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Simulations of arsenic and boron co-implanted in silicon during RTA for ultra-shallow junctions realizations

A. Merabet *

Laboratoire de Physique et Mécanique des Matériaux Métalliques, Département d'O.M.P., Faculté des Sciences de l'Ingénieur, Université de Sétif, 19000 Sétif, Algérie

Abstract

We have used the simulator of TITAN process. The latter uses the finished elements method for the equations resolution of codiffusion. We have simulated arsenic (10^{16} atoms cm^{-2}, 100 keV) and boron (2×10^{15} atoms cm^{-2}, 30 keV) codiffusion profiles in the monosilicon, after rapid thermal annealing (RTA) by using the parameters by defect of simulator. We have noted the difference between the experimental distribution profiles measured with secondary ion mass spectrometry (SIMS) and those simulated. This lead us to readjust the profiles, changing the dopant diffusion coefficient in order to obtain the simulated profiles corresponding in a better way to the experimental profiles. The arsenic diffusivity values vary from 2×10^{-13} to 2×10^{-12} cm^2/s in the amorphised zone; and from 4×10^{-16} to 6×10^{-14} cm^2/s in the crystalline zone. As far as boron is concerned, they are from 10^{-15} to 6×10^{-14} cm^2/s and from 10^{-14} to 4×10^{-13} cm^2/s in the two zones cited, respectively.
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1. Introduction

Ionic implantation techniques are commonly used in the ultra large scale integrated (ULSI) area. They permit the reduction of impurities in depth with accuracy. The formation of thin junctions is realized by arsenic preamorphisation of substrate (heavy ion) followed by the boron implantation (light ion). After that, we carried out rapid thermal annealing (RTA) which permits obtaining simultaneously the recrystallisation of the amorphous layer and the activation of impurities.

Our work is a contribution to the study of the ULSI technology. There are many ways to be envisaged for the junction realization, among them, the boron implantation in the silicon substrate preamorphised, followed by a rapid thermal annealing. This leads the apparition of the “end of range” (EOR) under the old interface amorphous/crystalline (a/c). Many models have been proposed to explain the origins of defects EOR. After confrontations of TEM observations with simulations by Bergaud [1], the model that has been retained stipulates that this formation is the result of an agglomeration of particles under the interface. These particles appear during preamorphisation step while a great number of heavy ions are implanted producing an important punctual defects concentration.

Ultra-shallow junction formation is a crucial phase for the production of integrated circuit in an ultra scale (ULSI). The necessary annealing permits the created defect elimination during the boron implantation; this leads to boron diffusion implantation in a large scale depth, which limits the possibility of reducing the thickness of the junction. These phenomena which affect the performance of the ultra-short components, named transient enhanced diffusion (TED), can be reduced by ion co-implantation to limit the diffusion [2–4]. In microelectronics, the realization of nano-metric components requires serious control of the dopant diffusion. A simulator process semiconductor component fabrication permits to study the technology feasibility and its optimization in different adjusted parameters. So, we can reduce the experimental cost.

2. Experimental procedure

The substrates used for these experiments are boron-doped (1 0 0) Czochralski-grown 4-in. diameter wafers with resistivity of 8–15 ohm cm and a thickness of 520 μm. The samples were chemically cleaned and oxidized in dry O_2 to grow 20 nm before implanting. Afterwards, the silicon substrate received a double implantation starting with arsenic and followed by boron. The doses and energies of implantation were 10^{16} atoms cm^{-2} and

* Tel.: +213 36 91 26 81; fax: +213 36 92 51 34.
E-mail address: merabet_abdelali@yahoo.fr.

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100 keV for arsenic and 2×10^{15} atoms cm^{-2} and 30 keV for boron. The rapid thermal annealing is performed in a 30 kW ADDAX R1000 machine under Ar atmosphere. The samples were annealed for 20 s at temperatures ranging from 1000 to 1150 °C. The SIMS analysis was achieved by a Cameca IMS-4f instrument using Cs^+ and O_2^+ primary ions and a beam current of 80 nA. We have used the simulator of TITAN process [5]. It is a two-dimensional simulation program of the fabrication steps of elementary components in the integrated circuits. This simulator uses the finished elements method for the equation resolution of codiffusion. The main simulated phenomena are:

- The ionic implantation (Gaussian profiles or Pearson),
- The diffusion of one or more impurities (boron, arsenic, and phosphor) under an inert or oxide atmosphere, or during the epitaxy,
- The interface movement during the oxidation.

3. Results and discussion

The doping diffusion–annealing phase is described in terms of flux. The flux of the impurity (e) in an isotropic field contains (*j*) impurities, knowing that the only parameters are the power of chemical potential gradient and the electric field, which can be expressed by [6,7]:

$$F_e = -D_e \nabla C_e + Z_e \mu_e C_e E \tag{1}$$

where D_e is the diffusivity coefficient of impurity e; C_e, the concentration of impurity; μ_e, the mobility of impurity e; Z_e, the impurity charge, positive for donors and negative for acceptors; and E is the internal electrical field.According to Fair [8], the essential characteristic of kinetic diffusion is the punctual defects effect, extended, pre-existed or generated during the implantation or eventually during the annealing cycle, on the dopant diffusion. The defects can be presented under different electrical states: neutral defects, positively charged defects or negatively charged defects. The diffusion coefficient D_e is the sum of various diffusion coefficients, including impurity diffusion with one of these defects [9]:

$$D_e = D^0 + D^- \left(\frac{n}{n_i}\right) + D^+ \left(\frac{n_i}{n}\right) \tag{2}$$

By normalizing the different coefficients diffusion related to the intrinsic diffusion coefficient D_i and supposing that the diffusion should only be carried out for arsenic by intermediary's defects, and negatively charged, then:

$$D_d = D_{id} \frac{1 + \beta_d (n/n_i)}{1 + \beta_d} \quad \text{with} \quad \beta_d = \frac{D_i^-}{D^0} \tag{3}$$

As far as boron is concerned, and by supposing that the diffusion is carried out by intermediary neutral defects positively charged, then:

$$D_a = D_{ia} \frac{1 + \beta_a (n_i/n)}{1 + \beta_a} \quad \text{with} \quad \beta_a = \frac{D_i^+}{D^0} \tag{4}$$

where β is the factor representing the ratio diffusivity introduced by the defects charged once on the diffusivity due to neutral defects. Meanwhile, as far as temperatures are concerned, β can be considered constant [6]. TITAN simulator uses in particular Fair and Tsai [10] model for the expression: $D = D_i h$.The effective coefficient diffusion, which intervenes in the diffusion equation, takes the form:

$$D = D_i h \frac{1 + \beta f}{1 + \beta} \tag{5}$$

with

$$h = 1 + \frac{C}{2n_i} \left[\left(\frac{C}{2n_i} \right)^2 + 1 \right]^{-0.5} \tag{6}$$

and

$$f = \frac{C}{2n_i} + \left[\left(\frac{C}{2n_i} \right)^2 + 1 \right]^{0.5} \tag{7}$$

D_i and n_i design the diffusion and the intrinsic concentration, respectively; n_i essentially depends upon the gap and the temperature:

$$n_i = 7.6354 \times 10^{15} \times T^{3/2} \exp\left(\frac{-\text{Gap}}{2k_B T}\right) \quad \text{with}$$

$$\text{Gap} = 1.17 - \frac{4.73 \times 10^{-4} T^2}{(636\,\text{K} + T)}$$

The intrinsic diffusion coefficient D_i follows Arrhenius law:

$$D_i = D_0 \exp\left(\frac{-E_0}{kT}\right)$$

As far as arsenic is concerned, the usual parameters used during classical annealing are [5,11,12]:

$$D_{0As} = 22.83\,\text{cm}^2/\text{s} \qquad E_{0As} = 4.1\,\text{eV} \qquad \beta = 100$$

As far as boron is concerned [5,11]:

$$D_{0B} = 0.5554\,\text{cm}^2/\text{s} \qquad E_{0B} = 3.426\,\text{eV} \qquad \beta = 19$$

The physical model used for studying the coupled diffusion of two impurities should include, as in the case of one impurity, the effect of the internal electrical field and the defects influences in diffusion. Then, we have a system of two coupled equations (Fick's second law) [6]:

$$\frac{\partial C_{As}}{\partial t} = D_{i,As} \frac{\partial}{\partial x} \left[\frac{1 + \beta_{As} f}{1 + \beta_{As}} \left(h_{As} \frac{\partial C_{As}}{\partial x} - (h_{As} - 1) \frac{\partial C_B}{\partial x} \right) \right] \tag{8}$$

$$\frac{\partial C_B}{\partial t} = D_{i,B} \frac{\partial}{\partial x} \left[\frac{1 + \beta_B / f}{1 + \beta_B} \left(h_B \frac{\partial C_B}{\partial x} - (h_B - 1) \frac{\partial C_{As}}{\partial x} \right) \right] \tag{9}$$

with:

$$h = 1 + \left(\frac{C}{2n_i} \right) \left[\left(\frac{C_{As} - C_B}{2n_i} \right)^2 + 1 \right]^{-0.5} \tag{10}$$

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