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New Deconvolution Technique to Improve the Depth Resolution in Secondary Ion Mass Spectrometry

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This paper presents an efficient method for recovery of SIMS signals from strongly noised blurred discrete data. This technique is based on Tikhonov-Miller regularization where a priori model of solution is included. The latter is a denoisy signal obtained using the Kalman filter. This is an interesting estimation method, but it can only be used when the system is described precisely.

By comparing the results of the proposed technique with those of the literature, our algorithm gives the best results without artifacts and oscillations related to noise and significant improvement of the depth resolution. While, the gain in FWHM is less improved than those obtained by the wavelet technique. Therefore, this new algorithm can push the limits of SIMS measurements towards its ultimate resolution.

Keywords: Kalman filter, Denoising techniques, SIMS depth profiles, Wavelet shrinkage, Tikhonov-Miller regularization, Depth resolution.

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1. INTRODUCTION

Continuous developments in manufacturing technologies for microelectronic components imposes new requirements for analysis techniques in-depth. In this context, secondary ions mass spectrometry, SIMS, is classified at the front range of techniques of characterization in-depth, because of its ability to detect all elements, high sensitivity, large dynamic range and depth resolution. It is an effective and powerful technique for analyzing almost any non-volatile material and for characterizing very large and very thin structures [1-4]. Despite the considerable improvements carried out on SIMS technique, development of SIMS analysis is not as pronounced and rapid than that of manufacturing techniques of materials. The depth resolution in SIMS analysis remains limited to meet the challenge imposed by modern microelectronics. It is therefore necessary to explore other ways to help the depth resolution to cross its instrumental and physical limitations so that it is synchronized with the needs of modern microelectronic technologies. The most used way to achieve this object is the signal processing. A prototype of this kind of signal processing is the deconvolution procedure. This is to go back to a better approach of the actual profile from the experimental profile.

Deconvolution is a required operation in many signal processing applications such as system identification, spectroscopy, seismic processing, image deblurring, to name a few. This is an active area of research with many publications [2]. No universal algorithm has been developed so far. The reason lies in a diversity of applications and in the intrinsic ill-posedness of the problem [5-8].

The deconvolution of depth profiling data in SIMS analysis amounts to the solution of an appropriate ill-posed problem in that any random noise in data leads to no unique and no stable solution (oscillatory signal with negative components, which are physically not acceptable in SIMS analysis). Thus, the results must be regularized.

The removal of noise and restoration of signals has been one of the most interesting researches in the field of signal processing during the last years. Our algorithm is an iterative algorithm, which is based on Tikhonov-Miller regularization and a model of solution. This latter is a denoised signal using Kalman filter, we are interested in the idea of denoising the signal from the measure, as a first step of treatment before applying other techniques of digital signal processing.

2. EXPERIMENTAL

2.1 SIMS System

The equation characterizing the SIMS system is as follows:

$$y_n(t) = h(t) * x(t) + n(t) = y(t) + n(t), \quad (1)$$

where $y_n(t)$ is the noised output signal, $h(t)$ is the impulse response, $x(t)$ is the input signal and $n(t)$ is the noise.

In the Fourier space, this equation becomes

$$Y_n(f) = H(f).X(f) + N(f) = Y(f) + N(f). \quad (2)$$

Dividing the two members of this equation by $H(f)$, we obtain

$$\tilde{X}(f) = X(f) + \frac{N(f)}{H(f)}, \quad (3)$$

$\tilde{X}(f)$ is an estimate of $X(f)$ obtained by dividing $Y_n(f)$ by $H(f)$. The noise takes on all its importance in this equation; $\tilde{X}(f)$ is composed of the real profile $X(f)$ plus the noise $N(f)$ strongly amplified by the term $H^{-1}(f)$. Therefore, $\tilde{X}(f)$ has a "saturated" noise spectrum at high frequencies and its image $\tilde{x}(t)$ in the time domain is highly oscillatory and unstable signal.

Unfortunately, a signal is corrupted by various factors which produce a noise during acquisition or transmission. These noisy effects decrease the performance of visual and computerized analysis. It is clear that the suppression of noise from the signal makes the processing easier. The denoising process can be described as to remove the noise while retaining and not distorting the quality of processed signal or image. The traditional way of denoising to remove the noise from a signal or an image is to use a low or band pass filter with cut off frequencies. However, the traditional filtering techniques are able to remove a relevant of the noise but they are incapable if the noise is present in the band of the signal to analyze [9]. Therefore, many denoising techniques are proposed to overcome this problem [10-14].

2.2 Denoising Using the Kalman Filter

It is an infinite impulse response filter that estimates the states of a dynamic system from a series of incomplete or noisy measurements. Due to its effectiveness and efficiency, the Kalman filter is one of the most used algorithms in all areas of control systems. Many teaching and research have been presented in this area. It is a topic of discussion of different authors in several application fields [15-19].

The strength of this filter is its ability to predict parameters and rectify errors, not only of the sensors, but also of the model itself!

The operation of the Kalman filter can be divided into two stages:

- The first step is to predict the estimation according to the model of the system. To do this, the Kalman filter takes the previous estimate of the parameters and the error and predicts the new parameters and the new error as a function of the system modelling.
- The second step will update the prediction with the new measurements. These measurements, are noisy, will make it possible to obtain an estimation of the parameters and the error from the made prediction. If the model has any errors, this update step will correct them.

This study is based on the formula of the Kalman filter used in [21]. This filter can be applied to the signals of the following set:

$$\Sigma(\beta, L) = \begin{Bmatrix} k \text{ derivates exists}, \left(f^{(0)}, f^{(1)}, \dots, f^{(k)}\right) \\ f: \left|f^{(k)}(t_2) - f^{(k)}(t_1)\right| \le L|t_2 - t_1|^{\alpha}, \\ \forall\, t_1, t_2, \alpha \in (0,1]; \\ \beta = k + \alpha \end{Bmatrix} \quad (4)$$

This filter is of the following form:

$$\hat{F}^n(t_i) = \hat{F}^n(t_{i-1}) + \frac{1}{n}\alpha\hat{F}^n(t_{i-1}) + q_n\left(X_i - A\hat{F}^n(t_{i-1})\right) \quad (5)$$

In this study, we use the Kalman filter for $k = 0$.

2.3 Proposed Algorithm

The iterative methods make it possible to approach the desired solution by a series of iterations. Instead to apply the direct deconvolution of the measured profile, that is to say the inverse operation of the convolution, first of all, it must be denoised with a signal denoising technique (using the estimation by the Kalman filter), and then restore it (to retrieve the original profile based on the Tikhonov-Miller regularization). In our algorithm, the idea is to introduce a model of solution, which is a denoisy signal ($\hat{F}(t_i)$), using the Kalman filter.

This algorithm is iterative, its mathematical formulation, in the Fourier space, is the following:

$$\begin{cases} \hat{X}_{n+1} = \frac{H^{*}Y + \alpha|D|^2 X_{mod\,n}}{|H|^2 + \alpha|D|^2} \\ X_{mod\,0} = TF\left[\hat{F}(t_i)\right] \\ \hat{x}_n = TF^{-1}\left[\hat{X}_n\right] \end{cases} \quad (6)$$

3. RESULTS AND DISCUSSION

3.1 Denoising of SIMS Profiles

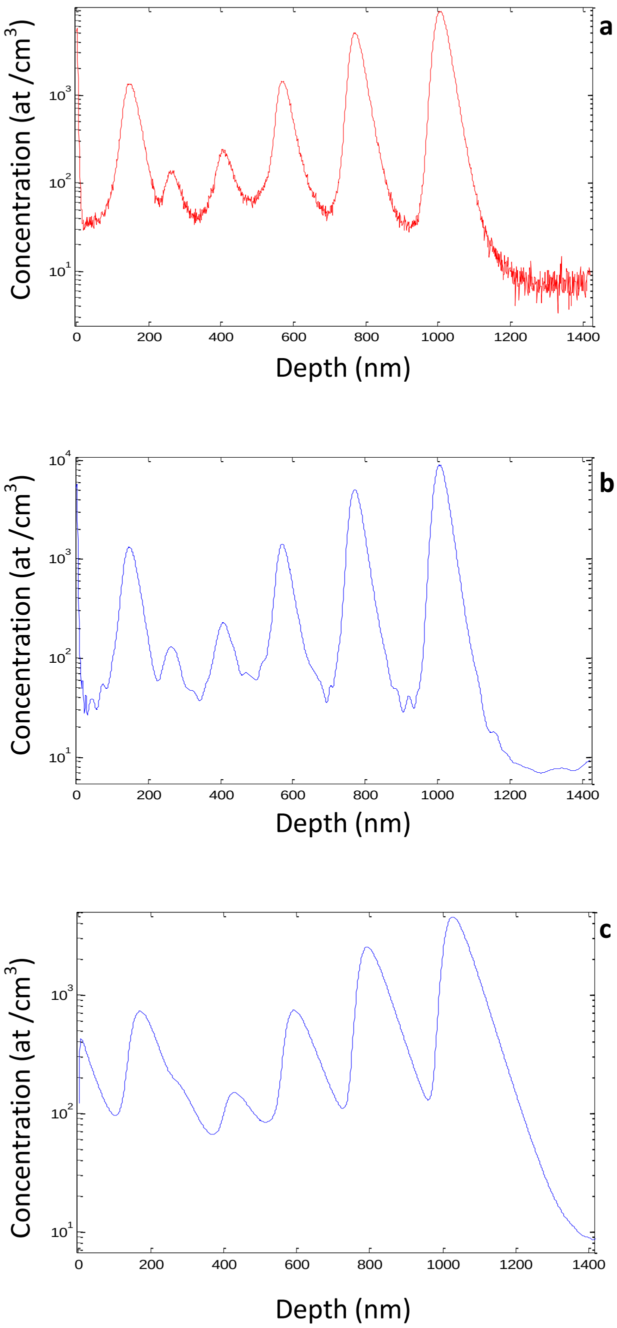

Fig. 1 – Results of denoising: (a) original signal, (b) denoised signal by wavelet shrinkage, (c) denoised signal by Kalman filter

In this section, the denoising of the sample MD6, which contains six delta layers of boron in silicon, using two techniques (wavelets and the Kalman filter), is presented.

The wavelet denoising techniques offers high quality and flexibility for the noise problem of signals and image. The wavelet transform (WT) is a powerful tool of signal and image processing that have been successfully used in many scientific fields such as signal processing, image compression, computer graphics, and pattern recognition [2, 20].

It results that the signal obtained using the wavelets follows the original profile by using this process; high-frequency components above a certain threshold can be removed. A raw SIMS profile and the corresponding denoisy profile are shown in Fig. 1. In particular, this figure shows that low-frequency components, which usually represent the main structure of the signal, are separated from high-frequency components. These preliminary results demonstrate the superior capabilities of the wavelet approach in SIMS profiles analysis rather than the traditional techniques.

In this section the study is qualitative. While, in the case of denoising by the Kalman filter, it is noted that the second peak has disappeared. An important limitation of such a method is that the Kalman filter makes it possible to take into account only a Gaussian noise model. The noise can generally be modeled by a Gaussian model, but in some cases, another type of noise is required (Poisson noise). This restriction limits the use of the Kalman filter.

3.2 Deconvolution of SIMS Profiles

The results of the deconvolution of the sample MD6 (six delta layer) in logarithmic scales is illustrated in Fig. 2.

The deconvolution of this sample gives a good improvement in depth resolution and recovery of the original signal shape. The exponential slopes have been completely removed giving well separated and symmetrical peaks. Compared with the results of the deconvolution by Gautier's algorithm [22], the profiles obtained by our approach are smooth and without artifacts which disturb the interpretation of the results obtained.

Gautier proposes to apply an empirical local confidence level deducted from the reconstruction error on deconvoluted profiles. The goal is to separate the parts of the original signal profile of those artificially generated by the inversion process (deconvolution artifacts). In our view, a confidence level, that allows to take into account certain parts of the signal and prevent others, does not provide any information on the quality of information and does not find a meaning in the case of a SIMS signal. One of advantages of SIMS analysis is the high dynamic signal that limits the deconvoluted signal to a dynamic, that does not exceed two decades, does not reflect the original signal and the filtered parts by the confidence level can provide valuable information on the analysed sample.

Mancina [23] showed that the artifacts are not always aberrations of the deconvolution, they may be structures but of low concentrations. An "artifact" that appears during deconvolution, can ultimately be an existing structure in the real profile, but it may be completely hidden during the measurement or a poor distribution of the dose due to the deconvolution method.

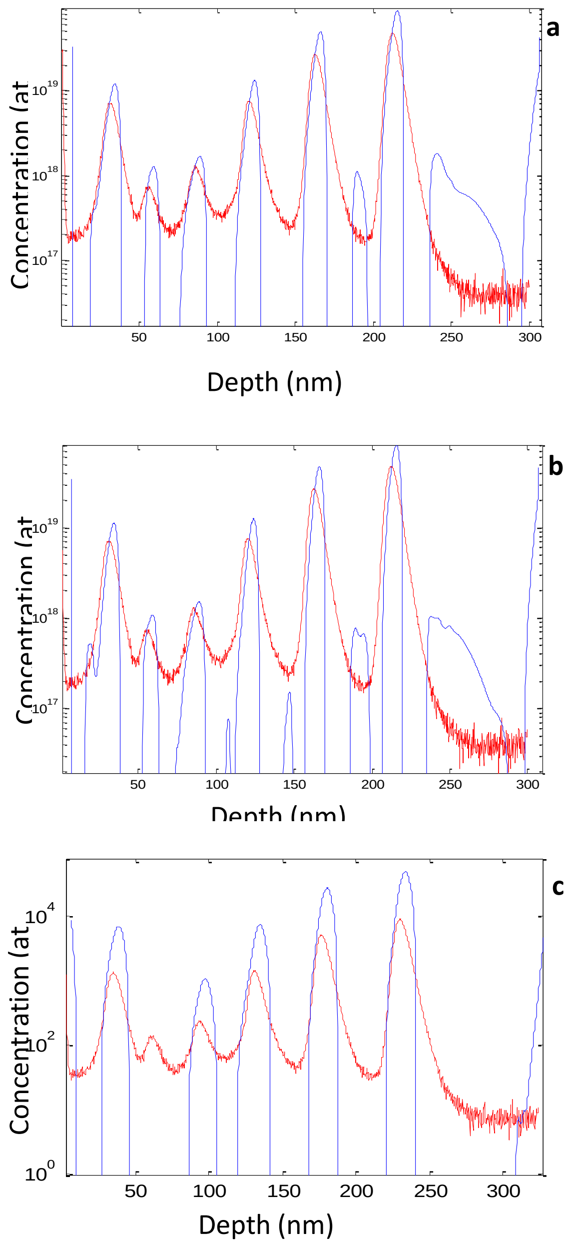

Fig. 2 – Results of deconvolution of MD6 sample of boron in silicon; (a) result of deconvolution using WT, (DRF1: $\lambda_d = 19.8$; $\lambda_u = 8.16$; $\sigma_g = 17.3$), (b) result of deconvolution using WT, (DRF2: $\lambda_d = 29.98$; $\lambda_u = 10.74$; $\sigma_g = 19.18$), (c) result of deconvolution using Kalman filter, (DRF2: $\lambda_d = 29.98$; $\lambda_u = 10.74$ and $\sigma_g = 19.18$)

The interpretation of the artifacts must be measured, especially if their dose is not negligible, and we cannot eliminate them from the profiles. Analysis of Mancina is very clear in our case, because we see the presence of a more pronounced peak between peaks 5 and 6 to a depth of 190 nm in both cases of deconvolution (see Fig. 1a). The question that arises here is what can be considered that this peak is an artifact?

The answer is clear: the fact that this small peak has not disappeared like other artifacts located in depths of 110 and 145 nm (see Fig. 1b) when changing the DRF, we can consider that this peak is not generated by the analysis but it is an intrinsic characteristic of the sample, so it is a full structure in which the concentration is not negligible, at 9.1018/cm³. The interpretation of the artifacts should be cautious, especially if their dose is not negligible. It is important to report that we cannot remove it automatically from the profiles.

In the case of the Kalman filter, one notices that the deconvolved profile is totally devoid of artifacts. In addition, the second peak does not appear. In a conventional estimation method (for example, the least squares method), a simple error in the modeling of the system leads to an error in the estimation. The strength of the Kalman filter is to integrate a term of inaccuracy on the model itself, which allows it to give correct estimates in spite of the modeling errors.

The strength of this filter is its ability to predict parameters and rectify errors, not only of the catch, but also of the model itself!

4. CONCLUSIONS

This work focused on the improvement of depth resolution in secondary ions mass spectrometry. In this context, an algorithm, based on Tikhonov-Miller regularization and a model of solution, has been developed and compared with others proposed in the literature.

In comparison, the results obtained by the Kalman filter are devoid of artifacts and oscillations. While, the gain in FWHM is less improved than those obtained by the wavelet technique. But the gain of peak's maximum is better, for example, in peak 6, the gain of maximum is 1.82 in the case of wavelet (Fig. 1a) but in the case of Kalman filter (Fig. 1c) the gain is 1.94.

The Kalman filter is therefore an interesting estimation method, but it can only be used when we can describe our system precisely. If it is impossible to find the modeling of the system, then it is preferable to turn to other methods (such as the Monté-Carlo method, for example, which is a statistical method, but which requires considerable computing power). Another important limitation of such a method is that the Kalman filter makes it possible to take into account only a Gaussian noise model. In general, the noise can be modeled in a Gaussian way, but in some cases, another type of noise is required (notably in image processing where Poisson sounds are frequently used). This restriction then limits the use of the Kalman filter.

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Нова технологія деконволюції для вдосконалення глибини різкості в мас-спектрометрії вторинних іонів

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У роботі запропоновано ефективний метод відновлення сигналів SIMS від сильно розмитих дискретних піків. Ця методика ґрунтується на регуляризації Тихонова-Міллера, де включена апріорна модель розв'язку. Останній – це шумопригнічуючий сигнал, отриманий при використанні фільтра Калмана. Це цікавий методом оцінки, але він може бути використаний тільки тоді, коли ми можемо точно описати наш зразок.

Порівнюючи результати запропонованої методики з результатами літератури, наш алгоритм дає найкращі результати без артефактів і коливань, пов'язаних з шумом, і значного поліпшення глибинного аналізу, у той час як коефіцієнт підсилення менш поліпшений, ніж коефіцієнт, отриманий методом вейвлетів. Таким чином, цей новий алгоритм може розширити межі вимірювань SIMS до граничної роздільної здатності.

Ключові слова: Фільтр Калмана, Техніка шумопригнічення, Глибинні профілі SIMS, Вейвлет-усадка, Регуляризація Тихонова-Міллера, Глибина різкості.