# A TRANSIENT ACTIVATION MODEL FOR PHOSPHORUS AFTER SUB-AMORPHIZING CHANNELING IMPLANTS

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**Abstract**

*We present a diffusion model for the activation of phosphorus after a sub-amorphizing channeling implant into bare silicon under intrinsic conditions. A coupled diffusion model has been developed to take into account the basic impurity diffusion mechanisms as well as point-defect generation-recombination mechanisms occuring during thermal treatment of doped silicon. The role of the vacancy based Frank-Turnbull recombination was investigated for the activation process.*

## 1. Introduction

As most of the dopants are electrically inactive after ion implantation, thermal activation by annealing has to be performed. The global trend towards shallow high doped junctions enforced the usage of high temperature – short time annealing processing (RTA). Our approach presented here is contrary to the global trend and allows the activation of phosphorus at relatively low temperatures. Simulations as well as experiments were carried out to get a better understanding of the complicated behavior of phosphorus activation in silicon. Due to the fact that both common measurement methods SIMS and SRP are available, we can present a diffusion model taking into account all established reactions between point-defects and dopant-defect pairs.

## 2. Experimental

Bare <100>-oriented p-type bulk silicon wafers with a background doping level of $10^{15} cm^{-3}$ were implanted with $30 keV$ phosphorus at a dose of $3 \cdot 10^{13} cm^{-2}$. Then the wafers were annealed for $30 min$ at $850°C$,$875°C$, and $900°C$ in a furnace equipment in $N_2$ ambient. Fig.1 shows the SIMS and SRP results for the above experiments in the same plot.

## 3. Phosphorus Activation Model

The present models of point-defect impurity diffusion in silicon favors the pairing of substitutional dopants with point-defects [1][2]. This models are based on full activated initial dopant profiles and on diffusion systems including enhancement due to point-defects. In our case we want to investigate the activation process as well as the diffusion process and so we start up with an unactivated dopant stream assuming pairing of dopants at interstitial sites with interstitial point-defects. Due to recombination these dopant-defect pairs are split into substitutional dopants and recombining point-defects (I-V). To include the unactivated dopant stream into our PDE system we have to extend a conventional five-stream diffusion model by a sixth stream. The basic rate equations are given in (1)-(6) taking into account the actual state of the species, where $i$ means interstitial, $s$ substitutional, and $p$ paired at the lattice position:

$$A_i + I_i \rightleftharpoons AI_p \qquad (1) \qquad\qquad AV_p + I_i \rightleftharpoons A_s \qquad (4)$$

$$A_i + V_s \rightleftharpoons AV_p \qquad (2) \qquad\qquad AV_p + AI_p \rightleftharpoons 2A_s \qquad (5)$$

$$AI_p + V_s \rightleftharpoons A_s \qquad (3) \qquad\qquad I_i + V_s \rightleftharpoons 0 \qquad (6)$$

$I$,$V$,and $A$ are representing interstitial, vacancy, and dopant species. (1) is known as kick-out reaction, (2) describes the according vacancy mechanism, where (3) is the Frank-Turnbull mechanism and (4) the opposite vacancy reaction. Finally, (5) represents the pair/pair recombination and (6) the bulk recombination. Note that there are three states possible for the dopant (interstitial, substitutional, and paired) during the diffusion process. Starting form a full description of a coupled diffusion equation system [1], we can apply some simplifications due to our doping conditions. We can neglect pair/pair interactions, because this effect occurs only at high concentrations. Also from oxidation and nitridation experiments it is known that phosphorus diffuses only via interstitial mechanisms under intrinsic conditions [3]. With the above assumptions the system of diffusion equations for intrinsic phosphorus reads:

$$\frac{\partial C_{P^i}}{\partial t} = -R_{P/I} \qquad\qquad \frac{\partial C_{PV}}{\partial t} = 0$$

$$\frac{\partial C_{P^s}}{\partial t} = +R_{PI/V} \qquad\qquad \frac{\partial C_I}{\partial t} = \mathrm{div} J_I - R_{P/I} - R_{I/V}$$

$$\frac{\partial C_{PI}}{\partial t} = \mathrm{div} J_{PI} + R_{P/I} - R_{PI/V} \qquad\qquad \frac{\partial C_V}{\partial t} = \mathrm{div} J_V - R_{I/V} - R_{PI/V}$$

where $R_x$ refers to the generation/recombination reactions and $J_x$ refers to the diffusion flux of the species. Only paired dopants or the point-defects themself are able to diffuse, the substitutional or interstitial dopant stream can only vary by rate reactions. There is also negligible field enhancement at intrinsic conditions, which leads to the simple diffusion flux

$$J_x = D_x \cdot \mathrm{grad}\ C_x, \qquad (7)$$

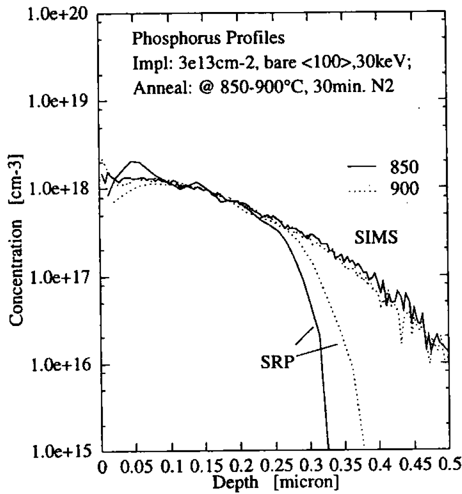


Figure 1: SIMS and SRP phosphorus measurements for channeling implant with subsequent furnace anneal.

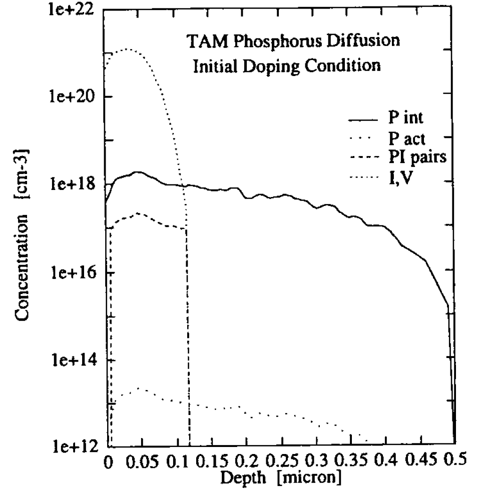


Figure 2: Initial setup for point-defects and dopant streams after implantation

where $D_x$ is the charge dependent diffusivity of the diffusing species $I$,$V$,$AI$. Because of the fast electronic interactions compared to the atomic diffusion processes, we can assume that all ionization processes are near equilibrium, and because of intrinsic conditions we do not need to decide between different charge levels of the dopants and can lump the forward and backward reaction rates in neutral charge related rates. This simplifies the structure of the net pairing rates to one equilibrium reaction rate constant for each generation/recombination term to extract. The values for the equilibrium point defect concentrations are taken from [4]. A crucial role in the model setup is the assumption of the initial point-defect concentrations. We used Monte Carlo simulations to get the initial guess for interstitials and vacancies [5]. The dopant concentration itself is taken from a crystalline Monte Carlo calculation. Fig.2 shows the initial setup for the diffusion system.

## 4. Simulation Results

Fig. 3 gives the simulation results for the temperature range $850°C$ - $900°C$ including measurements, where the total phosphorus concentration is compared to the SIMS profile and the subsitutional or active concentration to the SRP profiles. Interstitial dopants in the tail region are available, but they cannot be paired, because the interstitials have already diffused into the bulk. On the other hand they cannot be activated because there is no recombination vehicle within the reaction radius. So the vacancy concentration in combination with the paired dopant stream plays the key role in activation.

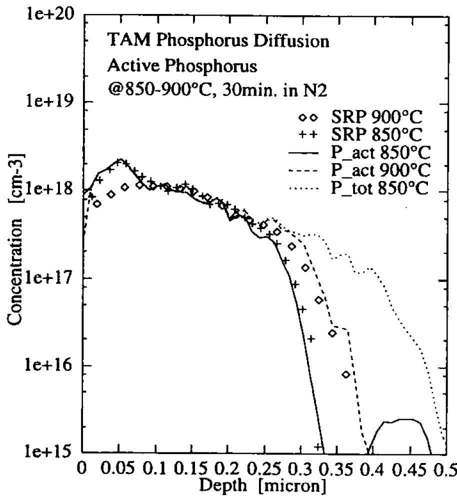


Figure 3: Simulation results of phosphorus activation for temperature range 850°$C$ - 900°$C$ and comparison of active profiles with SRP.

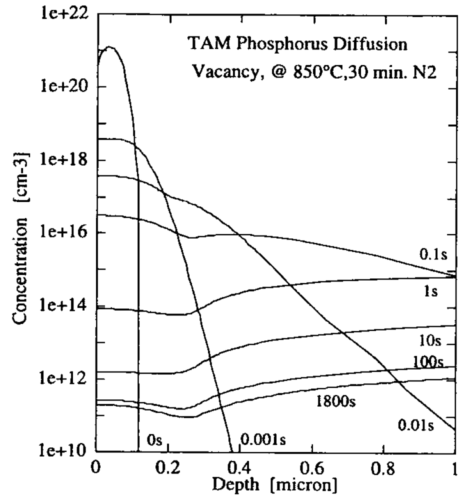


Figure 4: Transient vacancy distribution during annealing

Fig. 4 gives the transient profiles of the vacancy distribution. The vacancy concentration decreases at activation cites by Frank-Turnbull recombination and in the whole substrate by bulk recombination. Note that the activation process is a very short term process and is nearly finished after a time period of 0.1$s$. After this activation time there are not enough vacancies at the same lattice position with dopant pairs to continue activation. The simulation results show that it is possible to scale the activation process with the temperature, but at temperatures above 900°$C$ all of the implanted dopants will be activated during annealing because of the high diffusivity of the point defects.

# References

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