SIMS Deconvolution of Delta Layers in Silicon

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SIMS deconvolution of boron-nitride delta-doped multilayers has been successfully performed using the Cameca "SIMSDeconvol^{TM}" software. Two samples with the spacing of 5 nm and 18 nm of 0.05 nm thick delta layers have been used for the study. The depth profile of the 5 nm spacing multilayer has been deconvolved with the depth resolution function obtained by the first delta layer of the 18 nm spacing sample. Effects of various deconvolution parameters such as regularization parameter, number of iterations on the depth profile have been examined. Further investigations of SIMS deconvolution of boron implanted and arsenic delta-doped samples are needed using the method described in this work.

1. Introduction

The techniques of materials elaboration are nowadays able to produce thin and ultra-thin layers which thickness does not exceed one monolayer (ML). The SIMS analysis of such structures requires an optimal high depth resolution, the ultimate researched depth resolution limit being the atomic layer. Sputtering and internal atomic mixing irreversibly degrades the real depth profile, leading to broadening of thin peaks and inseparability of very close details of the profile. Instrumental improvements can be achieved by using very low primary energy. But a complementary way of improvement of depth resolution consists in processing the measured depth profiles with a numerical deconvolution procedure [1-3].

In this work, we used the Cameca "SIMSDeconvol^{TM}" software to investigate the deconvolution of boron-nitride delta layers in silicon samples. Effects of various deconvolution parameters such as regularization parameter, number of iterations and tolerance on the depth profiles will be discussed.

2. Experimental

Boron-nitride delta layers and silicon spacer layers were sputter-deposited alternately at NTT. We used two samples with the spacing of delta layers of 5 nm and 18 nm. The thickness of the boron-nitride delta layers was 0.05 nm, which corresponds to 0.15 ML. The structure of the boron-nitride delta-doped multilayers is Si / BN / Si / BN / Si / BN / Si / BN / Si / BN / Si / Substrate (Si). The sample has total five boron-nitride delta layers.

The SIMS depth profiling of the multilayers was performed using Cameca IMS 6f at Hyundai Hynix. The following experimental conditions were used for the depth profiling - Primary Ion:

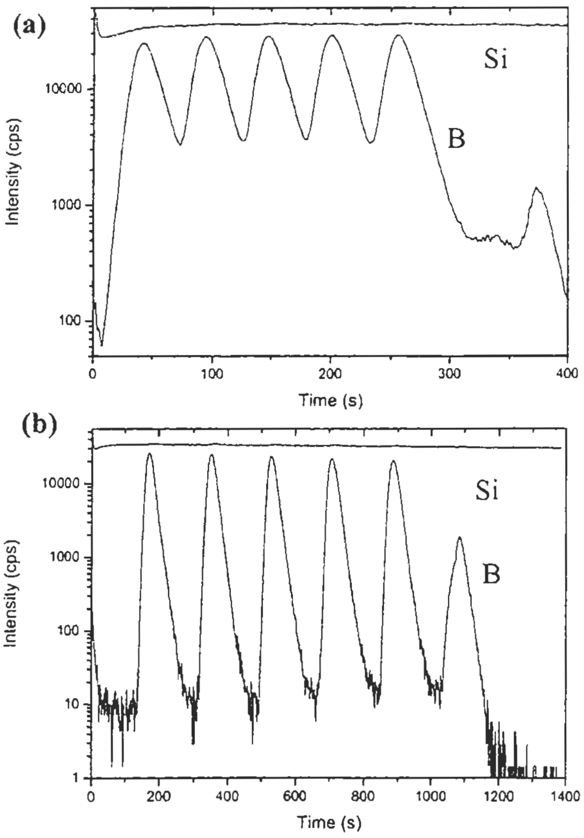

Fig. 1 SIMS depth profile of (a) 5 nm and (b) 18 nm spacing boron-nitride delta layers.

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O_2^+, Acceleration voltage: 2.01 kV, Raster Size: 200 μm, Sample bias: 1 kV, with oxygen flooding. So, the impact energy of the primary ion beam was 1.01 kV. The impact angle was 44.9°. Fig. 1 shows the SIMS depth profiles of (a) 5 nm and (b) 18 nm spacing boron-nitride delta layers.

3. Deconvolution Procedure

Determination of the depth resolution function (DRF) is the first important step in SIMS deconvolution procedure. The SIMS DRF completely characterizes the loss of depth resolution of any SIMS depth profile due to primary beam induced relocation of dopants in the target. The DRF is defined as the SIMS depth profile of a perfect delta layer containing dopant atoms located virtually at z=0 in an homogenous matrix and is usually noted as h(z) and normalized to the unit area.

Following the work of M. G. Dowsett et. al. [4], a semi-empirical analytical function is used for describing the response function measured in SIMS depth profile of an delta layer. The mathematical form of the DRF is the following :

$$h(z) = \frac{1}{2(\lambda_u + \lambda_d)} \times \left[\begin{array}{l} \exp\left(\frac{z - z_0}{\lambda_u} + \frac{\sigma_g{}^2}{2\lambda_u^2}\right)\left[1 - erf\left(\frac{z - z_0}{\sqrt{2}\,\sigma_g} + \frac{\sigma_g}{\sqrt{2}\,\lambda_u}\right)\right] + \\ \exp\left(\frac{-(z - z_0)}{\lambda_d} + \frac{\sigma_g{}^2}{2\lambda_d^2}\right)\left[1 + erf\left(\frac{z - z_0}{\sqrt{2}\,\sigma_g} - \frac{\sigma_g}{\sqrt{2}\,\lambda_d}\right)\right] \end{array} \right]$$

The analytical expression of the DRF is governed by four parameters: λ_u and λ_d represents the exponential growth and decay length of the DRF, respectively. σ_g represents the standard deviation of the convoluting Gaussian function encountered in the definition of the analytical form. z_0 represents the apparent position of the peak of the double exponential function.

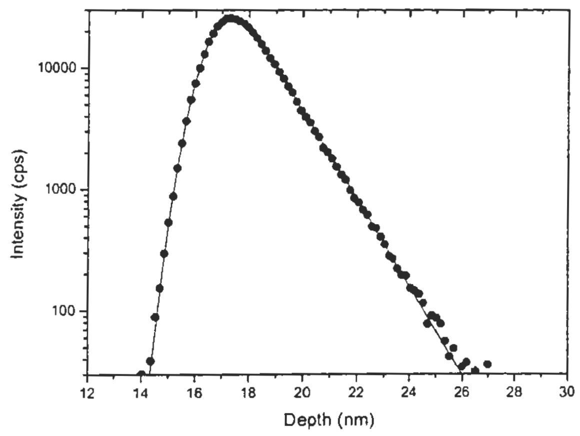

Fig. 2 Nonlinear curve fitting of the measured delta layer with the analytical DRF.

In order to get the four DRF parameters, fitting of the experimental data with the analytical DRF has to be performed, as can be seen in Fig. 2 representing the measurement of the first delta layer of the 18 nm spacing sample.

Among various commercial software, Origin 6.1 of Microcal™ has been used to extract the DRF parameters with a nonlinear least squares curve fitting: λ_u = 0.15 nm, λ_d = 1.20 nm, σ_g = 0.70 nm and z_0 = 16.8 nm.

The procedure of deconvolution of the Cameca "SIMSDeconvol™" software uses an iterative algorithm with hard constraints of positivity and Miller regularization, the parameter of the regularization being calculated by the generalized cross-validation. The deconvolved depth profile at the n^th^ iteration is computed by the following relation:

$$\mathbf{x}^{(n+1)} = \mathbf{C}\mathbf{x}^{n} + \left[\mathbf{H}^{T}\mathbf{y} - \left(\mathbf{H}^{T}\mathbf{H} + \lambda\mathbf{D}^{T}\mathbf{D}\right)\mathbf{x}^{(n)}\right]$$

$$\mathbf{x}^{(0)} = \mathbf{H}^{T}\mathbf{y}$$

where y is the measured depth profile vector, $x^{(n)}$ the deconvolved depth profile vector at the n^{th} iteration, H the Toeplitz matrix built from the DRF, H^T the transposed matrix, λ the regularization parameter, D the regularization operator and C the positive constraints operator.

The Cameca SIMS Depth Profile of the 5 nm spacing sample with the file extension .dp_ascii has to be opened. The depth of the SIMS profile is calibrated by selecting the "SIMS erosion conditions" semi calibrated option with 97.69 nm crater depth. The three DRF parameters λ_{up} = 0.15 nm, λ_{down} = 1.20 nm and σ_g = 0.70 nm is put in the input field at the custom DRF mode option. We can now adjust the regularization parameter, number of iterations and tolerance at the deconvolution parameter window

4. Results and Discussion

Fig. 3 shows the deconvolved delta layers of the 5 nm spacing sample with various number of (a) iteration at the regularization parameter of 1×10^{-4} and (b) regularization parameter at the iteration number of 25. Regularization parameters do not affect very much on the convergence of the deconvolved delta layers while the number of iteration has improved the sharpness of the depth profile. The profile of the first delta layer is distorted and its depth appears shallower. These

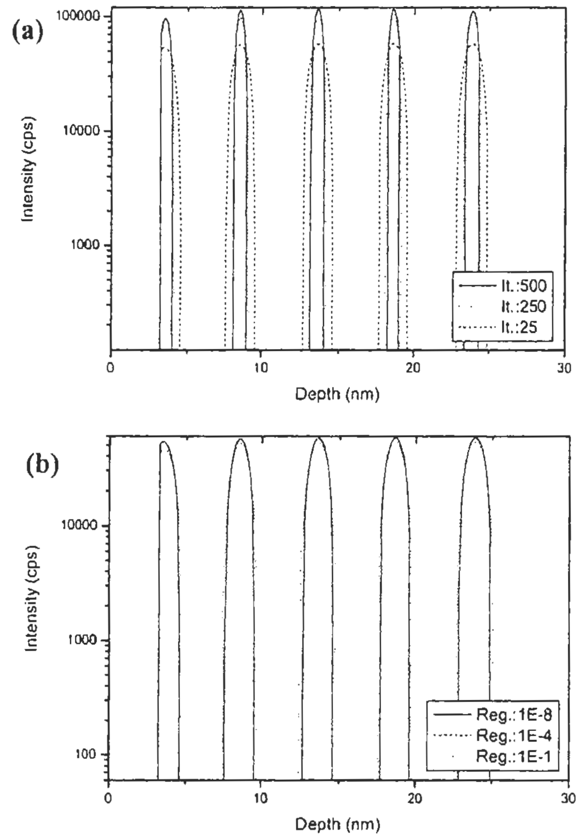

Fig. 3 Deconvolved delta layers of the 5 nm spacing sample with various number of (a) iteration at the regularization parameter of 1×10^{-4} and (b) regularization parameter at the iteration number of 25.

might be due to the larger sputtering rate in the initial transient region.

Fig. 4 shows the result of the deconvolution of the 5 nm spacing multilayers with the DRF obtained by the first delta layer of the 18 nm spacing sample. The regularization parameter was set to 1×10^{-4} and the tolerance 1×10^{-8}, which were the default numbers of the software. The number of iteration was 684, which was the number of the measured data points. The peak positions of the delta layers are 3.57, 8.57, 13.57, 18.63 and 23.85 nm with the average thickness of about 0.77 nm, which is the width at a low intensity. The deconvolved thickness of the delta layer is thicker than expected, which can be affected by roughness and diffusion. The measured and the reconstructed profile show a good agreement with each other except for the small discrepancy at the background level, which may come from the analytic form of the DRF.

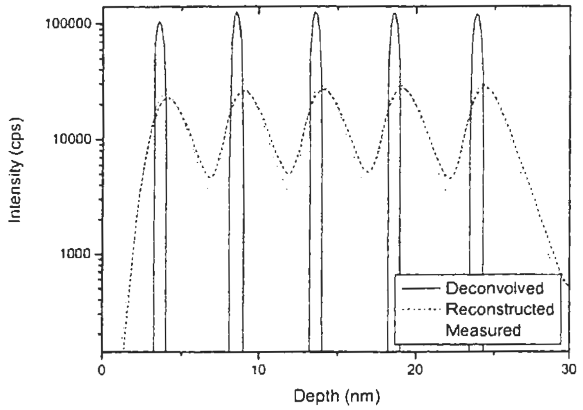

Fig. 4 Result of the deconvolution of the 5 nm spacing multilayers with the DRF obtained by the first delta layer of the 18 nm spacing sample.

5. Summary

SIMS deconvolution of boron-nitride delta-doped multilayers has been successfully performed using the Cameca "SIMSDeconvol^{TM}" software. The depth profile of the 5 nm spacing multilayer has been deconvolved with the DRF obtained by the first delta layer of the 18 nm spacing sample. The fitted parameters were λ_u = 0.15 nm, λ_d = 1.20 nm and σ_g = 0.70 nm. Effects of regularization parameter and number of iterations on the depth profile have been also examined. Further investigations of SIMS deconvolution of boron implanted and arsenic delta-doped samples are needed using the method described in this work.

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