The simple approach to determination of active diffused phosphorus density in silicon

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Abstract. The diffusion of Phosphorus in silicon using a $POCl_3$ source has been considered. In the base of Fair-Tsai model of P-diffusion an empirical equation for calculation of active diffused phosphorus density (Q_{el}), is proposed. In this equation, a relationship between (Q_{el}), diffusion time, temperature and junction depth of *P*-diffused layer (X_j), is presented. The value of sheet resistance (R_s), which is taken from theoretical determination at 900°C, has a good agreement with experimental result.

Keywords: phosphorus, silicon, diffusion, sheet resistance.

1. Introduction

Research on dopant diffusion in crystalline silicon has provided a wealth of detailed including atomistic diffusion models as well as the influence of various process conditions in the fabrication of integrated circuits. Nevertheless, dopant distribution in new device technology can hardly be predicted without going through several cycles of short loop technology experiments to calibrate the diffusion models used for technology computer aided design [1]. This talk addresses the question of how research on physical models can support process simulation to reach the goal of replacing costly experiments in the development of new technologies. Diffusion of phosphorus, is one of the important steps, which is used in silicon based MEMS technology. Therefore, the presentation of a simple equation for determination of active diffused phosphorus density and prediction of depth junction can be useful in silicon based MEMS technology [2].

In practice, it is shown that at high concentration, the diffusion of phosphorus (P), into silicon (Si), produces an impurity atom distribution, which considerably differs from the standard profile of diffusion theory [3–7]. In order to explain the anomalous diffusion of phosphorus pair different models have been developed. In the first model or Fair-Tsai model, only one type of dopant-defect pair namely, the dopant-vacancy pairs have been considered [8]. Hu [9], has shown that in order to simu-

late high concentration phosphorus diffusion both dopant interstitial and dopant vacancy pair have to be included. The number of coupled differential equations and the unknown parameters were still acceptable. However, in his model no electrical charge states of species have been taken into consideration. In the next model suggested by Richardson and Mulvaney [10], the different charge states of each species have also been included. This model comprises a relatively large number of coupled differential equations, as they write one equation for each charge state of species. Moreover, the number of unknown parameters increases rapidly with the number of considered charge state of the defects in these models. Budil [11], has defined the total concentration for each species as the sum of the concentrations of charged species and the neutral one. Assuming local equilibrium for electronic processes, he derived a pair diffusion model with only on equation per species, considering all possible charge and average diffusivities. In this model, however, not all-possible reactions between point defects and dopant defect pairs have been considered. Baccus [12], has suggested a general pair diffusion model. However, in his model there is still a huge number of unknown parameters. Dunham [13,14], has introduced another model with using some of the assumptions of Baccus. In the model proposed by Dunham, the number of parameters is reduced but the special case of intrinsic concentrations is not automatically considered. Ghaderi [15], has reduced same pa-

rameters of Dunham s model and presented another model for diffusion of phosphorus in silicon. But, there are several complicate equations and unknown parameters in all of these models. Therefore, the determination of active diffused dopant and depth of junction as two important parameters for evaluation of diffusion process, are difficult. The goal of the present work is, to introduce a simple equation for determination of active diffused phosphorus density (Q_{el}), in perdeposition. According to that equitation, the junction depth and sheet resistance has been calculated.

2. Theory

Numerous models have been proposed to explain the anomalous deviation from simple diffusion theory of diffused phosphorus in silicon. Fair and Tsai [8], have suggested a model for this purpose and have concluded that the distribution of phosphorus in silicon during predeposition has a profile, which is shown in Fig. 1. The experimental results of dopant profile show that the best model for prediction of phosphorus distribution in silicon during predeposition process is Fair-Tsai model. According to that model the profile of dopant distribution can be divided into two parts, one associated with total doping per square centimeter, Q_{st}, and the concentration level in this region is almost approximately constant. In the second part that is associated with a tail region, the total doping per square centimeter is Q_{tail}. The Q_{el} is sum of the two total dopant concentrations in diffusion region (Q_{st} +Q_{tail}). Also the junction depth of P-diffused layer in silicon is introduced as X_j. At that case, the criteria for evaluation of diffusion process is determination of sheet resistance (R_s). According to Fair-Tsai model the relationship between R_s and Q_{el} is as follows:

$$R_s = \frac{1}{q(75 \times Q_{el} + 1.8 \times 10^{20} \times X_j)} \; (\Omega \cdot \mathrm{cm}^{-2}) \qquad (1)$$

Therefore, in the Fair-Tsai model for determination of (R_s), we need to calculate Q_{el}. Fair [16], have also suggested that Q_{el} and X_j can be calculated from two following equations:

$$X_j = X_0 + 2\sqrt{D_{tail} \times t}\left(erfc^{-1}\left(\frac{c_B}{c_K} \right) \right) (\mathrm{cm}) \qquad (2)$$

$$Q_{el} = n_s^{\frac{3}{2}} \times \sqrt{\frac{t}{n_i}} \times \left[\sqrt{\frac{2D_i^{=} n_s}{n_i}} + \right.$$
$$\left. + \frac{1}{2} \times \sqrt{D_i^{-}\left(1 + \exp\left(\frac{0.3ev}{KT} \right) \right)} \right] \quad \mathrm{cm}^{-2} \qquad (3)$$

where $D_{tail} = 3.85 \exp\left(\frac{-3.66ev}{KT} \right) + \frac{D_i^{-} n_s^3}{n_e^2 \times n_i}\left[1 + \exp\left(\frac{0.3ev}{KT} \right) \right]$,

$D_i^{=} = 44.2 \exp\left(\frac{-4.37ev}{KT} \right)$ and $D_i^{-} = 4.44 \exp\left(\frac{-4ev}{KT} \right) (\mathrm{cm}^2 \mathrm{s}^{-1})$.

In Eq. 2, X_0 is depth of the first region and (t) is the diffusion time in terms of second and K is the Boltzman constant. Also c_B is the initial concentration of dopant in the silicon before perdeposition and c_k is the concentration of P at the kink in the diffusion profile (Fig. 1). In the Eq. 3 n_s is the surface concentration that can be obtained from Fig. 2. Here n_i is the intrinsic concentration that can be determined from [17]:
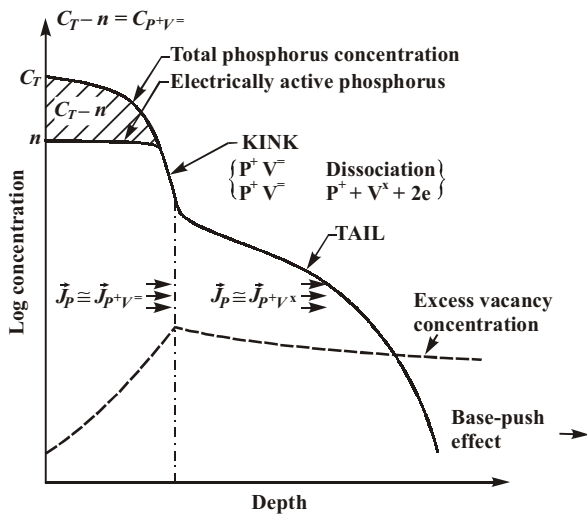

Fig. 1. Phosphorus diffusion model based upon the work of Fair-Tsai [8].
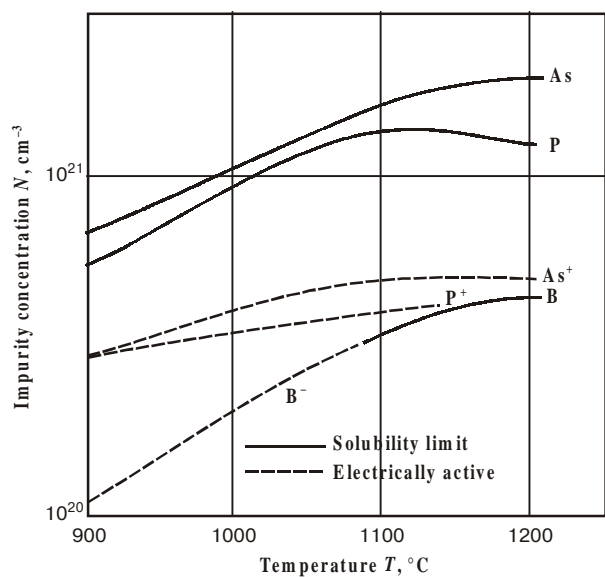

Fig. 2. Amount of inactive dopant for common dopants, solid lines are solid solubility; dashed lines are limits of electrically active dopant concentration.

$$n_i = 5.17 \times 10^{20} \exp\left(\frac{-5420}{T}\right) (\text{cm}^{-1}) \qquad (4)$$

Tsai [18] has proposed the equation for determination of X_0. But X_0 obtained from his research has some discrepancy with experimental results. Our study has shown this uncertainty could be compensated using the equation given below:

$$X_0 = \alpha \times t \text{ (cm)} \qquad (5)$$

where $\alpha = 6.057 \exp(\frac{-2.12 \text{ eV}}{k_B T})$

However, Fair and Tsai have presented some simplifier hypotheses for providing of above equations, the calculation of the sheet resistance and active diffused phosphorus density using Eqs 1 and 3 are difficult. Therefore, it will be favorable to find a simple way for calculation of Q_{el}. In order to drive a suitable equation for Q_{el}, we should consider the variation of sheet resistance with respect to diffusion time and temperature. The well-known experimentally approved equation for R_s in planar silicon technology is as follows:

$$R_s = R_{so} \frac{e^{\frac{a}{T}}}{\sqrt{t}} \ (\Omega \cdot \text{cm}^{-2}) \qquad (6)$$

where R_{so} and a are two constants. In that equation, R_s is inversely proportional to $t1/2$. Thus, the Q_{el}, must be function of $t1/2$. On the other hand, and in the base of data analysis process, the relationship between sheet resistance and diffusion time can be shown with a mathematical function such as $f(R_c) = [\sqrt{t} \times \ln(c)]^{-1}$.

According to that function, we need to define the variable of $\ln c$ in terms of sheet resistance behavior for diffused phosphorus in silicon, and providing an equation for calculating the Q_{el}. For this reason, different works for obtaining that goal have been carried out, and it was found that Q_{el} can be calculated by:

$$Q_{el} = -B\sqrt{t}\ln\left(X_j - \alpha t\right) \qquad (7)$$

where B is a constant for given temperature and t is time (in seconds). The X_j can be given from Eq. 2. Q_{el} for se-
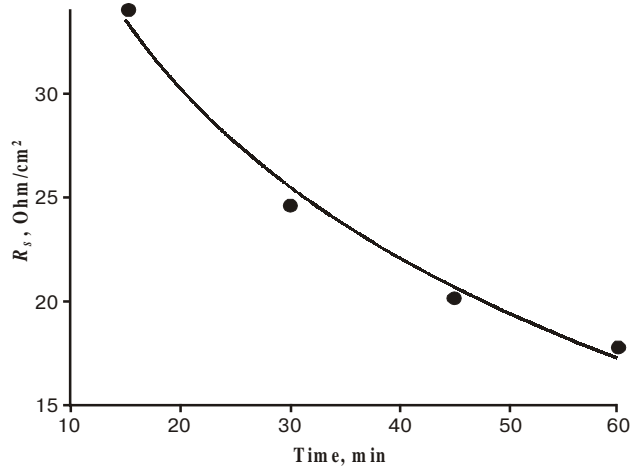

Fig. 3. Sheet resistance vs. diffusion time with POCl$_3$ source.

veral different diffusion temperatures and times have been calculated by using Eqs 3 and 7 and compared with experimental results given in Table 1.

3. Experiment

In order to evaluate the precision of Eq. 7, we have to predict the sheet resistance and diffusion depth of diffused layer by that equation and compare with experimental results. The experiment of phosphorus diffusion process has been carried out in Centrotherm open tube furnace. The silicon wafers, which have been used in the process, were P-type with 10^{17} atom/cm^2 impurity concentration. For P-source, we have used POCl$_3$ prepared by purging of 50cc/min N$_2$ gas bubblier. Preheating and postheating times were 10 minutes. The sheet resistance of diffusion region has been measured by four-point probe technique. The variation of sheet resistance via diffusion time was illustrated in Fig. 3. The experimental results of sheet resistance measuring and calculation of that parameter with Eq. 7 are in good accordance. The comparison of the sheet resistance calculated with two different equations 3 and 7 have been presented in Table 2.

Table 1. The variation of Qel with time in the base of two different Eqs 3 and 7.

Time (min)	X_0, (cm)	X_j, (cm)	Q_{el} Eq. (7)	Q_{el} Eq. (3)
15	$4.124 \cdot 10^{-6}$	$3.76 \cdot 10^{-5}$	$1.84 \cdot 10^{15}$	$3 \cdot 10^{15}$
30	$8.388 \cdot 10^{-6}$	$5.72 \cdot 10^{-5}$	$2.517 \cdot 10^{15}$	$4.24 \cdot 10^{15}$
60	$16.78 \cdot 10^{-6}$	$8.58 \cdot 10^{-5}$	$3.436 \cdot 10^{15}$	$6.02 \cdot 10^{15}$

$T = 900°C$, $\alpha = 4.67 \cdot 10^{-9}$, $n_i = 5.1 \cdot 10^{18}$, $n_e = 9.83 \cdot 10^{19}$, $c_B = 1 \cdot 10^{17}$, $n_s = 3 \cdot 10^{20}$, $c_k = 10^{23} \exp(-0.79 \text{eV/KT})$

Table 2. The comparison of the sheet resistances calculated using two different Eqs 3 and 7.

Time (min)	R_s Eq. (3)	R_s Eq. (7)	R_s Ref. [19]
15	20.38	33.94	34
30	14.67	24.65	24.15
45	12.02	20.5	19.91
60	10.38	17.69	17.2

4. Conclusions

Sheet resistance is being accepted as a criteria for diffusion control during semiconductor device fabrication, and it has an inversely proportional to active diffused phosphorus density (Q_{el}) and junction depth (X_j). In this work, we first presented a mathematical function (Eq. 7) for prediction of the experimental results and parameters included to this equation. Experimental results have shown that Q_{el} obtained form Eq. 7 is longer than previously proposed by the formula (equation (3) of the ref. [16]). Hence, our equation for calculation of Q_{el} in its turn produces a bigger R_s, which is in better agreement with the experimental data, including our experimental measurements at 900°C at the diffusiion time and those of [19, 20].

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