

Platinum in Silicon after Post-Implantation Annealing: From Experiments to Process and Device Simulations

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Abstract—Based on experimental findings of platinum clusters, a model of post-implantation annealing of platinum in silicon has been developed for the temperature range from 850 to 900 °C and the dose range from 1×10^{12} to 1×10^{13} cm⁻². The model has been implemented in a full TCAD simulation chain to predict the electrical behaviour of platinum-diffused diodes.

Index Terms—platinum implantation, silicon, diffusion, process simulation, device simulation

I. INTRODUCTION

Platinum is used for lifetime engineering in power devices. It can be introduced from a Pt silicide or by ion implantation. One possible advantage of ion implantation in comparison to Pt from a silicide is that the same platinum depth profiles can be obtained with a lower thermal budget [1]. However, a thorough understanding is still needed to fully utilize this technology.

Post-implantation annealing of platinum in silicon has previously been studied by Badr *et al.* [1] at diffusion temperatures from 765 to 900 °C. They showed that it is necessary to take into account the incomplete activation of the implanted platinum. In this paper, new depth profiles of substitutional platinum after post-implantation annealing at 850 and 900 °C are presented together with a simulation model which can describe the experimental results available. It will also be shown that this model can be implemented in a full TCAD (technology computer-aided design) simulation chain to predict the electrical behavior of a platinum-diffused diode.

II. EXPERIMENTAL

For the experiments, dislocation-free silicon wafers were used; (111)-oriented, n-type, P-doped, FZ-grown, 625 µm thick wafers, with a resistivity of 4 Ωcm for the ones implanted with 3×10^{12} cm⁻²; (100)-oriented, n-type, P-doped, CZ-grown, 725 µm thick wafers, with a resistivity of 2 Ωcm for the rest.

In all cases, an oxidation step was performed first to eliminate grown-in voids, as in the work of Badr *et al.* [1]. The resulting oxide was removed. The platinum was implanted at the frontside (depth = 0) with 150 keV in the dose range from 1×10^{12} to 1×10^{13} cm⁻² at room temperature. No significant wafer heating is expected for the implantation conditions. Next, the wafers were annealed as described by Badr *et al.*

[1] for 2 hours (30 min in O₂, 90 min in N₂) at a nominal process temperature of 850 or 900 °C.

The concentration of substitutional platinum C_{Pt_s} was measured by DLTS (deep level transient spectroscopy) with an accuracy of approximately 30% [2] using a Hera-DLTS system from PhysTech. The samples for DLTS were prepared as described by Badr *et al.* [3].

III. PROCESS SIMULATIONS

A. Platinum diffusion

Platinum diffusion in silicon has been studied by several authors [1]–[6], however mainly for the introduction of platinum from a Pt silicide. Platinum is a hybrid element in silicon, it diffuses as interstitial platinum Pt_i and resides mainly at substitutional sites (not considering Pt-clustering). The diffusion proceeds via interaction with point defects; vacancies V (the Frank Turnbull mechanism [7]) and self-interstitials I (the kick-out mechanism [8]). IV-recombination is also considered. A more detailed description of these (basic) mechanisms and the parameters used for the simulations can be found in the publication of Johnsson *et al.* [6]. The equilibrium concentration of self-interstitials C_I^{eq} not explicitly specified in [6], was here taken from Badr *et al.* [1].

The Pt_i atoms diffuse rapidly and establish a nearly uniform distribution across the wafer depth regardless whether the source is a Pt silicide or from Pt implantation. As the interactions with intrinsic point defects proceed, the system locally approaches steady state. For the concentration of substitutional platinum C_{Pt_s} to increase further, via the Frank-Turnbull mechanism or the kick-out mechanism, vacancies have to diffuse in from the surfaces or self-interstitials have to diffuse out to the surfaces. Therefore, C_{Pt_s} increases faster at depths with a shorter distance to the surface. This typically results in U-shaped profiles of C_{Pt_s} .

The Pt_s concentration in the bulk $C_{Pt_s}^{bulk}$ after annealing may also be influenced by the initial concentrations of I and V present in the wafer before Pt is introduced (C_I^0 and C_V^0). If there is a surplus of vacancies, it leads to a higher $C_{Pt_s}^{bulk}$: Pt_i diffuses in rapidly and decorates the excess of vacancies. On the other hand, if there is a surplus of self-interstitials, it results in a lower $C_{Pt_s}^{bulk}$ since Pt_i can only proceed to go into substitutional sites as the excess of I's in the bulk is transported

to the surfaces. However, the initial concentrations only have a significant influence if the surplus of either I or V is in the range of $C_{Pt_s}^{bulk}$ obtained after annealing. For our process conditions, we expect C_I^0 and C_V^0 to be low because of the prior oxidation-step, and therefore not to have a significant influence on $C_{Pt_s}^{bulk}$.

B. Implantation damage

3-D Kinetic Monte Carlo (KMC) simulations were performed with Sentaurus Process [9] to investigate if the damage related to an implanted dose of $1 \times 10^{13} \text{ cm}^{-2}$ is close to the amorphization limit. KMC simulations give some information about the evolution from point defects into smaller amorphous regions, amorphous pockets, and finally the formation of amorphous layers. Amorphous regions are defined as regions where the damage concentration is higher than some threshold. The default amorphization threshold of $1.5 \times 10^{22} \text{ cm}^{-3}$ [9] was used in the simulations. The results indicated that regions of amorphous pockets were formed for an implanted dose of $1 \times 10^{13} \text{ cm}^{-2}$, but no continuous amorphous layer. It would require doses $> 2 \times 10^{13} \text{ cm}^{-2}$ according to this approach.

The simplifying +1 model from Giles [10] was used to model the damage distribution after ion implantation in this work. It assumes that the generated intrinsic point defects quickly recombine during the initial phase of annealing and that the implanted ions quickly occupy substitutional sites. What remains is one self-interstitial (+1) per implanted ion. The excess of I's is assumed to follow the same concentration profile as the implanted ions. This model was developed for implantation below the amorphization threshold and has been employed by many authors, for example [1], [11].

During annealing, the supersaturation of self-interstitials leads to the formation of immobile clusters which undergo Ostwald ripening. The Si clustering was described by the model of Zechner *et al.* [11] which considers small clusters up to I_4 , and thereafter a moment-based model to describe the formation and growth of $\{311\}$ -defects. The model parameters were adjusted since other parameters for the intrinsic point defects were used in this work compared to [11].

C. Platinum clusters

The knowledge about post-implantation annealing of platinum in silicon is incomplete. A series of experiments with similar experimental conditions to this work was reported by Badr *et al.* [1]. For some cases, depending on the implanted dose and the annealing temperature, they observed that only a fraction of the implanted platinum was found to be Pt_s by DLTS measurements. Similar findings were made in this work.

The concentration of platinum in the implanted region exceeds solid solubility, and Pt is therefore assumed to have formed clusters or precipitates during annealing. Badr *et al.* [1] suggested an empirical dynamic cluster model based on the experiments available at the time. It predicts that all Pt clusters are dissolved already for an annealing temperature of 825°C (2 h) for doses up to at least $1 \times 10^{13} \text{ cm}^{-2}$. This model could describe most of the profiles presented in this

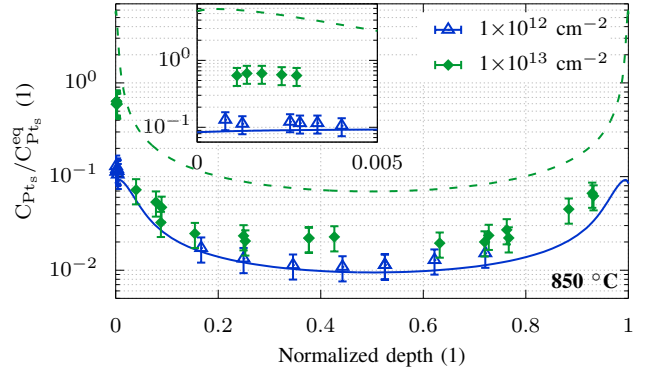


Fig. 1. DLTS measurements and simulation results of C_{Pt_s} after annealing at 850°C for two doses: $1 \times 10^{12} \text{ cm}^{-2}$ (—) and $1 \times 10^{13} \text{ cm}^{-2}$ (- - -). The lines show the simulation results using the model by Badr *et al.* [1]. The inset shows the concentrations close to the surface.

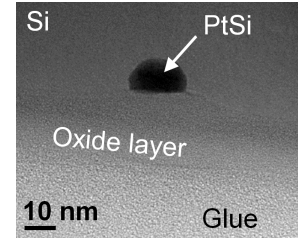


Fig. 2. HR EFTEM image (by Institut für Oberflächen- und Schichtanalytik GmbH, Kaiserslautern, Germany) after post-implantation annealing of platinum in silicon ($1 \times 10^{14} \text{ cm}^{-2}$, 150 keV, 900°C , 30 min). The dark spot in the middle was identified as a PtSi precipitate by EDX.

work, but not all. As an example, Fig. 1 shows a good fit using their model for an implanted dose of $1 \times 10^{12} \text{ cm}^{-2}$; a dose where virtually all of the implanted Pt was found as Pt_s . However, their model strongly overestimates C_{Pt_s} for an implanted dose of $1 \times 10^{13} \text{ cm}^{-2}$. C_{Pt_s} in the figures is scaled with the equilibrium concentration of Pt_s , $C_{Pt_s}^{eq}$, at the nominal process temperature and the depth is scaled by the wafer thickness.

Another indication of Pt clusters, or rather precipitates, was found with HR EFTEM (high-resolution energy-filtered transmission electron microscopy). Fig. 2 shows a dark area close to the implanted surface after post-implantation annealing for an implantation dose of $1 \times 10^{14} \text{ cm}^{-2}$ and an annealing temperature of 900°C (30 min), which was identified as a PtSi precipitate using EDX (energy dispersive X-ray spectroscopy).

To get an idea of the differences between Pt-implantation and Pt from a Pt silicide for similar conditions, the experimental results with an implanted dose of $1 \times 10^{13} \text{ cm}^{-2}$ were compared to simulations of Pt diffusion from a PtSi layer in Fig. 3. The simulation results are in close agreement with the measured data after post-implantation annealing. Based on this we worked with the assumption that large PtSi precipitates, like the one shown in Fig. 2, act similar to a PtSi layer.

An approach suggested by Pichler [12] was used to model Pt clustering. It is an empirical cluster model, derived on the basis of classical nucleation theory, which incorporates a saturation of the monomer concentration associated with large

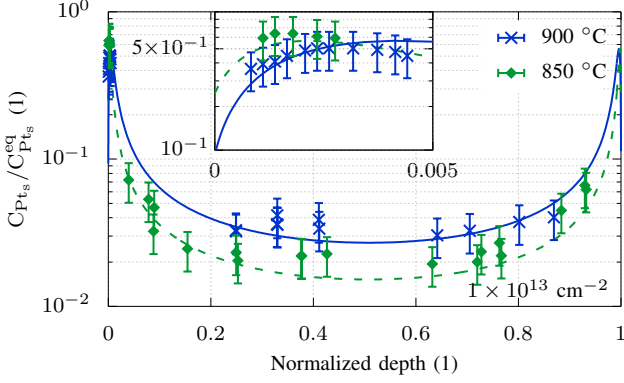
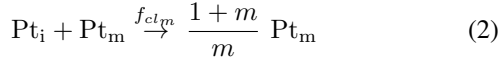
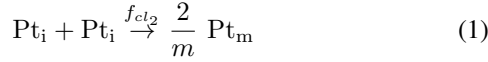


Fig. 3. DLTS measurements and simulation results of C_{Pt_s} after annealing at 850 (—) and 900 °C (---) with an implanted dose of $1 \times 10^{13} \text{ cm}^{-2}$. The lines show the simulation results of Pt diffusion from a PtSi layer using the model from Johnsson *et al.* [6] with C_i^{eq} from Badr *et al.* [1]. The inset shows the concentrations close to the surface.

precipitates. The Pt clustering was realized considering only three reactions, reducing the number of equations compared to classical nucleation theory considerably. The clusters were assumed to be immobile and of size m with two paths for cluster formation/growth; either via the reaction of two Pt interstitials, or when a Pt_i reacts with a Pt cluster (Pt_m).



The clusters are assumed to dissolve into m Pt interstitials.



f_{cl_2} , f_{cl_m} , and b_{cl} are the reaction rate constants.

D. Simulations of platinum diffusion

The simulation model was implemented in and solved by the general-purpose solver PROMIS [13]. Initial concentrations close to 0 were assumed for I and V before the Pt implantation. The as-implanted profile was obtained via Monte Carlo simulations using MCSIM [14]. It was read in by PROMIS as the initial concentration profile for Pt_s and I (+1 model). Dirichlet boundary conditions with the respective equilibrium concentrations were used for I and V, and Neumann boundary conditions were used for Pt_i (same at both surfaces). The Pt-cluster parameters were calibrated to fit the available data. The oversaturation of self-interstitials during the oxidation phase was not found to have a significant impact on the results and was therefore not considered in the simulations.

The measured data are compared to the simulation results in Fig. 4. The measurements after annealing at 850 °C are shown in (a) and (b), and the measurements after annealing at 900 °C are shown in (c), where data from Badr *et al.* [1] is also included (900 °C, 2 h, $5 \times 10^{12} \text{ cm}^{-2}$, 150 keV, 520 μm).

The simulation results fit all of the considered profiles in the bulk region. The fit for the case with a dose of $1 \times 10^{13} \text{ cm}^{-2}$ annealed at 850 °C is considerably improved compared to the results in Fig. 1. The activation energy of the dissolution rate

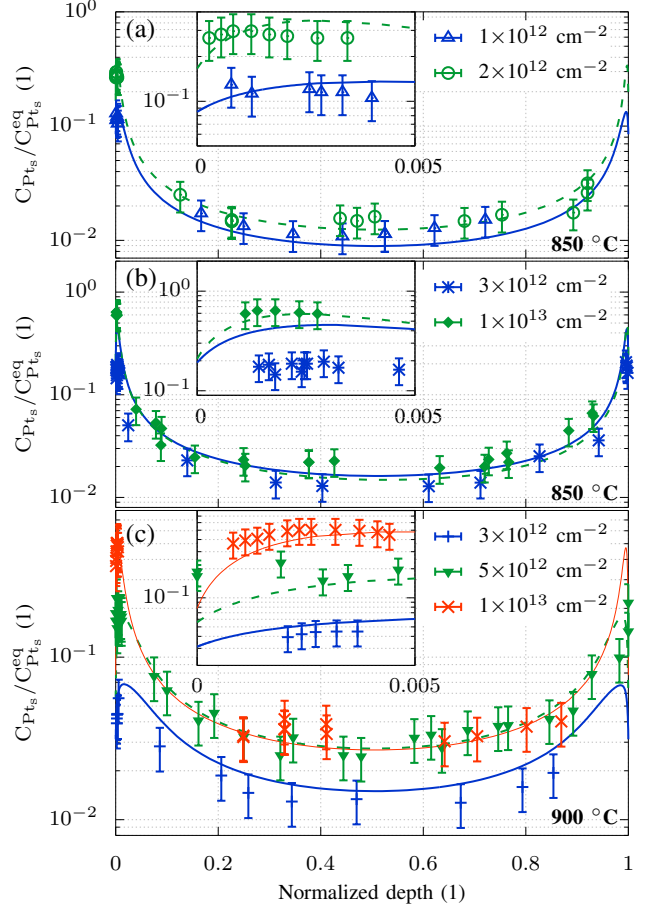


Fig. 4. DLTS measurements of C_{Pt_s} and the simulation results: a) 1×10^{12} (—), 2×10^{12} (---) and b) 3×10^{12} (—), 1×10^{13} (---) after annealing at 850 °C, and c) 3×10^{12} (—), 5×10^{12} (---), 1×10^{13} (—) at 900 °C. The $5 \times 10^{12} \text{ cm}^{-2}$ data was taken from Badr *et al.* [1]. The insets show the concentrations close to the surface.

b_{cl} is approximately 3.6 eV, which appears more reasonable than the 33 eV in the model of Badr *et al.* [1].

The fit close to the surface is good for all profiles but one. The new model predicts a too high concentration for the case with a dose of $3 \times 10^{12} \text{ cm}^{-2}$ annealed at 850 °C. It is noteworthy, that the concentration close to the surface is lower for a dose of $3 \times 10^{12} \text{ cm}^{-2}$ than for a dose of $2 \times 10^{12} \text{ cm}^{-2}$ (850 °C). This feature cannot be captured with the type of model suggested in this work.

IV. DEVICE SIMULATIONS

Hauf *et al.* [15] recently developed a TCAD simulation flow to predict and optimize the electrical performance of silicon power diodes. In this work, the Pt cluster model was implemented into the simulation flow to simulate a silicon diode with a Pt implantation energy of 80 keV, a dose of $5 \times 10^{12} \text{ cm}^{-2}$, and a diffusion temperature of 820 °C. In Fig. 5a, the simulation output of the Pt model of this work, as well as the output of the model by Badr *et al.* [1] are compared to measurements of the reverse recovery current transient of a diode during IGBT turn-on in a half-bridge configuration at nominal current and maximum operating temperature. The

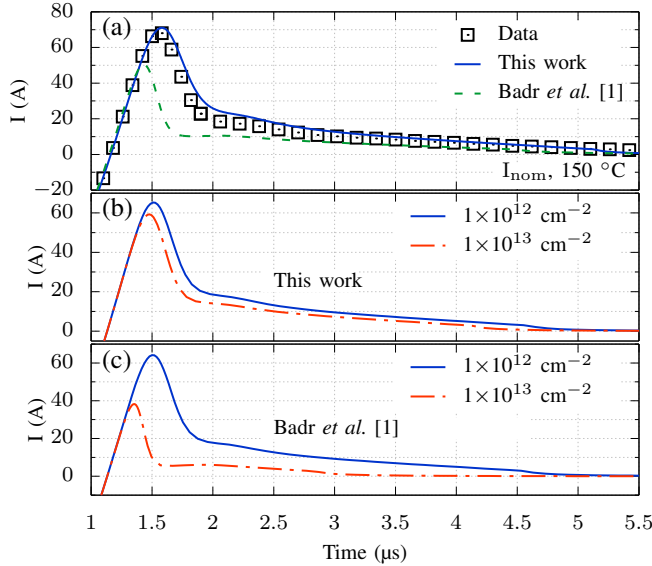


Fig. 5. Reverse recovery of a diode during IGBT turn-on in a half bridge configuration: (a) Comparison of simulations and experiment (black symbols) using the trap profile output of the model by Badr *et al.* [1] and the model from this work without any further adjustments. (b) and (c) show simulation results of the diode current for a Pt-diffusion temperature of 850 °C and implantation doses of 1×10^{12} and $1 \times 10^{13} \text{ cm}^{-2}$ using the model from this work and the model by Badr *et al.* [1], respectively.

developed model delivers more accurate results out of the box compared to the model by Badr *et al.*

Assuming a correct implementation of the physical properties of Pt_s in device simulation, it can be observed that the model by Badr *et al.* significantly overestimates the amount of Pt for the given process conditions, resulting in a too low reverse recovery current of the simulation. The Pt cluster model of this work, however, only slightly underestimates the amount of Pt_s . It should be noted that no measurements of the Pt_s profile for these process conditions are available and that the model was developed based on data in a higher temperature range (850 – 900 °C). The deviation between simulation and experiment for the reverse recovery charge Q_{rr} , and the reverse recovery losses of the diode E_{rec} amount to 13 % and 15 % for the new Pt cluster model, whereas the deviation is about –50 % and –49 % for the model by Badr *et al.*

When scaling the Pt_s profile to fit the dynamic reverse recovery behavior of the diode, an overall increase of 50 % is required. This value has to be compared to an overall reduction by a factor of four, which is required for the model by Badr *et al.* The 50 % deviation is close to the size of the error bars of the DLTS measurement (± 30 %).

The benefit of the newly developed Pt cluster model can also be demonstrated by comparing the simulated diode performance for the different models in Figs. 5b and 5c. Here, the simulated diode current transients are shown for a Pt-diffusion temperature of 850 °C and implantation doses of 1×10^{12} and $1 \times 10^{13} \text{ cm}^{-2}$. This corresponds to the process conditions of Fig. 1. The model from this work accurately reflects the minor increase in the Pt_s profile, which leads to a slight decrease of the reverse recovery current (Fig. 5b). In contrast, the model

by Badr *et al.* strongly increases the Pt_s profile for the higher dose, leading to a significant decrease in the diode current (Fig. 5c).

V. CONCLUSIONS

Some of the DLTS-measured profiles within this work show indications of platinum clustering/precipitation at higher temperatures than previously predicted [1]. It was most visible after annealing at 850 °C. HR EFTEM measurements and spectrum imaging indicated that the excess of platinum may form PtSi precipitates for high doses. It was possible to describe the experimental data to a large degree with the developed model for the investigated temperature range (850 – 900 °C). The model captures the incomplete incorporation of Pt at substitutional sites with increasing dose, which was observed in the measurements. The post-implantation annealing model was implemented in the full TCAD simulations and it showed significant improvement compared to the previously available model.

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