the minimal value of the average deviation of the calculated from the measured profiles is achieved. The final input X(z) is the reconstructed, original in-depth distribution of composition.

3. Results and discussion

To demonstrate the application of the analytical MRI model, the measured SIMS depth profiles of $Si_{0.73}Ge_{0.27}$ superficial layer and $Si_{0.4}Ge_{0.6}$/Ge 10-period quantum well (QW) on Si substrate [2, 12] will be quantified. Both layer structures were deposited on Si substrate by chemical vapor deposition (CVD). The $Si_{1-x}Ge_x$ superficial layer thickness is determined as 26.6 ± 0.5nm [2]. The $Si_{0.4}Ge_{0.6}$/Ge 10-period QW thickness values determined from HR-XTEM picture are listed in Table 1 [12]. The SIMS profiling was performed with an Atomika 4500 instrument using primary ions of O_2^+ with a range of energies (0.25–1keV) at near normal incidence. An area of 220x220 mm was scanned, and the $30Si^+$ and $70Ge^+$ secondary ions were recorded.

Table 1. $Si_{0.4}Ge_{0.6}$/Ge QW thickness values determined by XTEM [12].

Period number	1	2	3	4	5	6	7	8	9	10
Si0.4Ge0.6 layer (nm)	8.6	8.6	8.6	8.5	8.5	8.5	8.4	8.5	8.4	8.6
Ge layer (nm)	12.6	12.7	12.6	12.6	12.7	12.7	12.7	12.7	13.0	12.8

Figure 2 shows the measured and normalized Ge SIMS depth profiles as open circles for $Si_{0.73}Ge_{0.27}$ superficial layer on Si substrate using different O_2^+ beam energies from 0.4-2.0 keV. The best fits for each measured depth profile using Eq. (9) are shown as solid lines in Figure 2. The corresponding MRI parameters are listed in Table 1 together with the depth resolution values calculated from Eq. 6. It shows clearly that upon increasing the O_2^+ beam energy, the atomic mixing length increases from 1.1nm to 3.0nm and the roughness parameter increases from 0.4 nm to 1.0 nm, yielded the increasing of depth resolution, i.e. the degradation of measured depth profile.

Table 2. The best fits of the MRI parameter and the corresponding depth resolution values.

	400 eV	500 eV	1keV	1.5 keV	2 keV
***w* (nm)**	1.1	1.3	2.0	2.6	3.0
***σ* (nm)**	0.4	0.4	0.7	0.8	1.0
Depth resolution (nm)	2.0	2.3	3.6	4.7	5.4

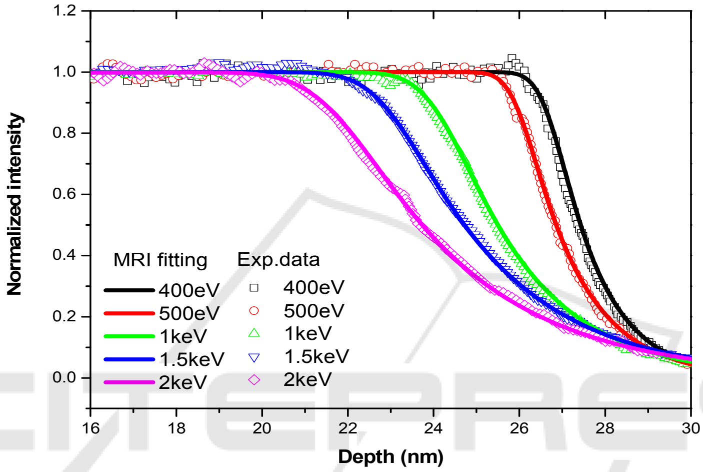

Figure 2. The measured SIMS profiles (open circles) [2] and the fitted profiles (solid lines) using the MRI analytical depth resolution function.

Table 3. The best fits of the MRI parameter and sputtering rate values.

	250 eV	500 eV
***w* (nm)**	0.9	0.1
***σ* (nm)**	1.2	1.2
Sputtering rate (nm/s)	0.01	0.03

Figure 3 shows the measured and normalized Si SIMS depth profiles as open circles for $Si_{0.4}Ge_{0.6}$/Ge 10-period QW structure on Si substrate using (a) 250 eV and (b) 500eV O_2^+ beam energy sputtering. The best fits for the measured depth profiles using Eq. (9) are shown as solid lines in the respective figure. The corresponding MRI parameters are listed in Table 2 together with the average sputtering rate of $Si_{0.4}Ge_{0.6}$ layer. Both the MRI fits are based on the same QW layered structure that is taken as one of fitting parameters. The fitted individual layer thickness of each period is shown by different symbols in Figure 4 and is compared with the value listed in Table 1. The maximum relative error between the fitted thickness and the one obtained by XTEM is less than 1.2%. This implies that the quantitative SIMS depth profiling can provide an alternative way for determination of nano-layered structure. Meanwhile, the fitted interface roughness of 1.2 nm in $Si_{0.4}Ge_{0.6}$/Ge QW structure is slight higher than that of 0.4 nm in $Si_{0.73}Ge_{0.27}$ superficial layer on Si substrate. This implies that both samples prepared by CVD are very smooth.

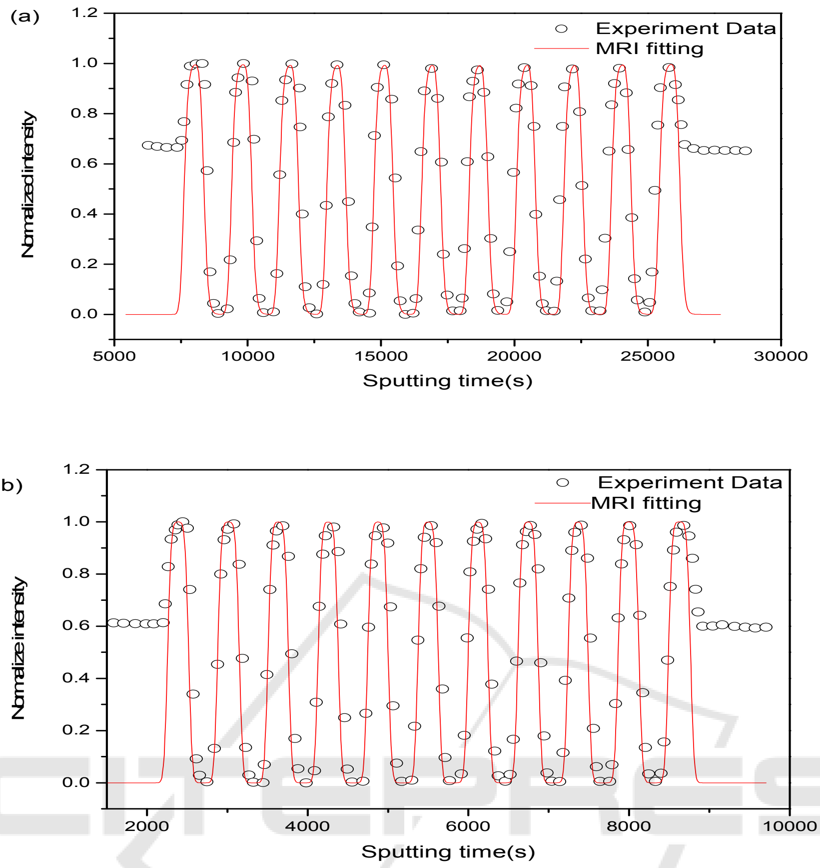

Figure 3. SIMS depth profiles [12] of Si (open circles) (a) 250 eV and (b) 500eV O_2^+ and MRI fitted profiles (solid lines) for $Si_{0.4}Ge_{0.6}$/Ge QW structure.

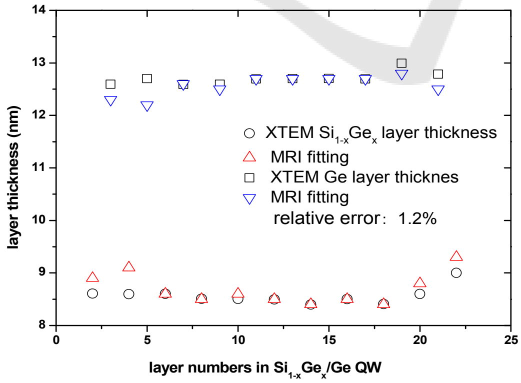

Figure 4. Comparison of the fitted and the measured (listed in Table 1) layer thickness values of $Si_{0.4}Ge_{0.6}$ and Ge sublayers in $Si_{0.4}Ge_{0.6}$/Ge QW structure.

4. Conclusions

The analytical DRF of the MRI model that is simple and user friendly has successfully been used to quantify the measured SIMS depth profiling data of nano-layered structures. The individual layer thickness, the interface roughness and the depth resolution values are determined accordingly. The extracted layer thickness values for $Si_{0.4}Ge_{0.6}$/Ge quantum-well structure are consistent with the ones determined by XTEM.

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