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Ultra-shallow Boron Profile Fitting Compensating for Surface Contamination by Utilizing Genetic Algorithms

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1. Introduction

Sub-keV ion implantation is an indispensable tool for the formation of ultra-shallow junctions and MOSFET scaling. Although 0.2 keV implantation is now available that can realize 10 nm junction depths with B^+, such shallow implantation is very sensitive to the surface condition of a wafer. In general, screen oxide is not feasible in the case of such ultra-shallow implantations. Even if wafers are cleaned immediately prior to implantation, it is impossible to completely remove the presence of composite oxide and deposits of organic contaminants, which lead to serious dose losses [1].

One method of estimating dose loss is ellipsometry, but this alone cannot estimate the influence of surface contamination on dopant depth. In contrast, SIMS (Secondary Ion Mass Spectrometry) is a very powerful tool for obtaining dopant profiles, although its quantitative accuracy can sometimes suffer for surface regions [2]. To solve these problems, we propose a profile fitting method with a modeling function to compensate for the presence of contaminants. Using this modeling function, it is possible to obtain more precise dopant profiles for the sub-keV implantation process. Moreover, once a fitting function is obtained for a process line, the level of contamination at the line can be estimated from a single SIMS measurement. Thus, our method is useful not only for Technology CAD but also for process-line control.

2. Fitting Function and Experimental Conditions

We propose an implantation modeling function based on the Dual-Pearson profile [3]. We describe how the influence of surface contamination is incorporated in the profile and how the model parameters are fitted to the SIMS data.

Dual-Pearson Profile

A Dual-Pearson profile is represented as a linear combination of Single-Pearson profiles, as shown in Figure 1. As each Single-Pearson profile has 4 fitting parameters, the Dual-Pearson profile has 9 parameters in total (4+4+1). We assume each parameter, *Pi*, to be represented as

$$P_i(d; m_{i1}, m_{i2}, m_{i3}) = m_{i1} + m_{i2} \times d^{m_{i3}} \qquad (1)$$

where d is the thickness of the contamination layer, m_{i1}, m_{i2}, m_{i3} are fitting parameters, and i is an index number for the nine parameters. Therefore, our model has 27 (= 3 x 9) fitting parameters in total. However, due to the presence of local minimums, the fitting process for SIMS data using traditional gradient-based methods, such as the Levenberg Marquardt (LM) algorithm sometimes fails, and often yields inadequate results. To overcome this difficulty, we adopt a fitting technique based on Genetic Algorithms (GAs) [4].

Fitting method based on Genetic Algorithms

For a trial fitting process, multiple SIMS profiles were prepared with oxide layers of various thicknesses. Thermal or chemical oxides, with thicknesses within 0.20 nm to 1.34 nm, were intentionally deposited on Si (100) wafers to imitate contamination. B^+ was implanted into the wafers at a dose of 5×10^{14} cm^{-2} after pre-amorphization with Ge^+ implantation.

The summation of the fitting errors (MSE) for each profile, as shown in Figure 2, was taken as an evaluation function, called *fitness* in GAs. The fitting errors where the B^+ concentration was between 10^{18} and 10^{21} were weighted by 10^4 to avoid errors due to surface transience and detection limits at the tail ends. The weight *r* in Figure 1 was set to 0.0 for simplicity (i.e. a Single-Pearson profile).

4. Experimental Results

Figures 3 and 4 show fitting results at implantation energies of 0.2 keV and 0.4 keV, respectively. The calibrated profiles clearly fit well to the data apart from the characteristics of SIMS at the surface (small notches and peaks) and at the tail end (a gentler slope). Figure 5 shows extracted parameters, *Rp*, (averaged over 10 individual runs) plotted against the thickness *d* for the artificial contamination layer. (*Rp* is the 1st order moment for the profile.) As expected, the *Rp* decreases as *d* increases. Also, the dose integrated from the profile decreases as *d* increases, as shown in Figures 3 and 4. The variances in all the extracted parameters were nearly 0.0.

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5. Conclusions

We have proposed an implantation modeling function to compensate for the presence of contamination. Experimental results show that our model with a GA-based fitting method fits well to the SIMS data. We believe that it is possible to estimate the degree of contamination at the process line using the fitting function, which represents the dependency of fitting parameters on the thickness of the contamination layer.

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$$f_{pearson}(x) = r f_1(x) + (1-r) f_2(x) \quad \text{where} \int f(x)dx = dose$$

$$\frac{df_i(s)}{ds} = \frac{(s-a_i) f(s)}{b_{0i} + b_{1i} s + b_{2i} s^2} \qquad s = x - R_{pi} \qquad (i=1,2)$$

$$\begin{cases} a_i = -\gamma_i \sigma_{pi} (\beta_i + 3) / A_i \\ b_{0i} = -\sigma_{pi}^2 (4\beta_i - 3\gamma_i^2) / A_i \\ b_{1i} = a_i \\ b_{2i} = -(2\beta_i - 3\gamma_i^2 - 6) / A_i \end{cases} \quad \text{where} \quad \begin{matrix} A_i = 10\beta_i - 12\gamma_i^2 - 18 \\ b_{1i}^2 - 4b_{0i}b_{2i} < 0, \; b_{2i} < 0 \end{matrix} \qquad (i=1,2)$$

Model parameters: $r, R_{p1}, R_{p2}, \sigma_{p1}, \sigma_{p2}, \gamma_1, \gamma_2, \beta_1, \beta_2$

Fig. 1 Dual-Pearson profile: Each profile has 9 parameters to be fitted

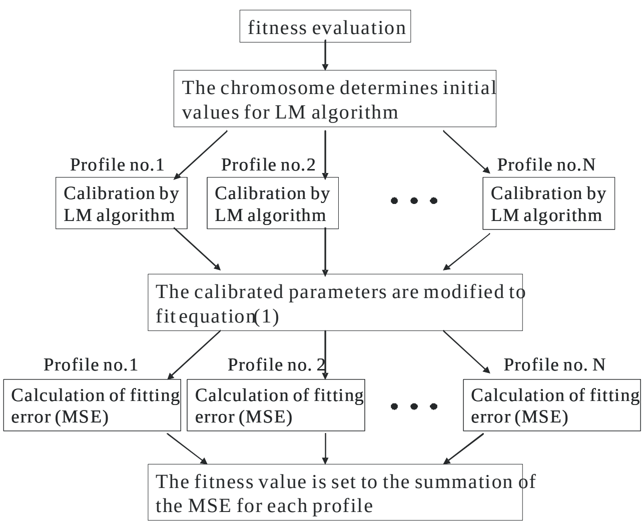

Fig. 2 Flowchart of the proposed GA fitness evaluation

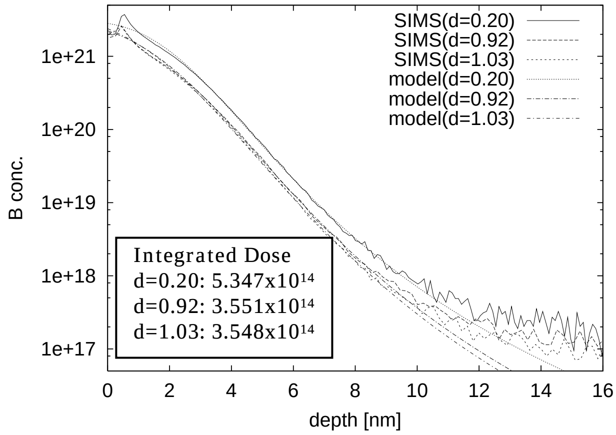

Fig. 3 SIMS measurement data and fitted model for an implantation energy of 0.2keV

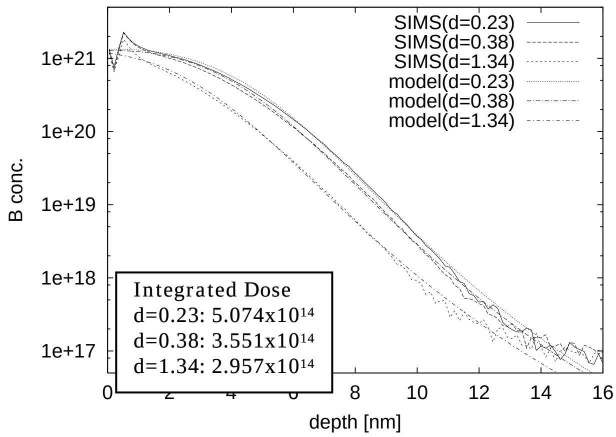

Fig. 4 SIMS measurement data and fitted model for an implantation energy of 0.4keV

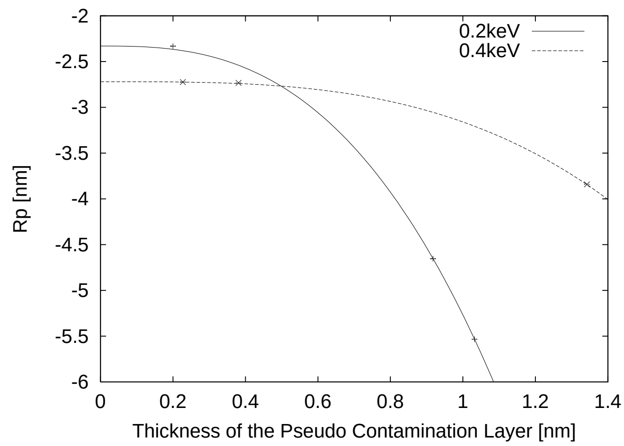

Fig. 5 Extracted Parameters Rp against thickness *d* for implantation energies of 0.2keV and 0.4keV