Analysis of Very High Energy Implantation Profiles at Channeling and Non-Channeling Conditions

Serguei I. Kondratenko Axcelis Technologies, Inc. 108 Cherry Hill Drive, MA, USA Serguei.Kondratenko@axcelis.com Leonard M. Rubin Axcelis Technologies, Inc. 108 Cherry Hill Drive, MA, USA Leonard.Rubin@axcelis.com Eric A. G. Webster OmniVision Technologies, Inc. 4275 Burton Dr. Santa Clara, CA, USA Eric.Webster@ovt.com

Abstract—This paper presents SIMS data for very high energy ion implantations of arsenic (1.9-8.0 MeV), boron (2.0-5.0 MeV), and phosphorus (4.0-8.0 MeV) from Axcelis' PurionTM VXE implanter with comparison to TCAD simulation results. Arsenic is found to be highly sensitive to implant angle, requiring beam angle control better than 0.05°, and to be relatively insensitive to damage and is generally in good agreement with simulation. It is reported for the first time that the As profile for tilt/twist=1°/0° is more channeled than 0.5°/22°, indicating the significance of planar channeling for this condition even at tilt angles ≤1.0°. Boron is well described by the TCAD model except for a 2.0 MeV highly channeled implant where it underestimates the channeling. Phosphorus is found to be the most challenging to simulate with a general overestimation of the channeling tail.

Keywords—ion implantation, high energy ions, dopant distribution profiles, TCAD modeling

I. INTRODUCTION

Technology development for advanced CMOS image sensors, discrete power devices, and non-volatile memory has resulted in requirements for high energy ion implanters that can operate at higher energy ranges. In particular, the need to improve the quantum efficiency of image sensors for red and near-infrared photons has driven the requirement for very high energy implants into the photodiode region with precise angle and dose control [1].

In this paper we present experimental and modeling results for very high energy ion implantations from Axcelis' PurionTM VXE implanter, which is based on an RF-linear accelerator architecture and was developed to extend the maximum energies of Purion XE serial high energy system [2]. It provides a maximum high energy capability of 5.0 MeV for boron and 8.0 MeV for phosphorus and arsenic. In many cases high energy ions are implanted at a normal angle to the crystalline substrate to minimize shadowing effects for structures with high aspect ratios and/or to use channeling effects to form deeper layers. This makes these implants very sensitive to beam angle alignment and control [3].

Prior to this work, few dopant profiles in silicon at these energies and angles have been published or compared to TCAD simulations. A shortage of reference data especially for high energy arsenic was another motivation for this work.

II. EXPERIMENTAL

SIMS analysis of dopant profiles was performed on (100) Si-wafers implanted with maximum energies of singly and multiply charged ions of boron, phosphorus, and arsenic. Certified test wafers with a slice angle offset from <001> of $<0.05^{\circ}$ were used for these experiments. Wafers from the same ingot were used for each particular test. The test wafer surface angle offset was verified using the TW V-curve method [5]. The angle of wafer cut offset was then accounted for in subsequent implants by changing the tool angle to achieve the desired implant. All implantations were performed on the Purion VXE single wafer implanter. The implanted dose was $1 \times 10^{13} \text{ at/cm}^2$ for most samples (unless otherwise specified) to provide reliable SIMS measurement with low background noise and minimize damage accumulation effects on dopant profiles.

Implant profiles were simulated using Synopsys Sentaurus Process Monte-Carlo using default parameters except where otherwise indicated [4]. A beam divergence of 0° was used for all simulations, a native oxide thickness was assumed on the wafer, and the number of simulated ions was 10,000.



Fig. 1. TW signal versus tilt angle for 4.5 MeV, $1x10^{13}at/cm^2$ arsenic implantation (a). Expanded TW V-curve around a normal angle together with actual tilt angle calculated values (b).

III. EXPERIMENTAL AND SIMULATION RESULTS

A. Arsenic SIMS Profiles and TCAD Modeling

A set of wafers from the same ingot were implanted with arsenic, 4.5 MeV. The tilt angle was varied from 0° to 1.5° with 22° twist angle. The Thermal Wave (TW) response versus tilt angle is shown in Fig. 1(a). Actual values of the implantation angles relative to the (100) plane were estimated using the TW curve around normal angle fitted with a 2nd order polynomial as shown in Fig. 1(b). Assuming

the curve minimum position corresponds to true zero implantation angle, an offset of 0.02° was estimated for the tilt angles relative to the (100) plane. The arsenic SIMS profiles are shown in Fig. 2. Significant channeling reduction was observed at tilt angles of 0.25° and higher. As expected, very high energy profiles are found to be highly sensitive to the ion beam incident angle. At tilt angles $\leq 0.25^{\circ}$ the SIMS profiles show some difference in channeling tails even for tilt angle variations as low as 0.04°. This drives higher requirements for the angle alignment and control during implantation relative to the wafer crystalline plane.



Fig. 2. SIMS profiles for As, 4.5MeV, $1x10^{13}at/cm^2$ for different implantation tilt angles, with a 22° twist angle.



Fig. 3. SIMS profiles for As, 4.5MeV, $1x10^{13}at/cm^2$. Tilt angles 0, 0.5° and $1.0^\circ.$ Comparison of 0° and 22° twist angles.

Arsenic SIMS profiles for twist angles of 0° and 22° are shown in Fig. 3. At zero twist angle the (004) planar channel is sufficiently deep that profiles for tilts 0.5° and 1.0° are very close. TW maps were measured for these wafers after implantation. As expected, the TW value was higher for 1.0° compared to 0.5°. This suggests that higher damage does not influence the arsenic profiles for this condition. The profile for tilt/twist=1°/0° is more channeled than for 0.5°/22°, indicating the significance of planar channeling for this condition even at tilt angles $\leq 1.0^\circ$. We also found that arsenic profiles did not show any dependence on the beam current during implantation for a 10X beam current change. Fig. 4 overlays arsenic SIMS profiles implanted at normal angle with energies of 1.9, 3.0, 4.5, and 8.0 MeV using multiply charged ions. All profiles show a deep channeling tail. Experimental and modeled As profiles at 8.0 MeV are shown in Fig. 5. For non-channeling angles (5°/27°) the model demonstrates a good agreement with SIMS data but slightly overestimates channeling tail of a random direction implant. For zero tilt angle a good agreement with experimental data is observed for different ion doses of 2.5×10^{12} , 5×10^{12} , and 1×10^{13} at/cm². All fits were achieved using the OVT model with the same input settings, which suggests negligible influence of damage and excellent angle control achieved on the implanter.



Fig. 4. SIMS profiles for As, 1×10^{13} at/cm² implanted at energies of 1.9, 3.0, 4.5, and 8.0 MeV. 0° tilt and twist.



Fig. 5. Experimental and simulated profiles for As, 8MeV. Dose 2.5×10^{12} , 5.0×10^{12} , and 1.0×10^{13} at/cm² (tilt/twist 0°/0°) and 5×10^{12} at/cm² (tilt/twist 5°/27°).

B. Boron SIMS Profiles and TCAD Modeling

In Fig. 6 boron experimental and modeled profiles are shown for a non-channeling implantation angle. Similar to arsenic, the simulated profiles agree well with experimental data except that TCAD slightly overestimates the channeling tail of all three implants. Changing default model parameters did not result in improved profile fits.

Normal implantation angle SIMS and TCAD profiles are shown in Fig. 7. Generally good agreement is seen between experimental data and simulated profiles using default model parameters. Interestingly, 3.6 MeV and 5.0 MeV agree better than 2.0 MeV, where the channeling concentration peak on the SIMS profile is significantly higher than on the TCADsimulated profile. The only way found to make the TCAD channeled peak higher than non-channeled peak was to increase the Debye temperature. With a higher Debye temperature, the TCAD profile fits better for both the channeled and un-channeled peak of 2.0 MeV boron, but the validity of this method is questionable. Further work on model improvement for 2.0 MeV boron is needed.



Fig. 6. Experimental and simulated profiles for B, 2.0 and 3.6 MeV $(1x10^{14}at/cm^2)$, and 5.0 MeV $(1x10^{13}at/cm^2)$. Tilt/twist angle 5°/27°.



Fig. 7. Experimental and simulated profiles for B, 2.0, 3.6, and 5.0 MeV. Tilt/twist angle $0^{\circ}/0^{\circ}$. For 2MeV simulated profiles are shown for two Debye temperatures 519K (default) and 1100K.

C. Phosphorus SIMS Profiles and TCAD Modeling

SIMS profiles and TCAD simulation for phosphorus at a non-channeling implant angle are shown in Fig. 8 for energies 4.0, 6.0, and 8.0 MeV. Similar to As and B, the model overestimates the channeling tails. In the phosphorus case this difference is higher, especially for 8.0 MeV and lower dose 1×10^{13} at/cm². Doubling the implantation damage de-channeling factor (amor.par) [4] for 4.0 and 6.0 MeV phosphorus brings TCAD very close to the SIMS profile (Fig. 8). However, for phosphorus 8MeV TCAD vastly overestimates channeling for the lower dose of 1×10^{13} at/cm². The TCAD damage de-channeling had to be unrealistically increased 64X to fit the channeling profile.

Phosphorus SIMS profiles for 4.0, 6.0, and 8.0 MeV at 0° tilt are presented in Fig. 9. Phosphorus profiles shapes are very different from to arsenic; no deep channeling tail is observed. The projected range and the distance between the channeled and un-channeled peaks increases sub-linearly with energy in this energy range. TCAD modeling applied using same default parameters for all three phosphorus energies shows poor agreement with experimental data. To

improve fitting to the SIMS profiles, the TCAD parameters had to be optimized separately for each energy.



Fig. 8. Experimental and simulated profiles for P at 4.0 and 6.0 MeV $(1x10^{14}at/cm^2)$, and 8.0 MeV $(1x10^{13}at/cm^2)$. Tilt/twist angle 5°/27°.



Fig. 9. Phosphorus SIMS profiles for 4.0, 6.0, and 8.0 MeV. Tilt/twist angle $0^{\rm o}/0^{\rm o}.$



Fig. 10. Experimental and simulated profiles for phosphorus, 4.0 MeV. Tilt/twist angle 0°/0°. TCAD modeling with different tilt angle.

Experimental and simulated profiles for phosphorus, 4 MeV at tilt 0° are shown in Fig. 10. TCAD suggests higher channeling as compared to SIMS profiles. Modeling with low tilt angles 0.1° , 0.2° , and 0.3° show that P 4.0 MeV at tilt=0° has the best agreement at TCAD tilt= 0.3° . Either this is the (unexpected) actual implant angle or the TCAD model needs improvement. Further investigation is required.



Fig. 11. Experimental and simulated profiles for phosphorus, 6.0 MeV. Tilt/twist angle $0^{\circ}/0^{\circ}$. TCAD modeling with different electronic stopping power (LSS.pre).



Fig. 12. Experimental and simulated profiles for phosphorus, 8.0 MeV. Tilt/twist angle 0°/0°; TCAD modeling with different implantation damage.



Fig. 13. P and As 8.0 MeV SIMS and TCAD profiles comparison. Tilt/twist angle $0^{\rm o}/0^{\rm o}.$ Default TCAD parameters.

For P 6.0 MeV implants, (Fig. 11) the profile peak position cannot be fit with the default TCAD parameters. The electronic stopping power in TCAD has to be reduced by ~8% to fit the SIMS peak position. This was not observed for other energies; all other phosphorus profiles fit with the default LSS.pre [4] parameter of 1.25. This unusual result suggests the TCAD model needs further improvement. For the maximum P energy of 8.0 MeV, increasing the TCAD damage de-channeling 4X slightly improves fitting in places (Fig. 12), but does not provide satisfactory agreement with the SIMS profile.

P and As profiles at 8.0 MeV are presented in Fig.13. The channeling profile shapes are significantly different between P and As (blue and green curves). The projected ranges are very close despite the large mass difference between P and As. It is thought possible that the relatively higher and complex influence of damage on phosphorus could contribute to the difficulty of modeling the profile. Further model adjustments are needed to match the phosphorus channeling profiles.

IV. CONCLUSIONS

We analyzed SIMS profiles of B ions with energies up to 5.0 MeV and P and As ions with energies up to 8.0 MeV implanted on Axcelis' Purion VXE implanter. By careful control of the ion beam parameters and the wafer crystal cut offset, we demonstrated that all species and specifically arsenic are extremely sensitive to tilt and twist angle. We report for the first time that the (004) planar channel causes an As implant at $1.0^{\circ}/0.0^{\circ}$ tilt/twist to be more channeled than at $0.5^{\circ}/22^{\circ}$! For energies > ~4.0 MeV, better than 0.05° beam angle control is required to control channeling effects.

TCAD modeling using default parameters for implantations at non-channeling conditions demonstrates good agreement with SIMS but with a slight overestimation of the channeling tail for all 3 species. Normal implants are more difficult to simulate than randomized conditions, with the B 2.0 MeV results suggesting something is missing from the TCAD model for boron. The phosphorus results for tilt 0° and 5° suggest a larger influence of implantation damage on channeling than for As or B. Consistent with the SIMS results, Arsenic channeling is found to be highly sensitive to the implant angle. TCAD overall performs well but requires improvement for the high energies achievable on the Purion VXE implanter.

ACKNOWLEDGMENT

The authors would like to thank EAG Laboratories for the SIMS analysis and Synopsys for TCAD model development and fruitful discussions on Debye temperature and beam parameters.

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