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New Iterative Algorithm for Improving Depth Resolution in Ionic Analysis: Effect of Iterations Number

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***Abstract*—**In this paper, the improvement by deconvolution of the depth resolution in Secondary Ion Mass Spectrometry (SIMS) analysis is considered. Indeed, we have developed a new Tikhonov-Miller deconvolution algorithm where a priori model of the solution is included. This is a denoisy and pre-deconvoluted signal obtained from: firstly, by the application of wavelet shrinkage algorithm, secondly by the introduction of the obtained denoisy signal in an iterative deconvolution algorithm. In particular, we have focused the light on the effect of the iterations number on the evolution of the deconvoluted signals. The SIMS profiles are multilayers of Boron in Silicon matrix.

***Keywords*—**DRF, in-depth resolution, multiresolution deconvolution, SIMS, wavelet shrinkage.

I. INTRODUCTION

SECONDARYion mass spectrometry (SIMS) is widely used in the semiconductor industry for dopant depth profiling as well as contamination monitoring because of its ability to detect all elements, its high sensitivity, its large dynamic range, its unrivalled depth resolution and minimal sample preparation. In the last few years, Improvement of depth resolution in secondary ion mass spectrometry (SIMS) analysis is a critical issue for depth profiling of silicon semiconductor films [1]-[3].

Developments of SIMS analysis are not as pronounced and rapid than those of the manufacturing techniques of materials in microelectronics. For progress in this domain, it is necessary to exceed the raw experimental results by including a post- erosion digital processing. This treatment must lead to a better approach of the real profile from the experimental one. In this sense, the different proposed monoresolution deconvolution methods in the SIMS fields showed a certain disability towards the noise, the consequences are mainly limiting the depth resolution of the deconvoluted profiles and especially the generation of oscillations and artifacts, which are not physically acceptable as negative concentrations. The origin of these artifacts is related to the presence of strong local components of high frequencies in the signal which form part of the noise. To overcome these limitations; it is useful to adopt a strong deconvolution algorithm that takes into account this nuisance parameter. For this, we have developed a new multiresolution deconvolution method based on Tikhonov-Miller regularization with model of solution as a denoisy signal, previously decomposed on a wavelet basis [3], [4].

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II. PRINCIPLE OF THE ALGORITHM

The deconvolution of depth profiling data in SIMS analysis amounts to the solution of an appropriate ill-posed problem and it requires the result to be regularized. To this end, the solution is superimposed with certain limitations by introducing some additional limitative operator, whose shape is chosen depending on the formalism used for the solution of the ill-posed problem, into a goal function (usually the goal function is the mismatch between the convolved solution and initial data) [5]. Gautier et al. [6],[7] have used a limitative operator that was determined as smoothness of the solution. Collins et al. [8] and Allen and Dowsett [9] have used the entropy function as a limitative operator.

Barakat et al. [10] have proposed a restoration method based on Tikhonov-Miller regularization with an integrated a priori model of solution. Mancina [11] has proposed an iterative constrained algorithm, based on Barakat algorithm, in which the model of solution is a pre-deconvolved signal. Nevertheless, the results of these approaches contain oscillations and artifacts with negative components, which are not physically accepted in SIMS analysis. The origin of these oscillations is the presence of strong local concentrations of high frequencies in the signal which belong to noise. For this reason, it is important to eliminate noise components from the signal [1]. Denoising with the sole purpose of extracting desired information from measured data has proven to be a crucial preliminarily steps in any analytical method. For this reason, it is important to remove noise components from the signal (in our case, the model of solution). The idea is to introduce a denoisy and pre-deconvoluted signal as model of solution in Barakat's approach. It is a signal denoised and reconstructed retaining only the approximation coefficients and detail thresholded coefficients [1], [3].

In this approach, the model of solution is as follows:

$$X_{mod}=\tilde{x}^{(j-1)}=\tilde{F}^{(j)}y_a^{(j)}+\tilde{G}\hat{y}_d^{(j)} \tag{1}$$

This algorithm is iterative, its mathematical formulation in Fourier space, is as follows:

$$\begin{cases} \hat{X}_{n+1} = \frac{H^{*}Y+\alpha|D|^2 X_{\mathrm{mod}_n}}{|H|^2+\alpha|D|^2} \\ X_{\mathrm{mod}_0} = TF\left[\tilde{x}^{(j-1)}\right] = TF\left[\tilde{F}^{(j)} y_a^{(j)} + \tilde{G}\hat{y}_d^{(j)}\right] \\ \hat{x}_n = TF^{-1}\left[\hat{X}_n\right] \end{cases} \qquad (2)$$

With $y_a^{(j)}$and $\hat{y}_d^{(j)}$are, respectively, the approximation signal and the thresholded details signal; α: regularization parameter; D: regularization operator; H: matrix constructed from the impulse response h; Y: vector constructed from the measured signal. For more details see [1].

III. Results and Discussion

Boron delta-doped multilayers are potential reference materials for the evaluation of depth resolution in secondary ion mass spectrometry (SIMS). These are ideal structures for applying a deconvolution method since it is the most affected by the effects of the convolution in SIMS analysis. Their deconvolution gives an idea of what we can expect from the depth resolution especially on the experimental plane after deconvolution. That is why we are interested to this type of samples.

A. Deconvolution of Sample MD5

The results of the deconvolution of five delta-layers sample (MD5) are illustrated in Fig. 1. Indeed, the deconvolution of this sample gives a great improvement of the depth resolution and recovery of the original signal shape. The exponential slopes are completely removed giving symmetrical and well separated peaks. By comparison these results with those obtained by the algorithm of [6], the profile obtained by our approach are smooth and don't contain artifacts.

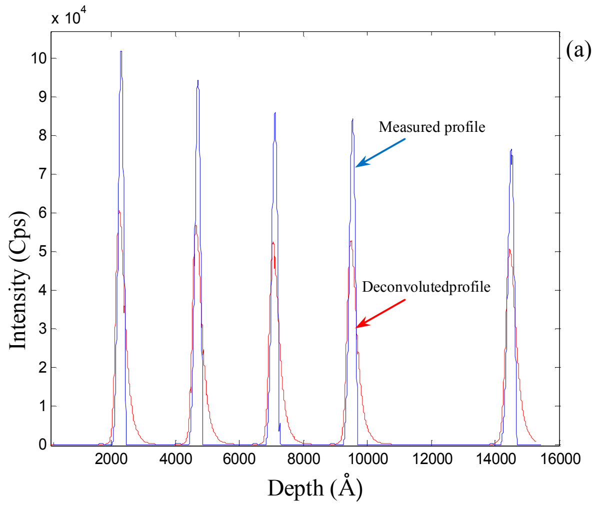

Fig. 1 (a) Results of deconvolution by Boulakroune's approch of SIMS profile containing five delta-layers of boron in silicon :Linear scale plot

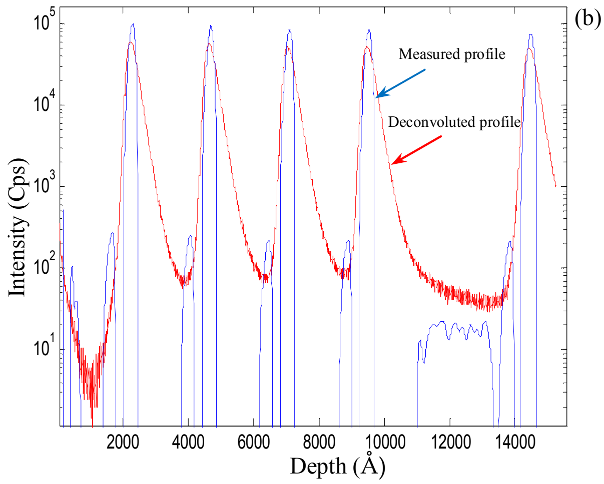

Fig. 1 (b) Results of deconvolution by Boulakroune's approch of SIMS profile containing five delta-layers of boron in silicon: Logarithmic scale plot

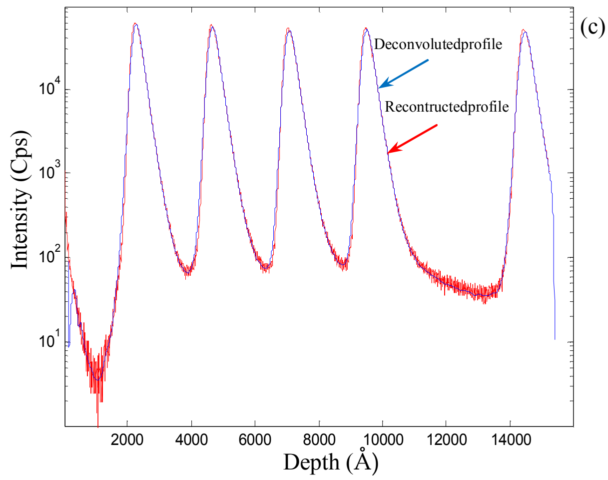

Fig. 1 (c) Reconstruction of the measured profile from the deconvoluted profile and the DRF

To eliminate these oscillations, [6], [7] proposed the application of local confidence level deduced empirically from the reconstruction error in the deconvoluted profiles. The goal of this confidence level is to separate the parts of the signal belonging to the original profile from those generated artificially by the process of deconvolution. According to these authors, when the signal falls to the noise level, at which point one cannot be confident in the deconvolution result, one must fix a limiting value of the deconvoluted signal below which one should not take into account the deconvolution result that likely belongs to the original signal. However, a confidence level that authorizes to take into account certain parts of the signal and eliminates the lower parts in which the signal should not be taken into account anymore, does not bring any information about the quality of information.

One of the advantages of SIMS analysis is the great dynamic range of the signal, and allowing the deconvoluted signal to be restricted to a dynamic range which does not exceed two decades and thus does not reflect the original signal. The parts filtered by the confidence level can provide precious information about the sample.

Mancina [11] showed that the artifacts are not always aberrations of the deconvolution; they can be structures with low concentrations. The interpretation of the artifacts must be measured, especially if their amount is not negligible, in which case, one cannot eliminate them from the deconvoluted profiles.

In deconvolution, a criterion of validation of a result is the reconstruction of measured signal from the deconvoluted signal and the impulse response which is in our case the DRF (Depth Resolution Function). More the reconstructed profile follows the measured profile, more the result is accurate. The reconstruction of our profiles is excellent, especially for high signal levels. The difference between the measured profile and the reconstructed profile is mainly at the junctions of concentration peaks, where the noise is dominant.

TABLE I
SUMMARY OF DEPTH RESOLUTION AND MAXIMUM OF PEAKS GAINS OBTAINED BY DECONVOLUTION

	Peak 1	Peak 2	Peak 3	Peak 4	Peak 5
Depth resolution Gain	1.53	1.51	1.53	1.35	1.51
Maximum of Peaks Gain	1.8	1.77	1.75	1.72	1.64

The values of obtained gains clearly give back the good quality of the deconvolution profiles.

B. Deconvolution of Sample md16. Discussion on the Effect of Iterations Number

This sample was made by the University of Warwick (England) for J. Bennett [12]. It contains sixteen delta-layers (MD16). We call it "sample Bennett".

Fig. 2 shows the evolution of the deconvoluted profile of the sample MD16 depending on the number of iterations (n = 200, n = 1000 and n = 10000). In particular, we have chosen to follow up the evolution of the deconvoluted profile of this sample for two reasons. The first reason is that the structure of this sample is complicated (five peaks spaced of 50 Å followed by nine peaks spaced of 150 Å, and after 100 Å we have two peaks spaced of 50 Å). The second reason is that the relatively high thickness of this sample and the number of delta - layers reflects the ability of the deconvolution algorithm to recover shape and signal dynamics of large and condensed structures. Evidently, the deconvolution of a thin sample containing a single delta-layer is easier and simpler than a thick and complicated structure. It should be also noted that the last two peaks allow us to see the limit of separation (contrast) that can achieve this algorithm.

To note that the separation limit is another criterion for evaluation of the depth resolution, i.e., the separation between two peaks which have been joined by the measure.

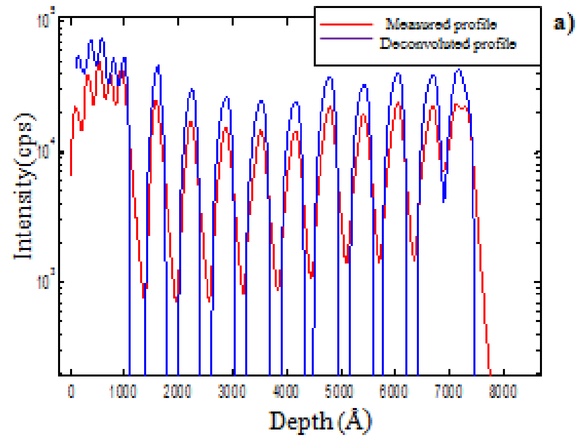

Fig. 2 (a) Evolution of the deconvoluted profile depending on the number of iterations n (n=200)

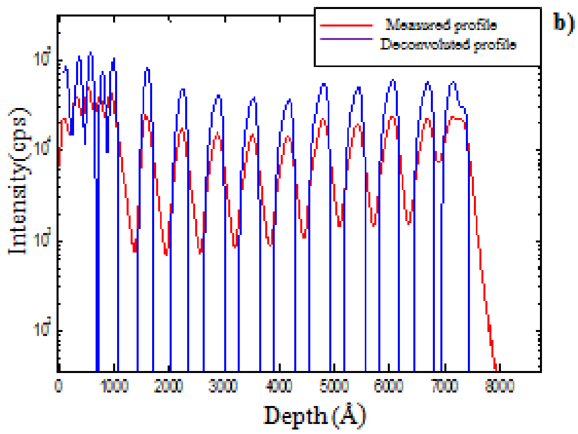

Fig. 2 (b) Evolution of the deconvoluted profile depending on the number of iterations n (n=1000)

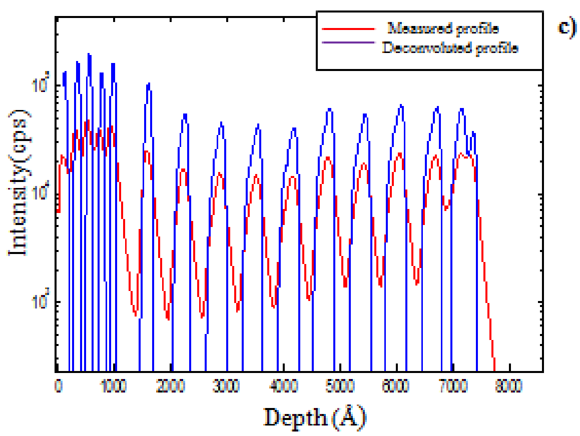

Fig. 2 (c) Evolution of the deconvoluted profile depending on the number of iterations n (n=10000)

Like the sample MD5, the deconvolution of the sample MD16 gives also a great improvement of the depth resolution and recovery of the original signal shape. The exponential slopes are completely removed giving symmetrical and well separated peaks. In particular, when observing the evolution of the deconvoluted profile depending on the number of iterations, we find that the quality of the deconvoluted profiles is improved significantly, this is characterized especially on the deconvolution of the last two peaks, which are well separated whose contrast exceeds 70 % (see Fig. 2 (c)). Obviously, in iterative algorithms the number of iterations plays an important role for the quality of the solution. Actually, a compromise has been made between the iterations number and the quality of the obtained peaks.

The obtained depth resolution gain is 1.8, so that the amplitude gain is 1.7. The values of these gains are relatively low, this is due to firstly, the good quality measurement at low energy and secondly the width of the delta – layers which are near to Gaussian form than the delta-layers. We note that the first delta- layer, which is buried at a depth of 50Å, should not be taken into account, because at this energy, it is still at the limit of the transient regime of the analysis. The advantage of deconvolution of this sample is the total absence of artifacts and oscillations in bottom of deconvoluted peaks despite the complicated structure which contains high concentrations gradient and noise.

IV. Conclusion

Physical limits reached by SIMS analysis makes difficult to envisage further technical improvements of the equipment without the cost becomes prohibitive. That’s why; the digital processing techniques such as deconvolution remain an effective way to achieve the ultimate depth resolution. This is a delicate operation should not be implemented without caution. It is necessary to control the process of restitution and to understand the different physical mechanisms, otherwise one obtains aberrant results. It is important to note that in the case of SIMS analysis, physical coherence is a paramount aspect, the deconvoluted profile must be physically acceptable. Thus, it is important to adopt a method whose result must be acceptable; otherwise the obtained result is mathematically right but with no connection with the physical reality. Also, the number of iterations is an important parameter to be taken into account in such iterative technique. An objective deconvolution leads to a good gain and good shape recovery without artifacts and oscillation. The greatest danger of deconvolution is to achieve a dazzling and brilliant result without ensuring that is accurate and it is not real and does not match the original profile.

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