Modeling the Effect of Source/Drain Sidewall Spacer Process on Boron Ultra Shallow Junctions

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***Abstract*— A novel model is developed to explain the effect of the source/drain sidewall spacer process on boron drain extension formation. A diffusion model for hydrogen in the source/drain sidewall spacer is developed and combined with a model for boron diffusion in oxides. The model is first calibrated to hydrogen out-diffusion data from Nuclear Reaction Analysis (NRA) and then to boron diffusion data from Secondary Ion Mass Spectroscopy (SIMS). Seemingly anomalous changes in boron junction depths with variation in sidewall spacer deposition conditions are explained by this model. The model is applied to TCAD process/device simulations to understand the effect of sidewall spacer on CMOS device performance.**

I. Introduction

Fig. 1 shows a schematic representation of a CMOS structure to illustrate the different layers after drain extension formation. After the PMOS drain extension boron implant, an oxide layer (oxide1) is deposited. This is followed by a nitride and then another oxide (oxide2) deposition. The oxide2 and nitride layers are then etched to form source/drain spacers. The deep source/drain is then implanted and an activation anneal is done. Recent work showed the importance of this source/drain sidewall spacer process on the diffusion and retention of boron in silicon [1]. In particular, changes in nitride deposition process (e.g. precursor, gas flow ratio (%N) during deposition) can lead to a large change in drain extension boron junction depth. Nitrides that retain higher concentrations of hydrogen in oxide1 were found to result in shallower junctions. Shallower junctions were a result of increased dose-loss of boron from the silicon to oxide. Hydrogen in oxide was suggested to increase this dose-loss by increasing boron diffusivity in oxide1 [1].

II. Proposed Model

Fig. 2 represents a schematic illustration of the models and interactions considered in this work. Primarily, we model the diffusion and segregation of hydrogen through the various spacers (Si/Oxide1/Nitride/Oxide2) and its effect on boron diffusion in silicon and oxide. Deposited oxides (oxide1) contain large amounts of hydrogen. The hydrogen in this oxide is highly mobile and diffuses out of the oxide readily. Oxides of interest in this work are less dense deposited oxides; therefore, we assume diffusion of hydrogen is mediated by only a neutral H^0. This assumption enables us to exclude ionic charge balance.

Various experiments in literature have found enhancement of boron diffusion in oxide with increasing hydrogen concentration [1], [2], [3]. Experiments on boron penetration have reported an increase in boron diffusivity in oxides with higher hydrogen concentrations [4]. We model boron diffusion in oxide as: $D_{\mathrm{B}} = D_{\mathrm{B}}^{\mathrm{Ox}}(1 + (\frac{C_{\mathrm{H}}}{C_{\mathrm{H}}^{\mathrm{ref}}})^n)$, where D^{Ox} is the diffusivity of boron in pure oxides, and C_{H} is the concentration of hydrogen in the oxide. A nitride on top of the oxide (oxide1) acts as a barrier to the diffusing hydrogen. Due to the different as-deposited density, different nitrides lead to different hydrogen concentration in the oxide during subsequent annealing. Higher concentrations of hydrogen in oxide1 increase boron diffusion in the oxide. This allows more boron to segregate out of the silicon and into the oxide. Consequently, this reduces the extent of boron diffusion in silicon as observed experimentally.

III. Model Verification

Hydrogen diffusion parameters are estimated by calibrating to hydrogen out-diffusion NRA data [1]. Fig. 3 shows comparison of the model to out-diffusion of hydrogen from a 1000Å oxide layer into the ambient. For our present study, we consider the effect of two different nitride deposition processes namely Nitride A and Nitride B. Nitride A uses a BTBAS precursor whereas Nitride B uses a Silane based precursor. Both of these are low temperature ($< 700°\mathrm{C}$) deposition processes. However, Nitride B is likely to be more dense than Nitride A due to the difference in deposition temperature. No visible dopant diffusion is observed during the deposition. Fig. 4 shows the effect of changing only the nitride process on hydrogen diffusion. After annealing Nitride B retains a higher hydrogen concentration in the oxide. Hydrogen segregation parameters capture this difference well.

A boron-interstitial cluster model calibrated to inert anneals is used as a reference for boron diffusion [6] in silicon (Fig. 5). Comparison of the model to boron SIMS profiles from Kohli *et al.* [1] is shown in Figs. 6–9. Fig. 6 shows model calibration representing effect of Nitride A process. As we observed in Fig. 4, Nitride A is a less effective barrier against hydrogen diffusion; hence the dose loss and reduction in junction depth is minimal. Fig. 7 shows the effect of the Nitride A deposition

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process on the boron profiles in oxide1 measured by Time Of Flight SIMS (TOF-SIMS). An enhancement in the boron diffusivity is observed after a 1050°C anneal and is captured by the model. Fig. 8 shows model calibration representing effect of Nitride B process. Nitride B is the more effective barrier to hydrogen diffusion. Hence this leads to increased dose loss and out-diffusion of boron into the oxide from silicon. Fig. 8 also shows a higher concentration of boron in the oxide relative to the reference (no nitride case). Thus, Nitride B also results in shallower junctions compared to Nitride A process (Fig. 9). Calibrating to experimental data (Figs. 6–9), we find a high order concentration dependence on the enhancement of boron diffusion in oxide ($n = 1.5$–2). A higher order (n) suggests complex interaction of boron with multiple hydrogen atoms.

IV. Application of Model

Comparison of PMOS devices fabricated using the two different nitride processes shows devices processed with Nitride B exhibit better short channel immunity. This is observed as a better rolloff in the saturation threshold voltage for the Nitride B process (Fig. 10). Nitride B also exhibits a lower gate to drain overlap capacitance (20%). Simulations incorporating our proposed model match the experimental observations (Fig. 10). This phenemenon is captured by the model and can be applied for further device optimization.

V. Conclusion

A new boron diffusion model is developed that predicts the observed large variation in boron junction depths (80Å) due to changes in spacer-nitride precursor chemistry. The nature of the nitride is shown to influence the hydrogen permeability and thus change boron diffusivity in oxides. The model incorporates diffusion of hydrogen in the sidewall spacer layers coupled with enhanced boron diffusion ($\sim 10000x$) by hydrogen in the oxide. The model is successfully applied to TCAD process/devices simulations to predict the effect of nitride sidewall spacers on device behavior.

References

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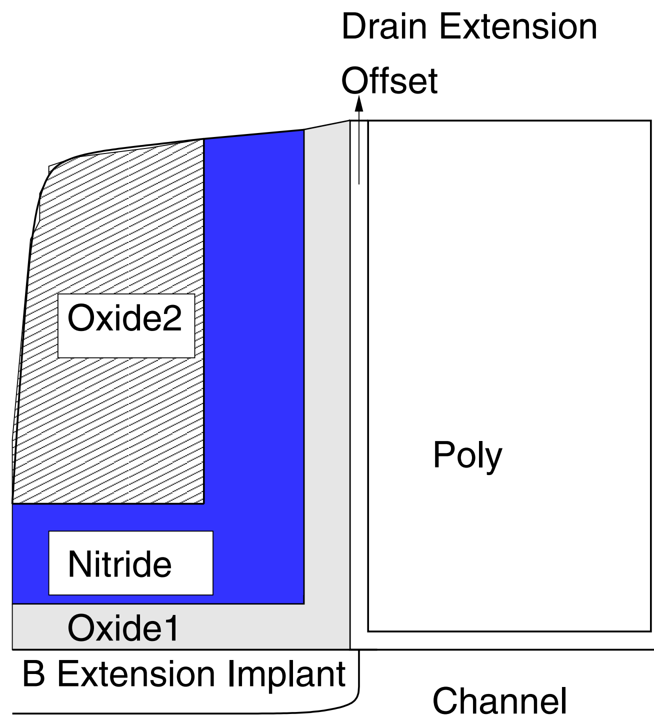

Fig. 1. Figure showing schematic illustration of various spacers during the formation of boron drain extensions.

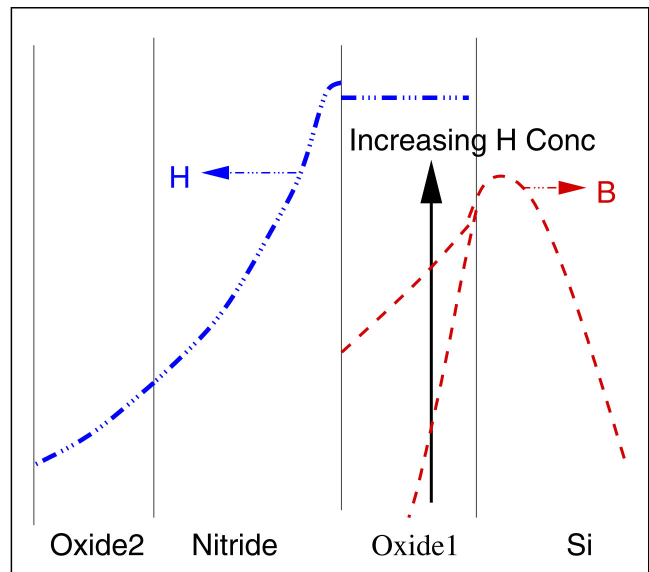

Fig. 2. Schematic illustration of the hydrogen model and boron diffusion in the spacer layers. The presence of hydrogen in the oxide enhances the boron diffusivity in the oxide. This increases the boron doseloss to the oxide from silicon.

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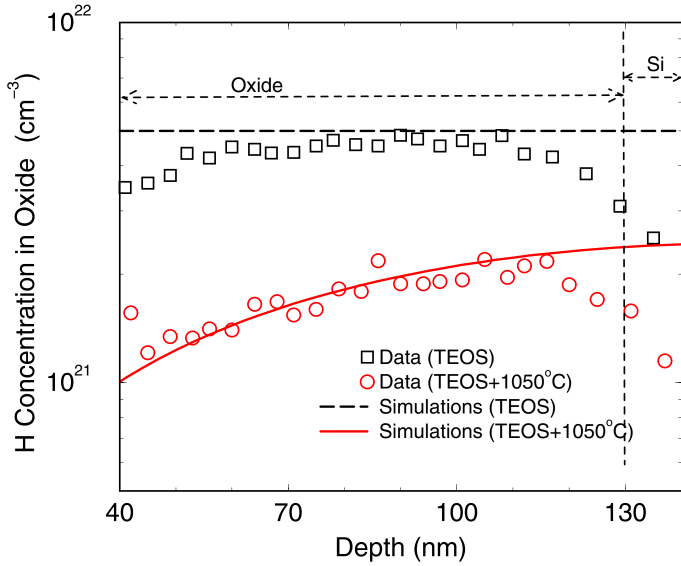

Fig. 3. Comparison of experimental hydrogen profiles (from NRA) to simulations illustrating hydrogen out-diffusion from a 1000Å oxide layer into the ambient.

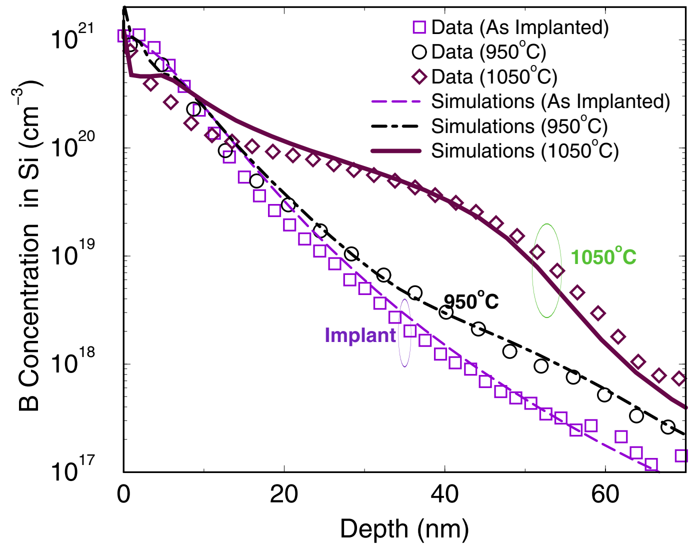

Fig. 5. Comparison of simulations to boron profiles in silicon after either a 950°C or 1050°C anneal. After implantation an oxide is deposited prior to annealing. The wafers however do not undergo a nitride process.

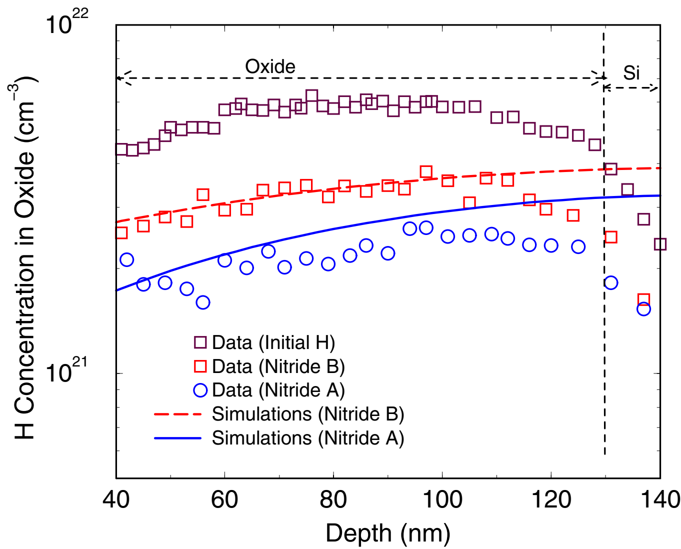

Fig. 4. Comparison of experimental hydrogen profiles (from NRA) to simulations for a 1000Å oxide layer deposited with either Nitride A or Nitride B. The wafers undergo a 1050°C anneal after the nitride deposition. The retained hydrogen is higher in case of Nitride B.

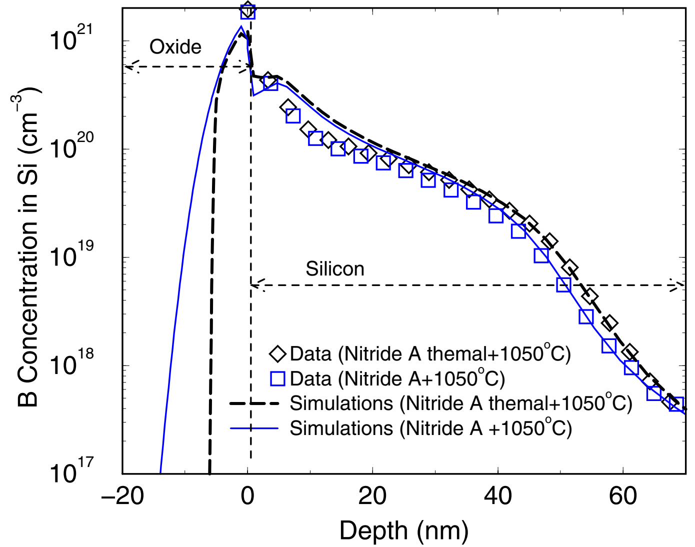

Fig. 6. Comparison of simulations to boron profiles in silicon after a 1050°C anneal. The wafer s undergo Nitride A deposition after the oxide1 deposition. The reference wafer (Nitride A thermal) undergoes the thermal budget of the Nitride A process with no actual nitride deposition.

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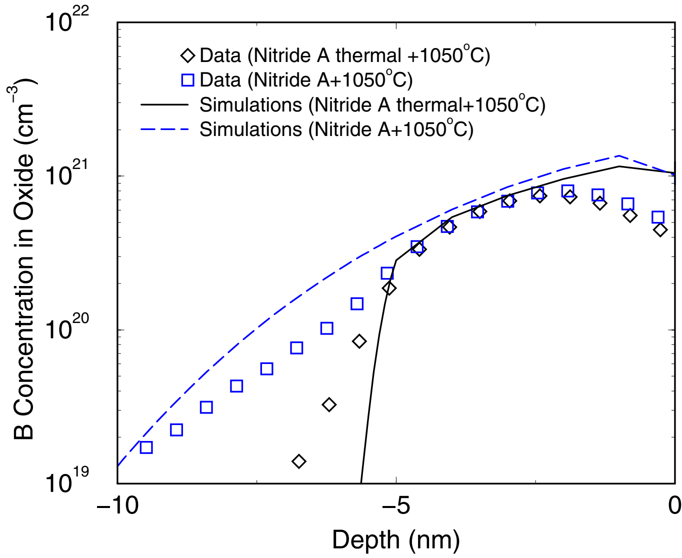

Fig. 7. Boron TOF-SIMS profiles in oxide1 after the 1050°C anneal for samples from Fig. 6 show impact of the presence of the Nitride A deposition process. The model compares well.

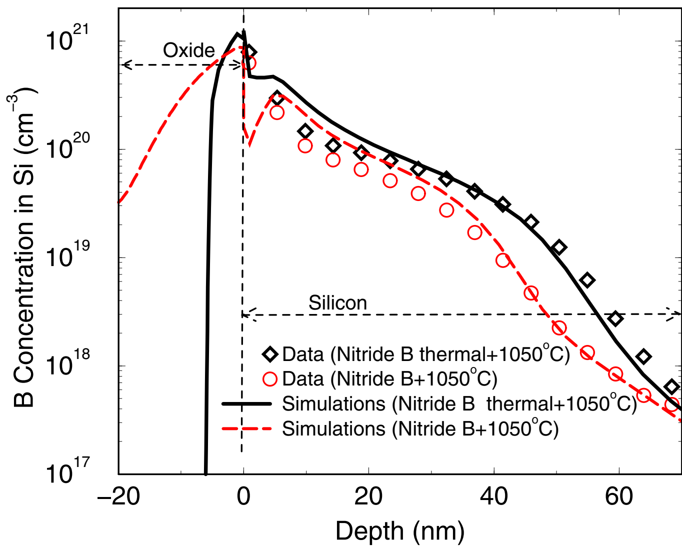

Fig. 8. Comparison of simulations to boron profiles in silicon after a 1050°C anneal. The wafers undergo a Nitride B deposition after the oxide1 deposition. The reference wafer (Nitride B thermal) undergoes the thermal budget of the Nitride B process with no actual nitride deposition.

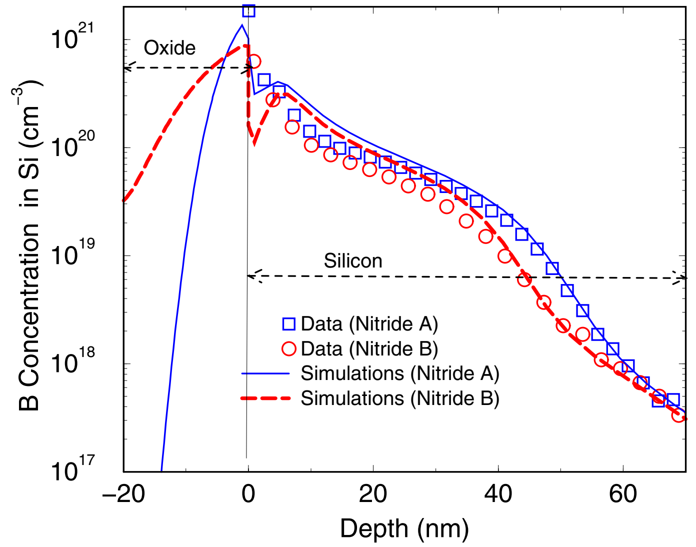

Fig. 9. Comparison of boron junctions formed using either a Nitride A or a Nitride B process. The Nitride B process retains a larger concentration of hydrogen in oxide (oxide1) leading to larger dose loss from silicon. Thus resulting in a shallower junction in silicon.

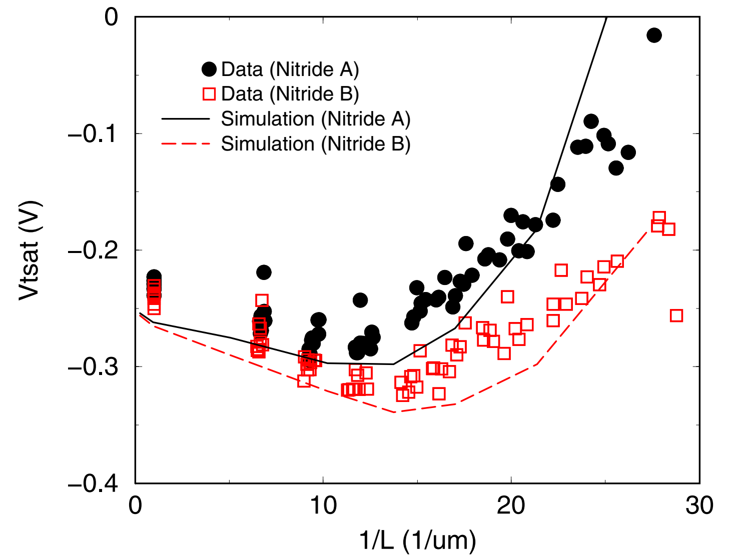

Fig. 10. Comparison of threshold voltage in saturation for PMOS devices fabricated using Nitride A and Nitride B process. Full flow process and device simulations show a similar change.

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