Change of electrical characteristics of a p-type MOSFET via hydrogen effect on boron redistribution

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***Abstract*—We present a hydrogen-assisted enhanced boron diffusion model in oxide. By introducing the B+OH reaction and BOH diffusion, the model could reproduce the enhanced B diffusion in the presence of high concentrations of hydrogen, which has been reported by previous studies. The model was applied to predict the B profile in the p-type MOSFET and the resulting B profiles were used to predict the threshold voltage (Vth) and the short channel effects (SCE). The simulation results are in good agreement with the measurements. Therefore, the model would be beneficial to optimize the H-involved process conditions.**

Keywords—Hydrogen, Boron diffusion, PMOSFET, Threshold voltage, Short channel effect.

I. INTRODUCTION

In semiconductor device fabrication processes, hydrogen is introduced into the device from many sources including hydrogen atmosphere annealing, precursor materials, etc. [1-4]. Due to the light mass of the hydrogen, it diffuses very fast and reaches to the various parts of a device causing unexpected changes in the device characteristics [5]. Previous studies have shown the enhanced boron diffusion in oxide in the presence of high concentrations of hydrogen at high temperatures above 800℃ [6-9]. They attributed the enhanced boron diffusion to the additional hopping network created by hydrogen-decorated oxygen (OH) sites having a lower diffusion activation barrier compared to the original hopping sites.

This phenomenon has a significant impact on the device characteristics of p-type MOSFETs (PMOSFETs) because the increased boron penetration through the gate oxide from the p-type polysilicon gate or stronger boron out-diffusion from the source/drain (S/D) to the oxide layers can significantly change the boron concentration in the channel or S/D. These accelerated boron movements result in two ways. The first one is lowering the absolute value of the threshold voltage ($|V_{th}|$) by increasing the boron concentration in the channel. Another one is reducing the short channel effects (SCE) with mitigating drain induced barrier lowering (DIBL) effect by reducing the boron concentration in the lightly doped drain (LDD) overlap.

In this paper, we propose a hydrogen-accelerated boron diffusion model in oxide. By constructing the boron reaction and diffusion equations affected by hydrogen concentration,

our model could reproduce experimental measurements in terms of $|V_{th}|$ and SCE under different concentrations of hydrogen.

II. Methods

Fig. 1 shows the doping of a typical PMOSFET and the two major transport pathways of boron affected by hydrogen concentration. The first diffusion path is from the highly boron doped polysilicon gate to the silicon channel region through the gate oxide. The other path is boron out-diffusion from the highly B doped S/D region to the gate spacer oxide [10, 11]. Higher hydrogen concentration accelerates the boron penetration via the first pathway, resulting in increased boron concentration in the channel region and decreased $|V_{th}|$. The enhanced out-diffusion via the second pathway is also expected to suppress the short channel effect (SCE) by reducing the amount of boron in the S/D regions.

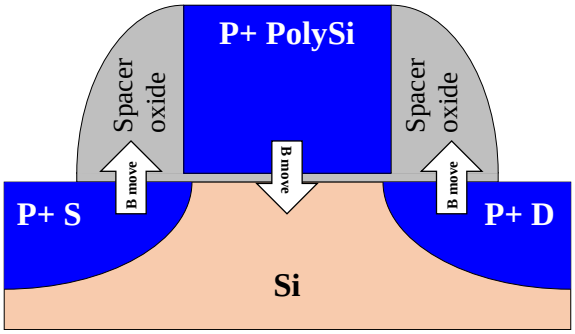

Fig. 1. The schematic image of a typical PMOSFET and hydrogen assisted boron movement.

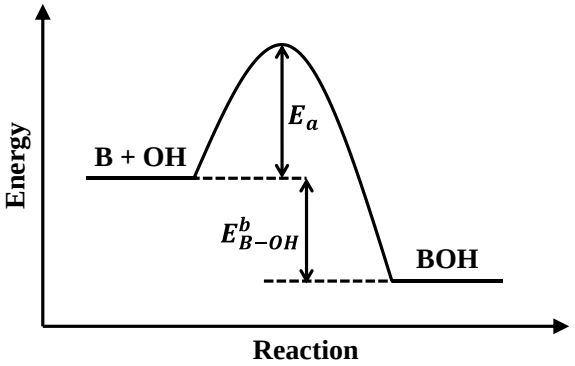

Fig. 2. The energy diagram of the reaction between boron (B) and hydroxide (OH) with the activation (E_a) and binding energy (E^b_{B-OH}) in the oxide.

To model the enhanced boron diffusion in the oxide bulk, we assumed that hydrogen atoms fully react with oxygen to form hydroxide (OH) and introduced the reaction between boron (B) and hydroxide (OH) in the oxide. Fig. 2 shows the energy diagram of this reaction with the activation (E_a) and binding (E^b_{B-OH}) energy. The reaction equations are given by

$$B + OH \leftrightarrow BOH, \quad \text{(Eq. 1)}$$

$$R = 4\pi r(D_B + D_{OH})\left(C_B \cdot C_{OH} - \frac{C_{BOH}}{K_{eq}}\right), \quad \text{(Eq. 2)}$$

$$K_{eq} = \frac{C^{eq}_{BOH}}{C^{eq}_B \cdot C^{eq}_{OH}} = \frac{\Theta}{C_0}\exp\left(-\frac{E^b_{B-OH}}{kT}\right), \quad \text{(Eq. 3)}$$

where R is the reaction rate, r is the capture radius of the pairing reaction, D_X is the diffusivity of the corresponding species X, C_X is the concentration of the species X, K_{eq} is the equilibrium constant of the reaction, C^{eq}_X is the equilibrium concentration of species X, Θ is the number of possible configuration of BOH, C_0 is the site density of oxygen in the oxide, and E^b_{B-OH} is the binding energy between B and OH. In Eq. 2, $D_B + D_{OH}$ is simplified to D_{OH} because OH diffuses much faster than B, which reflects our assumption of the uniform distribution of hydroxide (OH) in the oxide bulk.

In addition, we constructed diffusion equations for B (Eq. 4.) and BOH (Eq. 5) by taking into account the reaction rate (R) of both species. In the model, boron diffuses in two different flux forms described by

$$\frac{\partial C_B}{\partial t} = -\nabla(D_B \nabla C_B) - R, \quad \text{(Eq. 4)}$$

$$\frac{\partial C_{BOH}}{\partial t} = -\nabla(D_{BOH} \nabla C_{BOH}) + R, \quad \text{(Eq. 5)}$$

where D_{BOH} has a lower activation energy compared to D_B.

To enable BOH transport across the interface, the three-phase segregation model was applied. In the model, when BOH reaches the interface between the oxide and silicon, only B is trapped, leaving OH behind to minimize the disruption in the calibrated pre-existing model parameters in the polysilicon gate, silicon substrate and oxide. Fig. 3 represents the three-phase segregation model for the movement of BOH at the interface between the oxide and silicon. The grey arrows describe transport parts of the pre-existing model where boron diffuses in the form of boron atom (B) in the oxide and boron interstitial pair (BI) in the silicon. Whereas, the black arrows show the element movements influenced by the hydrogen concentration in the device.

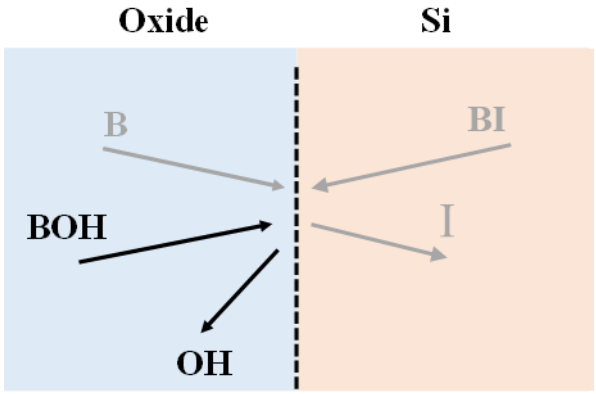

Fig. 3. The three-phase model at the interface between the oxide and silicon. The grey arrows show the transports of the pre-existing model with boron and boron interstitial pair. The black arrows show the movements of species affected by hydrogen concentration. At the interface, only B is trapped or emitted.

III. Results and Discussion

Fig. 4 (a) and (b) show the boron concentration and net doping profiles at the center of the PMOSFET channels for two hydrogen concentrations before and after annealing. Fig. 4 (a) displays a pile of boron at the top of the polysilicon gates caused by the ion implantation process for gate doping. This large amount of boron diffuses along the grain boundaries of

the polysilicon gates towards the interface between the polysilicon gate and gate oxide, forming a fairly uniform boron concentration in the gate [12-15]. At this interface, incoming boron atoms diffuse into the silicon substrate through the gate oxide. Since BOH has a greater diffusivity than B in the gate oxide due to its lower activation barrier, more boron migrates from the polysilicon gate to the silicon substrate via BOH formation under high hydrogen concentration.

In both cases, the net doping concentration in polysilicon gates increases due to boron activation during annealing processes. Since hydrogen enhances the boron migration from the polysilicon gate, higher hydrogen concentration results in lower net doping in the channel region. As a result, $|V_{th}|$ decreases. Fig. 4 (b) shows that the H-assisted boron transport even changes the sign of the net doping in higher hydrogen concentration case due to a large amount of boron penetration during annealing.

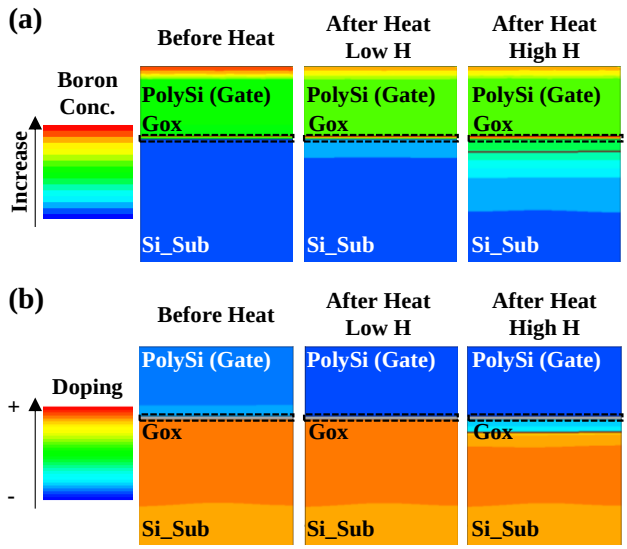

Fig. 4. (a) Boron concentration and (b) net doping distributions after annealing at the center of the channel in PMOSFET for the low and high hydrogen concentration cases.

On the other hand, boron escapes from silicon to oxide in the S/D region. Fig. 5 (a) and (b) show the net doping of the S/D region for the two cases. The simulation results show that a larger amount of boron moves from the S/D region to the spacer oxide region with a high hydrogen concentration in the oxide, which is driven by two mechanisms. The first is the attractive binding between B and OH which effectively increases the solubility of the B inside the oxide, causing B to segregate into the oxide through the silicon/spacer oxide interface. The second is the fast diffusion and reaction of BOH, which makes the system evolve towards the thermal equilibrium faster.

The evidence is shown in Fig. 5 (c), where the high hydrogen concentration leads to a higher B concentration in the spacer oxides as well as a higher segregation ratio [16]. In addition, the flatter profile in the oxide implies that the fast B diffusion via the BOH formation makes the system evolve to the thermal equilibrium faster at the high H concentration. As a consequence, the reduced boron concentration in the S/D region mitigates the SCE as shown in Fig. 5 (d), where the simulation results are in good agreement with the results of experiments in which the amount of hydrogen is controlled by adjusting the fabrication processes.

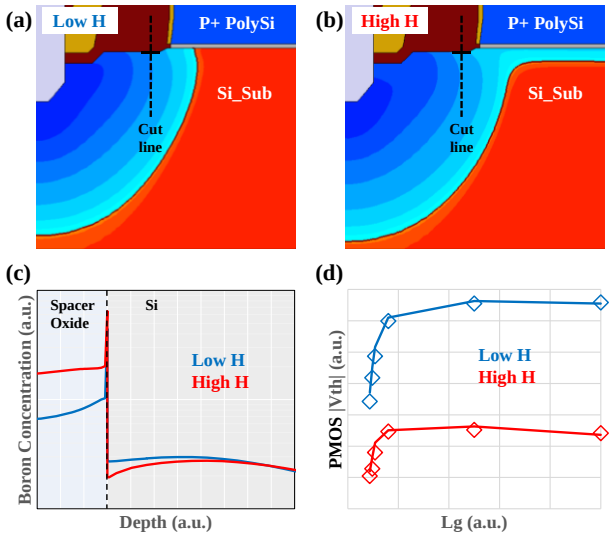

Fig. 5. Net doping distributions at the S/D regions for (a) the low and (b) high hydrogen concentration cases. (c) The boron concentration profiles following the cut lines. (d) Trend of the $|V_{th}|$ channel length (Lg) from measurements (symbols) and simulation (lines) for both the low and high hydrogen concentration cases

IV. Conclusion

The H-assisted accelerated B diffusion in oxide was described via the formation and fast diffusion of the B-OH complex. The attractive B-OH binding and the fast diffusion lead to high segregation at the S/D and spacer interfaces. The simulated hydrogen concentration dependent B profiles in the PMOSFET structure could reproduce the measured $|V_{th}|$ and the SCE. Therefore, this model was applied to predict the device characteristics of PMOSFETs in terms of the V_{th} and SCE.

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