Modeling and Simulation of Low Temperature Activation Processes

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Abstract—**A method for simulating dopant activation at low temperatures is proposed and tested, with a proof of concept showing the expected behavior implemented.**

Index Terms—**Simulation, Simulated Annealing, Doping, Activation Analysis, Integrated Circuit Doping**

I. Introduction

FOR thin film transistor applications, the original designs used amorphous silicon. While having advantages from a processing perspective, this imposes a limitation on the speed of the devices being fabricated, which led to the development of techniques for the fabricating single crystal silicon on glass. Single crystal silicon has a higher mobility than amorphous silicon, allowing faster transistors to be fabricated, but the use of this technology leads to other challenges. With amorphous silicon and polysilicon transistors, dopant can be introduced during the deposition process. In single crystal silicon designs, however, dopant must be introduced separately through techniques such as ion implantation, and then thermally activated. For standard CMOS processes, this is commonly achieved through anneals done at or above 1000° Celsius. These temperatures cannot be used for single crystal silicon on glass, however, as the melting point of the glass used is approximately 600° Celsius. Recent work has shown that it is possible to activate implanted dopant at lower temperatures [1]. A portion of the data collected during this work can be seen in Figure 1 below, showing a pattern of activation and deactivation at various anneal temperatures.

While there are existing models designed for modeling dopant activation, there are no models designed to work in this temperature range. As a basis for developing a calibrated model for dopant activation at these temperatures, two existing models in the Silvaco ATHENA simulator were investigated. The first of these models is the transient activation model, which is intended to be used with the fully-coupled dopant diffusion model. In this model, the rate of change of active dopant is modeled as being inversely proportional to a time constant, which is calculated using an Arrhenius expression, with the equilibrium state being determined by a solid solubility limit. The second model is the dopant-defect clustering model, which is part of the PLS model. In this model, the simulation software keeps track of clusters formed by various combinations of dopants and defects, with the equilibrium state existing when the forward and reverse reaction rates for the growth of these clusters becomes balanced. [2]

II. Experimental Procedure

All simulations were performed using the Silvaco ATHENA simulator with a $1x10^{15}$ cm^{-3} background boron concentration, 1000 Angstroms of deposited oxide, 92 keV implant energy, and the introduction of interstitial clusters for implant concentrations above $1x10^{17}$ cm^{-3} with cluster factor of 1.4. The size of the substrate varied depending on the simulation, with many of the early simulations being performed with an eight micron depth, though once the junction depth issues were dealt with a two micron depth was used. As the experiment consisted only of one-dimensional simulations, the width of the simulated substrate was not a factor.

III. Results and Analysis

Each of these models exhibit problems when used at these temperatures, however. When simulating using the transient activation model at 600° Celsius, the simulated profile has a sheet resistance far higher than the experimental data. In addition to the lower activation, the shape of the profile is also different. As can be seen from comparing figures 2 and 3, the simulated data exhibits a clipped profile that isn't present in the experimental data. This is due to the fact that the model does not account for solid phase epitaxy, which in the experimental data causes the active dopant to be above the solid solubility limit. Due to this, the focus was then switched to the dopant-defect clustering model.

The initial difficulty encountered with the dopant-defect clustering model was due to transient enhanced diffusion. Due to the concentration of interstitials present, the implanted

dopant would diffuse far deeper into the substrate than was supported by the experimental data. To counteract this, the dopant diffusivity was set to be nearly zero, so that any diffusion that would occur would be negligible. Once this issue was dealt with, the results showed sheet resistances relatively close to the experimental data, as seen in Figure 4. However, when the percentages of activated dopants are analyzed, as seen in Figure 5, the active dopant was shown to be too high for low dose implants and too low for high dose implants where solid phase epitaxy would occur. This is due to the fact that, like the transient activation model, the damage to the silicon lattice is not being accounted for directly.

Another flaw seen in both of these models is that they fail to account for the deactivation seen in Figure 1. To model this activation, the approach chosen was to implement an interstitial-dependant solid solubility limit. Lower temperature anneals, such as at 600°C or 650°C, lead to an increase in free interstitials, which corresponds to the observed deactivation, while higher temperature anneals like 800°C lead to a rapid decrease in free interstitials, while the same temperatures lead to an increase in activation. To test this concept, a proof of concept was implemented in ATHENA using the fully coupled model without transient activation, which can be seen in Figure 6. While the exact sheet resistance values do not match up with the experimental values, they do trend in the correct directions. With additional work, the expression relating the solid solubility limit to concentration could be improved, which would lead to a more accurate model. Other work that must be done is to make this model compatible with the activation models that are present in ATHENA, as well as testing it at finer time steps.

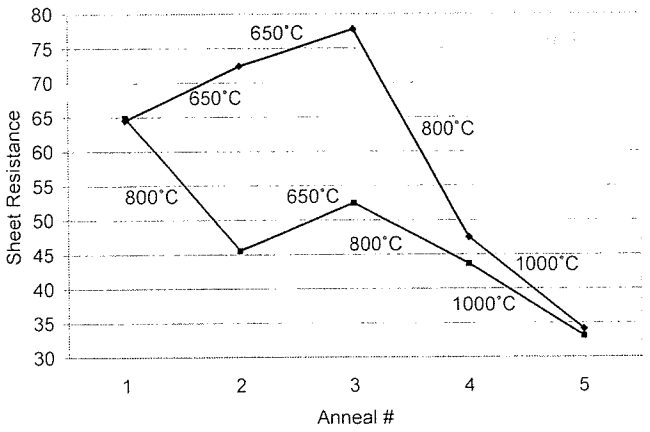

Fig. 1. Sheet resistance data collected after sequential anneal steps, showing the activation and deactivation of dopant over time.

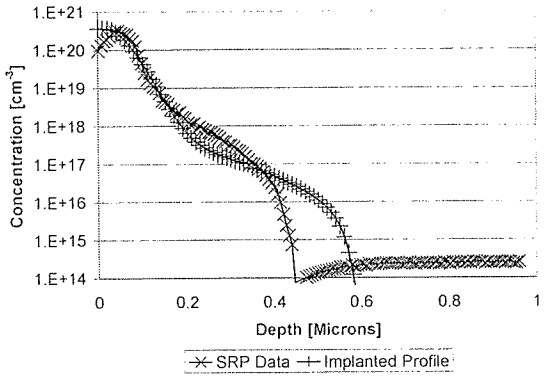

Fig. 2. SRP and implanted profile data for a $4x10^{15}$ cm^{-2} phosphorous dose implant after a one hour anneal at 600° Celsius

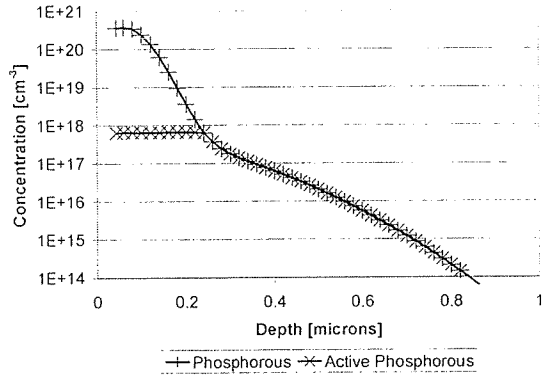

Fig. 3. Simulated chemical and active phosphorous profile data for a $4x10^{15}$ phosphorous dose implant after a one hour anneal at 600° Celsius, using the transient activation model

IV. Conclusions

The data collected in this experiment shows that it is possible to implement both activation and deactivation in ATHENA for use at low temperatures, though the functionality is not yet reached a usable level. The most promising design currently under consideration would be a combination of the PLS DDC model with the interstitial-dependent solid solubility limit, though the transienct activation model will remain under consideration

References

[1] Woodard, E.M., "Low Temperature Dopant Activation For Applications In Thin Film Silicon Devices." Master's Thesis, Rochester Institute of Technology, 2006.

[2] Silvaco, *ATHENA User's Manual*, Santa Clara: Silvaco, 1999.

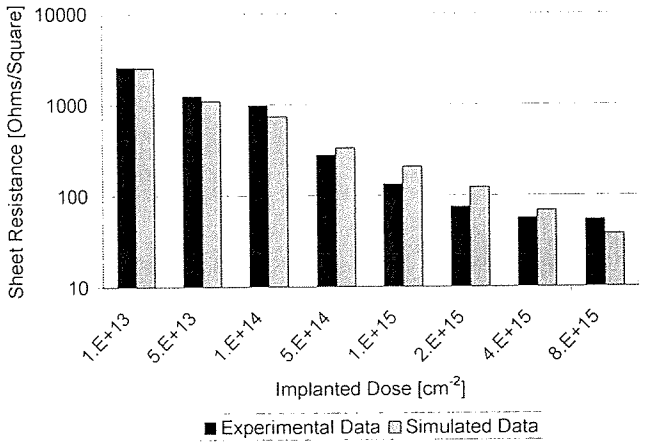

Fig. 4. Plot of sheet resistances for various doses after a one hour anneal at 600° Celsius, from both experimental data and simulations

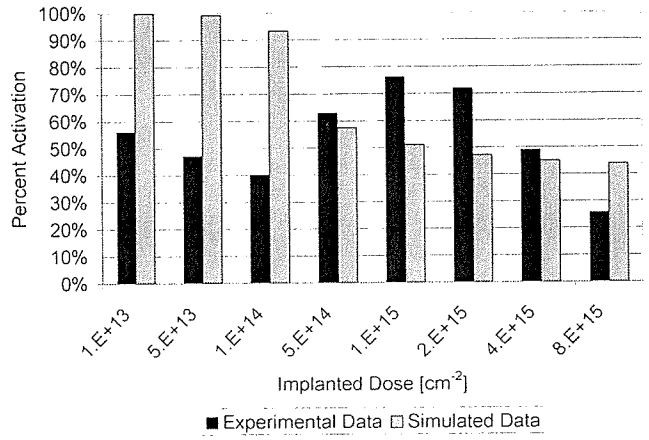

Fig. 5. Plot of percent activation for various doses after a one hour anneal at 600° Celsius, from both experimental data and simulations

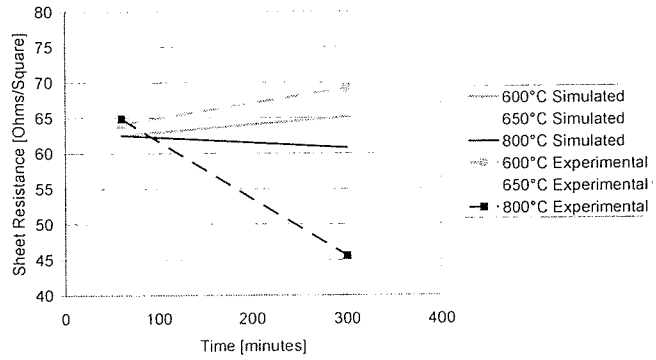

Fig. 6. Plot of experimental and simulated sheet resistance as a function of time for various anneal treatments using the interstitial-dependent solid solubility limit model. The initial point for all six data series is after a one hour anneal at 600°C.