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Signal Processing of Secondary Ion Mass Spectrometry Profiles. New Algorithm for Enhancement of Depth Resolution

[1]Nadia Dahraoui, [2]M'Hamed Boulakroune and [3]Djamel Benatia

[1,3]Electronics Department, Faculty of Engineer Sciences, University Hadj Lakhdar of Batna, Batna, Algeria
[1]nadiaelectro@gmail.com
[2]Electronics and Communication Department, Faculty of New Technologies of Information and Communication, University Kasdi Merbah of Ouargla, Ouargla, Algeria

Abstract

The aim of this work is signal processing of Secondary Ions Mass Spectrometry (SIMS) profiles for improving the depth resolution beyond its physical and instrumental limits. Indeed, we propose a new iterative deconvolution algorithm based on Tikhonov-Miller regularization where a priori model of solution is included. The latter is a denoisy and pre-deconvoluted signal obtained by wavelets shrinkage algorithm. It is shown that this new algorithm gives best results without artifacts and oscillations related to noise. This leads to a significant improvement of the depth resolution and peaks' maximums. The SIMS profiles are obtained by analysis of delta layers of boron in a silicon matrix using Cameca-Ims6f instrument at oblique incidence. In the light of the obtained results, the advantages and limitations of this new method as well as suggestions for future work are presented and discussed.

Keywords: *We multiresolution deconvolution, wavelet schrinkage, multilayers, SIMS, in-depth resolution*

1. Introduction

Secondary ion 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 [1-4].

Developments of SIMS analysis are not as pronounced and rapid than those of the manufacturing techniques of materials in microelectronics technology. For progressing in this domain, it is important to go beyond the experimental results by including a post-erosion digital processing. This treatment, called deconvolution, leads to a good approach to the original profile from the experimental one and the system response.

Actually, the deconvolution of depth profiling 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).

The different monoresolution deconvolution methods proposed in the SIMS field showed a certain disability to 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. Indeed, in image processing field Barakat *et al.* [5] proposed a restoration method based on Tikhonov-Miller regularization with an introduced *a priori* model of solution. In SIMS framework Mancina *et al.* [6] proposed an iterative constrained algorithm, based on Barakat algorithm, in which the model of solution is a pre-deconvoluted 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 related to 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 [2]. Denoising with the sole purpose of extracting desired information from measured data has proven to be a crucial preliminarily steps in any analytical method.

Noise reduction, as an integral part of signal estimation, has been studied for many years with practical applications. In this context, Morlet [7] proposed a powerful tool for data analysis: the wavelet theory. Indeed, in the last decade, interest in wavelets has grown at an exponential rate. Donoho and Johnstone [8] offered a method for reconstructing an unknown signal from noisy data. They employed thresholding in wavelet domain and showed it to be asymptotically near optimal for a wide class of signals corrupted by additive white Gaussian noise.

The aim of this work is to present an extension of Mancina algorithm [6]. Indeed, in the proposed algorithm the model of solution is a denoisy signal obtained by wavelet shrinkage and without application of any constraint operator. By denoising *a priori* of SIMS signal, the noise energy is then limited, only details which are greater than the shrinkage threshold are preserved. Thus, the contributions of high-frequency noise are removed to a great extent of the SIMS profiles.

This work is based on SIMS data, for which reason the results presented here are largely restricted to the conditions of SIMS. The case of multilayer boron-doped silicon, analyzed using Cameca-*Ims6f* at oblique incidence, is then considered.

2. Tikhonov-Miller regularization

The Tikhono-Miller regularization is achieved through a compromise between choosing a solution that both leads to a reconstructed signal close to the measured data and conform to some prior knowledge of the original signal [2, 4-6]. This means that the solution $\boldsymbol{x}$ is considered to be close to the data if the reconstruction signal $\boldsymbol{Hx}$ is close to the measured one $\boldsymbol{y}$, *i.e.* if $\|\boldsymbol{y}-\boldsymbol{Hx}\|^2$ is reasonably small. Where $\boldsymbol{H}$ is Toeplitz matrix constructed from the pulse response of the system $h(z)$.

The first task of deconvolution procedure is to minimize the quadratic distance between $\boldsymbol{y}$ and $\boldsymbol{Hx}$. Unfortunately; solutions that lead to very small values of $\|\boldsymbol{y}-\boldsymbol{Hx}\|^2$ are oscillating and unacceptable. In order to get a stable solution, one must choose another criterion that checks whether the solution conforms to what must be expected from the solution of the deconvolution problem: it must be physically accepted, i.e. a smoothed solution. The smoothness of the solution can be described by its regularity r^2, defined as

$$\|\boldsymbol{Dx}\|^2 \leq \boldsymbol{r}^2, \tag{1}$$

$\boldsymbol{D}$ is a stabilizing operator. The choice of $\boldsymbol{D}$ is based on the processing context and some a priori knowledge about the original signal. Indeed, $\boldsymbol{D}$ is usually designed to smooth the estimated signal, and then a gradient or a discrete Laplacien is conventionally chosen. Its spectrum is a high-pass filter [2, 9], this results in the minimisation of the quadratic functional proposed by Tikhonov:

$$\tilde{\boldsymbol{x}} = \arg\min(\|\boldsymbol{y}-\boldsymbol{H}\tilde{\boldsymbol{x}}\|^2 + \alpha(\|\boldsymbol{D}\tilde{\boldsymbol{x}}\|^2 - \mathrm{r}^2)), \tag{2}$$

where α is the regularization parameter and ‘argmin’ denotes the argument that minimizes the expression between brackets. Perfect fidelity to the data is achieved for α = 0, whereas perfect matching with *a priori* knowledge is achieved for α = ∞. It is therefore necessary

to find optimum α and, hence, such smoothing factor at which the solution of (2) is well-stabilized and still close to the actual distribution. This regularization parameter α can be estimated by a variety of techniques [2, 5, 6, 9]. In simulation where the regularity of the solution is known, $\alpha = \boldsymbol{n}^2/\boldsymbol{r}^2$, where $\boldsymbol{n}^2$ is a higher bound for the total power of the noise. Unfortunately, in the real case, there is no access to the regularity of the real profile, but it can be estimated by means of the generalized cross-validation [2] which is well applied for Gaussian white noise.
The regularized solution takes the following form:

$$\tilde{\boldsymbol{x}} = (\boldsymbol{H}^T \boldsymbol{H} + \alpha \boldsymbol{D}^T \boldsymbol{D})^{-1} \boldsymbol{H}^T \boldsymbol{y} = (\boldsymbol{H}^+)^{-1} \boldsymbol{H}^T \boldsymbol{y}, \quad (3)$$

with $\boldsymbol{H}^+ = \boldsymbol{H}^T \boldsymbol{H} + \alpha \boldsymbol{D}^T \boldsymbol{D}$.

The matrix $\boldsymbol{H}$ characterizing the deconvolution process before regularization is replaced by the generalized matrix $\boldsymbol{H}^+ = (\boldsymbol{H}^T\boldsymbol{H} + \alpha\boldsymbol{D}^T\boldsymbol{D})$ more conditioned. That is carried out by the modification of the eigenvalues of the system $\boldsymbol{H}$, thus the system becomes more stable. Figure 1 shows the spectra of the DRF (Depth Resolution Function: $\boldsymbol{H}$), the filter $\boldsymbol{D}$ and the generalized matrix $\boldsymbol{H}^+$.

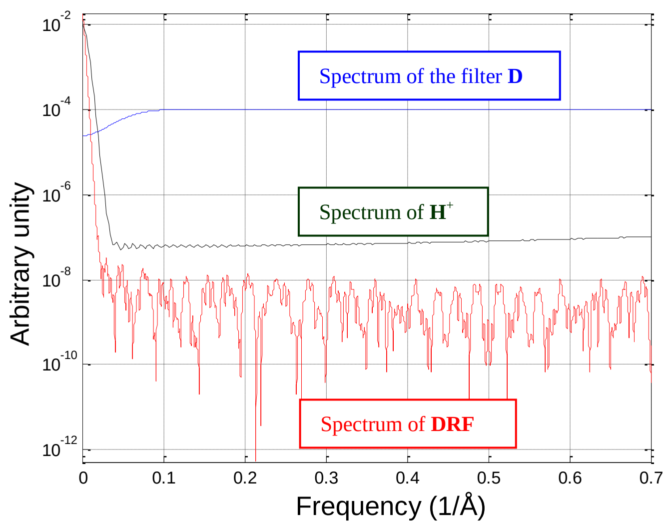


Figure 1. Spectra of: DRF (*H*), filter *D* and the generalized matrix *H*$^+$. Here the regularization parameter α is overestimated, which leads to well-conditioned *H*$^+$.

The choice of the regularization operator $\boldsymbol{D}$ should not constitute a difficulty since the rule on the modification of the eigenvalues is respected. The more determining choice for the reconstruction quality will be that of the regularization parameter α. Indeed, the bad calculation of this parameter leads to the evil conditioning of the matrix $\boldsymbol{H}$, consequently the solution will be degenerated.

The regularization can guarantee the unicity and stability of the solution but cannot lead to a very satisfactory result. The quantity of information brought is not sufficient to obtain a solution close to the ideal one, because this regularization provides global proprieties of the signal.

Barakat *et al.* [5] proposed a method based on Tikhonov regularization, combined with an *a priori* model of the solution. The idea of such model is to introduce local characteristics of the signal. This model may contain discontinuities whose locations and amplitudes are imposed. The new functional to be minimized with respect to $\boldsymbol{x}$, is defined as follows:

$$\mathrm{L} = \left\| \boldsymbol{y} - \boldsymbol{H}\tilde{\boldsymbol{x}} \right\|^2 + \alpha \left\| \boldsymbol{D}(\tilde{\boldsymbol{x}} - \boldsymbol{x}_{\mathrm{mod}}) \right\|^2, \quad (4)$$

where $\boldsymbol{x}_{\text{mod}}$ is an *a priori* model of the solution. The solution is given by:

$$\tilde{\boldsymbol{x}} = (\boldsymbol{H}^T\boldsymbol{H} + \alpha\boldsymbol{D}^T\boldsymbol{D})^{-1}(\boldsymbol{H}^T\boldsymbol{y} + \alpha\boldsymbol{D}^T\boldsymbol{D}\boldsymbol{x}_{\text{mod}}). \tag{5}$$

The strategy developed here is useful if the *a priori* information is quite precise and the quality of solution depends on the accuracy of *a priori* information.

Mancina *et al.* [6] proposed to reiterate the algorithm of Barakat *et al.* [5] and to use as model of solution a pre-deconvoluted signal (intermediate solution between the ideal solution *i.e.* the input signal and the measured one) with a sufficient regularization. The mathematic formulation of Mancina approach in Fourier space is as follows:

$$\begin{cases} \hat{\boldsymbol{X}}_{\boldsymbol{n}+1} = \dfrac{\boldsymbol{H}^*\boldsymbol{Y} + \alpha|\boldsymbol{D}|^2\boldsymbol{X}_{\text{mod}_n}}{|\boldsymbol{H}|^2 + \alpha|\boldsymbol{D}|^2} \\ \boldsymbol{X}_{\text{mod}_n} = \boldsymbol{TF}[\boldsymbol{C}\hat{\boldsymbol{x}}_{\boldsymbol{n}}] \\ \hat{\boldsymbol{x}}_{\boldsymbol{n}} = \boldsymbol{TF}^{-1}[\hat{\boldsymbol{X}}_{\boldsymbol{n}}] \\ \boldsymbol{X}_{\text{mod}_0} = 0 \end{cases} \tag{6}$$

Where $\boldsymbol{H}^*$ is the conjugate of $\boldsymbol{H}$ and $\boldsymbol{C}$ represents the constraint operator which must be applied in the time domain after an inverse Fourier transformation.

The accuracy of the solution is referred to the accuracy of the model which suggests a reasonable formulation. It is obvious that an important lack of precision in the *a priori* model leads to an error restoration more important than the usual one without model. Moreover, if the pre-deconvoluted signal is a noisy signal (which is the case of SIMS signal) or contains aberrations, the iterative process worsen these aberrations and the result is an oscillatory signal. This is a limitation of Mancina algorithm.

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 remove noise components from the signal. The tool more adapted to this mission is denoising by wavelets. Indeed, wavelet transformation has been a key technique in signal processing applications due to its capability of space frequency localization and provides a temporal (or spatial) resolution of the frequency information. This makes it an ideal tool to capture patterns at all relevant frequency scales as well as to denoise signals [8]. The following section addresses the wavelets transformation theory.

3. Discreet Wavelet Transform

3.1. Background

Nowadays, wavelet theory is developed into a methodology used in many disciplines. Wavelets also provide a rich source of useful tools for applications in many time-scale problems. The attention of wavelets was more attracted when Mallat [10] established a connection between wavelets and signal processing. Discrete Wavelet Transform (DWT) is an extremely fast algorithm that transforms a data into wavelet coefficients at discrete intervals of time and scale, instead of at all scales. It is based on dyadic scaling and translating and is possible if the scale parameter varies only along the dyadic sequence (dyadic scales and positions). It is basically a filtering procedure that separates high and low frequencies components of profiles measurements with high-pass and low-pass filters by multiresolution decomposition algorithm [10]. Hence, the DWT is represented by the following equation:

$$\boldsymbol{W}(\boldsymbol{j},\boldsymbol{k}) = \sum_{\boldsymbol{j}}\sum_{\boldsymbol{k}} \boldsymbol{y}(\boldsymbol{k})2^{-\frac{j}{2}}\psi(2^{-\boldsymbol{j}}\boldsymbol{n} - \boldsymbol{k}), \tag{7}$$

where $\boldsymbol{y}$ is descretized heights of the original profile measurements, ψ is discrete wavelet coefficients and n is a sample number. The translation parameter determines the location of the wavelet in the time domain, while the dilatation parameter determines the location in the frequency domain as well as the scale or the extent of the space-frequency localization.

DWT analysis can be performed using a fast, pyramidal algorithm by iteratively applying low-pass and high-pass filters, and subsequent down-sampling by 2 [10]. Each level of the decomposition algorithm then yields low-frequency components of the signal (approximations) and high-frequency components (details). This is computed by the equations

$$\boldsymbol{y}_{low}[\boldsymbol{k}]=\sum_{n}\boldsymbol{y}[\boldsymbol{n}]\,\boldsymbol{f}[2\boldsymbol{k}-\boldsymbol{n}], \tag{8}$$

$$\boldsymbol{y}_{high}[\boldsymbol{k}]=\sum_{n}\boldsymbol{y}[\boldsymbol{n}]\boldsymbol{g}[2\boldsymbol{k}-\boldsymbol{n}], \tag{9}$$

where $\boldsymbol{y}_{low}[k]$ and $\boldsymbol{y}_{high}[k]$ are the outputs of the low-pass (***f***) and high-pass (***g***) filters, respectively, after down sampling by 2. Due to the down-sampling during decomposition, the number of resulting wavelet coefficients (*i.e.,* approximations and details) at each level is exactly the same as the number of input points for this level. It is sufficient to keep all detail coefficients and the final approximation coefficient (at the coarsest level) in order to be able to reconstruct the original data.

In the matrix formalism, (8) and (9) can be written (the approximation and details at the resolution $2^{-(j+1)}$ are obtained from the approximation signal at the resolution 2^{-j}) as

$$\boldsymbol{y}_{a}^{(j+1)}=\boldsymbol{F}\ \boldsymbol{y}_{a}^{(j)},\ \ \boldsymbol{y}_{d}^{(j+1)}=\boldsymbol{G}\ \boldsymbol{y}_{a}^{(j)}, \tag{10}$$

where ***F*** and ***G*** are matrixes Toeplitz constructed from the filters ***f*** and ***g***, respectively.
The reconstruction algorithm then involves up-sampling (*i.e.* inserting zeros between data points) and filtering with dual filters. By carefully choosing filters for the decomposition and reconstruction phases that are closely related, one can achieve perfect reconstruction of the original signal in the inverse orthogonal wavelet transform [10].
The reconstructed signal is obtained from (10) by:

$$\tilde{\boldsymbol{y}}=\tilde{\boldsymbol{F}}\boldsymbol{y}_{a}^{(j)}+\tilde{\boldsymbol{G}}\boldsymbol{y}_{d}^{(j)}, \tag{11}$$

where $\tilde{\boldsymbol{F}}$ and $\tilde{\boldsymbol{G}}$ are Toeplitz matrixes constructed from the reconstruction filters $\tilde{f}$ and $\tilde{g}$, respectively.

The Mallat [10] algorithm is fast, linear operation that operates on a data vector whose length is an integer power of two, transforming it into numerically different vector of the same length. Many wavelet families are available. However only orthogonal wavelets (such as Haar, Daubichies, Coiflet and Symmlet wavelets) allow for perfect reconstruction of a signal by inverse discrete wavelet transform [7], *i.e.* the inverse transform is simply the transpose of the transform. Indeed, the selection of the most appropriate wavelet is based on the similarity between the derivatives of the signal and the number of wavelet vanishing moments. In practice wavelets with higher number of vanishing moments give higher coefficients and more stable performances. This study will be restricted to Symmlet, after some experimentation we have chosen "*Sym8*" wavelet with four vanishing moments. The following section addresses denoising of signals via wavelets shrinkage.

3.2. Denoising via Wavelet Shrinkage

In the wavelet decomposition of signals, as it is described in the previous section, the filter ***f*** is an averaging or smoothing filter (low-pass filter), while its mirror counterpart ***g*** produces details (high-pass filter) [10]. Since the signal will tend to dominate the low-frequency components it is expected that the majority of high-frequency components above a certain level are due to noise. With the exclusion of the last remaining smoothed components (usually one or two) all wavelet coefficients in the final decomposition corresponds to details. If the absolute value of a detail component is small and if we omit it (set it to zero) the general signal would not change much. Therefore, the thresholding of the wavelet coefficients is a good way of removing unimportant or undesired details from a signal and denoising it. Thresholding techniques are successfully used in numerous data processing domains, since in most cases a small number of wavelet coefficients with large amplitudes preserve most of the information about the original data set. Wavelet denoising methods in general use two different approaches: hard thresholding and soft thresholding. The hard thresholding philosophy is simply to cut all the wavelet coefficients below a certain threshold to zero. The soft thresholding reduces the value (referred to as 'shrinkage') of wavelet coefficients toward zero if they are below a certain value. For a certain wavelet coefficient *k* at scale *j* we have:

$$\hat{y}_d(\boldsymbol{k}) = \boldsymbol{sign}\left|\left|y(\boldsymbol{k})\right| - \lambda\right|, \tag{12}$$

where $\hat{y}_d$ is thresholded detail coefficients, sign returns the sign of the wavelet coefficient and λ is the threshold value. In the case of a gaussian white noise (which is the kind of noise in SIMS analysis), Donoho and Johnstone [8] modelled this threshold by:

$$\lambda = \sigma\sqrt{2\log(\boldsymbol{N})}\ , \tag{13}$$

where N is the number of the observed data, σ the standard deviation of noise. This standard deviation, in the case of white and Gaussian noise, is estimated by:

$$\hat{\sigma} = \boldsymbol{median}\left(\left|\boldsymbol{cd}^1(\boldsymbol{k})\right|\right/0.6754\,, \tag{14}$$

where ***median*** $(\boldsymbol{cd}^1(\boldsymbol{k}))$ is the median value of details coefficients at the first level of decomposition, which is considered attributed to noise.

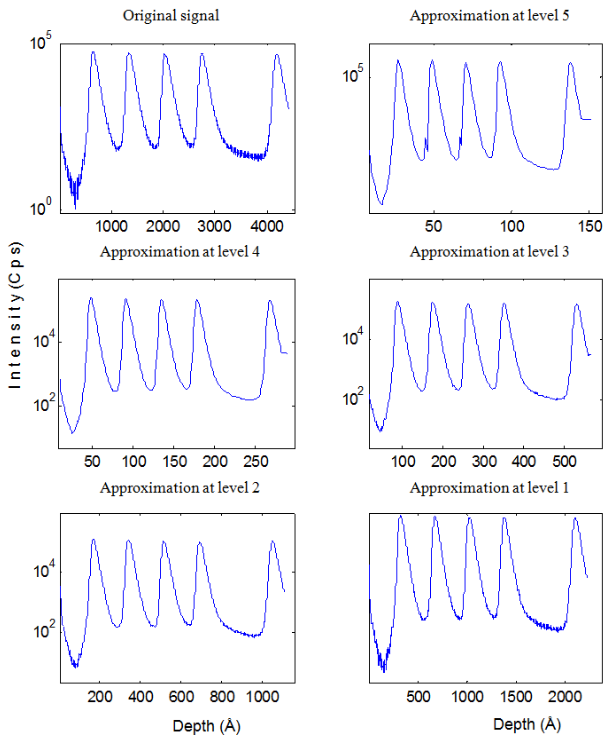
The reconstructed signal of (11) becomes after thresholding as follows:

$$\tilde{\boldsymbol{y}} = \tilde{\boldsymbol{F}}\boldsymbol{y}_a^{(j)} + \tilde{\boldsymbol{G}}\hat{\boldsymbol{y}}_d^{(j)}\ . \tag{15}$$

By this process, high-frequency components which (above a certain threshold) belong to noise can therefore be removed. It can be noted that the wavelet should be orthogonal. Then the noise in the approximation and detail signal remains white and Gaussian if the noise in the original is white and Gaussian.

The decomposition and denoising of MD5 sample (five delta layers of boron in silicon matrix) on a wavelet basis are illustrated in Figure 2. The used wavelet is *Sym8*.

(a)



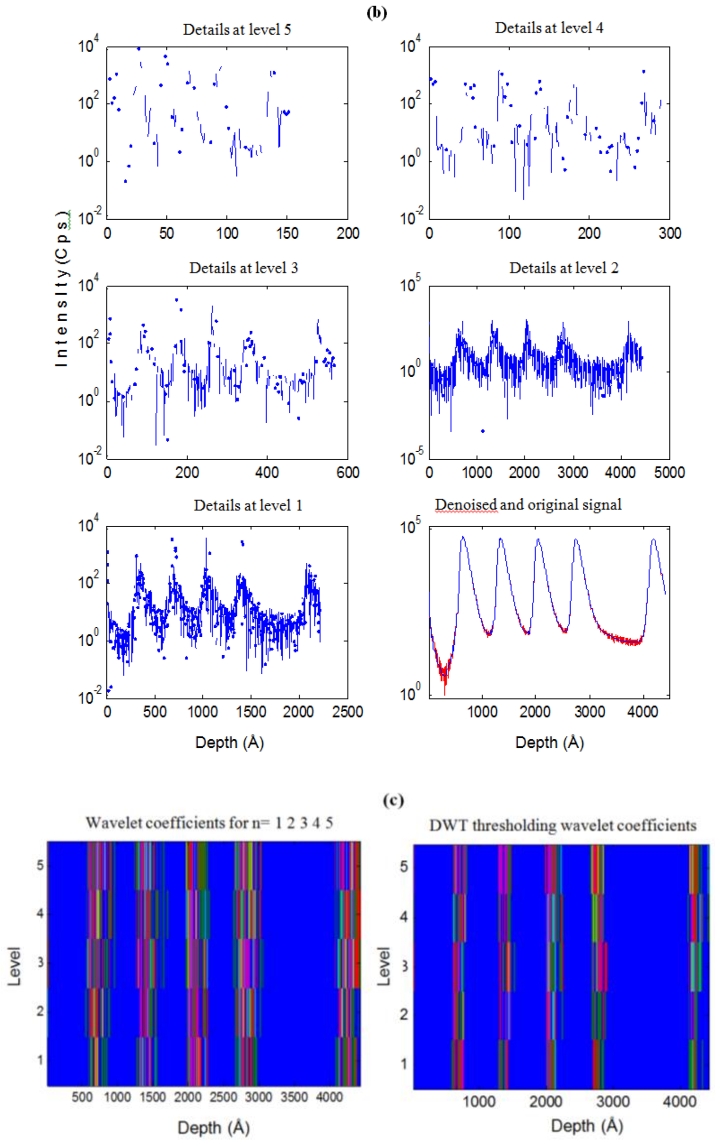


Figure 2. Wavelet decomposition of SIMS depth profile (8.5 keV / O_2^+, 38.1°), the used wavelet is *Sym8*; the decomposition level is 5. (a) The original measured profile with different approximation signals from level 1 to 5. (b) Details signals from 1 to 5 with denoised signal superposed on original signal. (c) Absolute wavelet coefficients with thresholded coefficients

In approximations' graphs (see Figure 2-a), starting from *a*1 and looking back to the level decomposition such that the approximation is a good candidate to be good estimator of the original signal. Thus, levels 4 and 5 are very good candidates for the useful signal.

Now look at the details (see Figure 2-b). Detail *d*1 is entirely composed by noise. *d*2 to *d*5 details have strong values concentrated in the abscissa corresponding to the positions of deltas - layers. We deduce that *d*4 and *d*5 details contain useful signal components versus uninformative noise. This phenomenon is also visible on the graph of the wavelet coefficients from level 5 to level 1.

The point that attracts all the attention here is the continuity between the denoised signal (deltas – layers) where it is supposed to be discontinuous. Classical denoising methods are incapable of such adaptation scale. Indeed, the approximation at level 5 is preserved as the noise is absent or much attenuated, complemented by the finest details clearly attributable to the useful signal. The thresholded wavelet coefficients give us an idea about the remaining details in the approximation (denoised signal) as part of the original signal (see Figure 2-c). These coefficients are concentrated in the area where the signal is very noisy (high frequencies), after thresholding there is only details which are higher than the specified threshold and likely to belong to the useful signal. The threshold obtained by the universal hard thresholding using the formula of Donoho and Johnstone [8] is $\lambda = 55.7831$ cps. The estimated noise level is SNR (signal to noise ratio) = 40.9212 dB.

4. The Proposed Algorithm

In the proposed algorithm, the idea is to introduce a model of solution which is a pre-decomposed signal on a wavelet basis. It is a denoised signal and reconstructed retaining only the approximation coefficients and details thresholded coefficients. In this approach, the model of solution is as follows:

$$X_{\text{mod}} = \boldsymbol{x}^{(j-1)} = \tilde{\boldsymbol{y}} = \tilde{\boldsymbol{F}}\boldsymbol{y}_{\boldsymbol{a}}^{(j)} + \tilde{\boldsymbol{G}}\hat{\boldsymbol{y}}_{\boldsymbol{d}}^{(j)}. \tag{16}$$

Hence, the proposed deconvolution scheme is constructed by the following steps:

1. Dyadic wavelet decomposition of the noisy signal at the resolution 2^{-j}.
2. Denoising of this signal by thresholding. One conserves only high-frequency components of details which are above the estimated threshold.
3. Reconstruction of the denoisy signal from the approximations and thresholded details using (15).
4. The obtained denoisy signal constitutes the model of solution in iterative Tikhonov-Miller regularization at the first iteration.

The mathematical formulation, in Fourier space, of this algorithm is as follows:

$$\begin{cases} \boldsymbol{X}_{\text{mod}_0} = \tilde{\boldsymbol{F}}\boldsymbol{y}_{\boldsymbol{a}}^{(j)} + \tilde{\boldsymbol{G}}\hat{\boldsymbol{y}}_{\boldsymbol{d}}^{(j)} \\ \hat{\boldsymbol{X}}_{\boldsymbol{n}+1} = \dfrac{\boldsymbol{H}^*\boldsymbol{Y} + \alpha\left|\boldsymbol{D}\right|^2 \boldsymbol{X}_{\text{mod}_n}}{\left|\boldsymbol{H}\right|^2 + \alpha\left|\boldsymbol{D}\right|^2}, \\ \boldsymbol{X}_{\text{mod}_n} = \hat{\boldsymbol{X}}_{\boldsymbol{n}+1} \end{cases} \tag{17}$$

It can be noted that denoising reduces the noise power in data; the regularization parameter should be evaluated by cross-validation in regards of the denoisy signal.

Since the noise is controlled by multiscale transforms, the regularization parameter does not have the same importance as in standard deconvolution methods. Clearly it will be lower than the one obtained without denoising.

5. Experimental

The profile we have chosen to process contains five delta-layers of boron in a silicon matrix (MD5). SIMS analysis was performed using Cameca-Ims6f magnetic sector instrument, corresponding to 8.5 keV / O_2^+ primary beam (38.1° incidence). The total sputter depth was determined from the crater measurements and the depth scale was established assuming a constant erosion rate. The DRF used in the deconvolution algorithm is taken from the first delta layer of the sample we deconvolve.

6. 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 the 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 in this type of samples.

The results of the deconvolution of multi delta-layers sample is illustrated in Figure 3. Indeed, the deconvolution of this sample gives a good improvement of the depth resolution and recovery of the original signal shape. Exponential slopes were completely removed giving symmetrical and well separated peaks. By comparison with the results of the deconvolution algorithm proposed by Gautier et al. [9], the profiles obtained by our approach are smooth and doesn't contain artifacts. The different gains of depth resolution and peaks maximum are summarized in Table1.

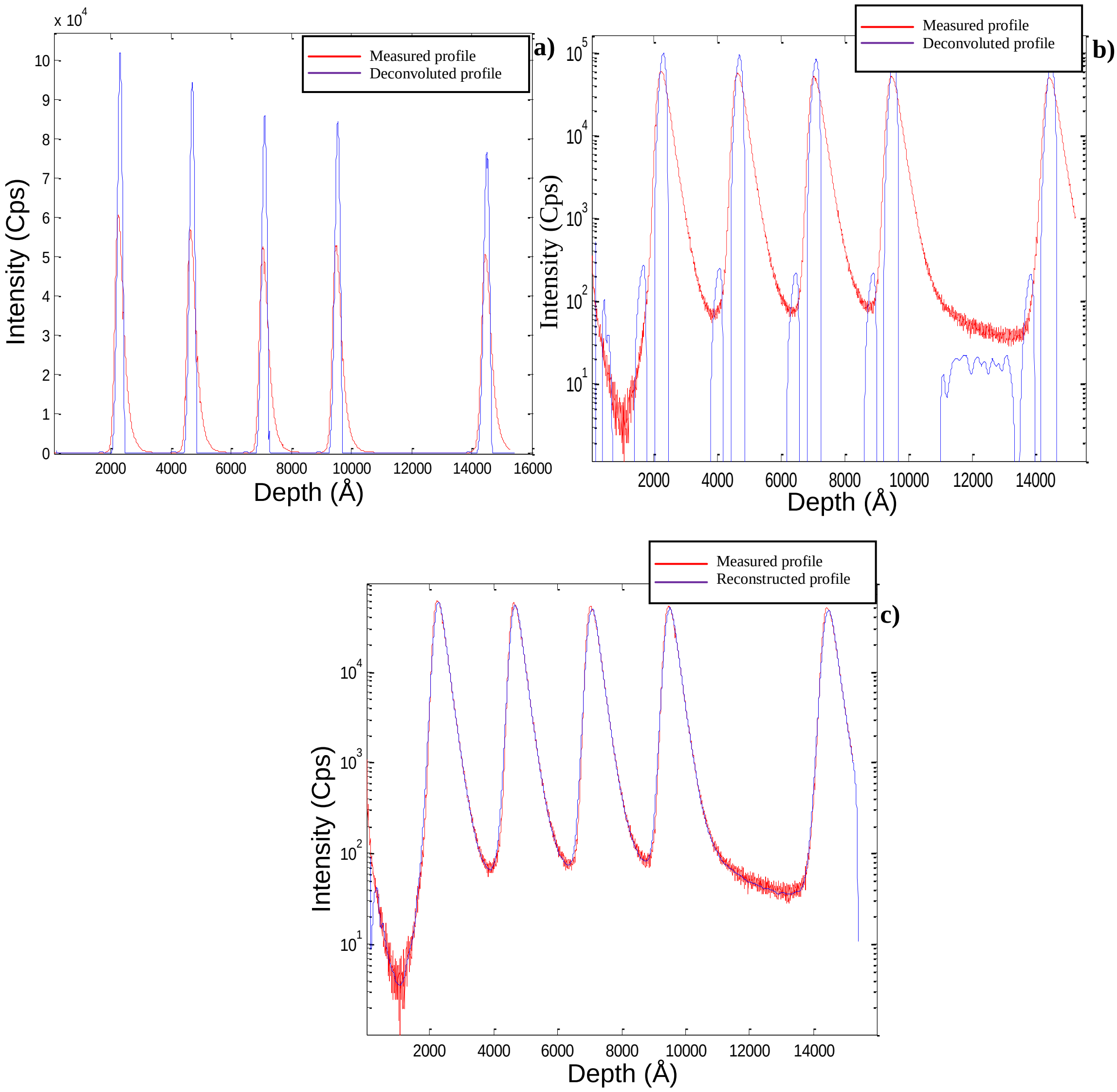


Figure 3. Results of deconvolution of SIMS profile containing five delta-layers of boron in silicon (8.5 keV / O_2^+, 38.1°). a) Linear scale plot. b) Logarithmic scale plot. c) Reconstruction of the measured profile from the deconvoluted profile and the DRF

Table 1. Summary of Gains of Depth Resolution and Peaks' Maximums 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

By observing the different values of gains, these results clearly show the good quality of the retrieval signal and good gains of depth resolution. Actually, the goal of the deconvolution procedure is to have a good gain of the depth resolution and good shape recovery of the entire signal without artifacts and oscillations and without ensuring that the solution is accurate! To eliminate these oscillations, Gautier et al. [9] 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 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 any more, 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.

In ref. [6], Mancina showed that artifacts are not always aberrations of the deconvolution; they can be structures with low concentrations. The interpretation of artifacts must be measured, especially if their amount is not negligible, in which case, one cannot eliminate them from the deconvoluted profiles. The greatest danger of deconvolution is to achieve a dazzling and brilliant result but it is not real and haven't no relationship with the original profile! In this context, a validation criterion of the deconvolution result is the reconstruction of the measured profile 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 one more the results are accurate. The reconstruction of the profiles is excellent, especially for high signal levels (see Figure 3-c). The differences between the measured profile and the reconstructed one are mainly at the junctions of concentration peaks, where the noise is dominant.

6. Conclusion

This paper proposes a new deconvoltion algorithm for the recovery of SIMS data, and hence, for the improvement of the depth resolution. In particular, deconvolution of delta layers is the most important depth profiling data deconvolution, since it gives not only the shape of the resolution function, but also the optimum data deconvolution conditions for a specific experimental setup. This algorithm can be characterized as a regularized wavelet transform, it combines ideas from Tikhonov Miller regularization, wavelet analysis and deconvolution algorithms in order to benefit from the advantages of each. Particularly, it shows how the denoising of wavelet coefficients plays an important role in the deconvolution procedure.

The results show that the SIMS profiles are recovered very satisfactory. The artifacts, which appear in almost all monoresolution deconvolution schemes, have been corrected.

In particular, the FWHM (Full Width at Half Maximum) of the deconvoluted peaks is equal to 10.46 nm, which corresponds to an improvement of the depth resolution by a factor around 1.75. The dynamic range is improved by a factor around 1.5 for almost peaks. Therefore, this new algorithm can push the limits of SIMS measurement towards its ultimate depth resolution.

The main advantage of this algorithm is the absence of oscillations with negative components which appear in almost monoresolution deconvolution results. The question for the SIMS user is to know whether these small peaks (oscillations) are to be considered as physical features or as deconvolution artifacts. In our opinion, the origin of these oscillations is the presence of strong local concentrations of the high frequencies of noise in the signal, and which cannot be correctly restored by a simple classical regularization.

This algorithm can be used in two-dimension applications and generally in many problems in science and engineering involving the recovery of an interest object from collected data. SIMS depth profiling is just one example thereof. Nevertheless, the major disadvantage of this approach is the longer computing time compared to monoresolution deconvolution methods. However, due to the increase of computer power during recent years, this disadvantage has become progressively less important.

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Authors

Nadia Dahraoui was born in El oued**,** Algeria, on February 22, 1986**,** She received her B.Sc and M. Sc.. Degree from the Department of Electronics and Communication University of Ouargla. Currently, she is a Ph. D. student in Electronics department, University of Batna. . Her research fields of interest are signal processing, Modeling, characterization techniques, Microwaves, etc.

M’Hamed Boulakroune was born in Constantine, Algeria, on January 28, 1971. He received his Ph.D. Degree in Electronics from the University of Batna, Algeria and UCL Belgium in 2008. He is currently associate Professor at the University of Ouargla, Algeria. His research concernsRF/Microwave circuits, Filters, DGSs behaviors, characterization of semiconductor materials, modeling, signal processing, improving the depth resolution of the SIMS technique, mono-resolution and multi-resolution deconvolution. Boulakroune is membership in the International SIMS Society, and the International Nanoscience Community and is a reviewer of several international journals and conferences.

Djamel Benatia was born in Constantine, Algeria, on January 19, 1967. He received his Ph.D. Degree in Electronics from the University of Constantine, Algeria in 1999. He is currently Professor at the University of Batna, Algeria. His research concernsRF/Microwave circuits, Filters, DGSs behaviors, mono-resolution and multi-resolution deconvolution, and satellite. Benatia is a reviewer of several international journals and conferences.