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Modeling boron dose loss in sidewall spacer stacks of complementary metal oxide semiconductor transistors

Z. Essa [a,b,c,*], B. Pelletier [a], P. Morin [a,*], P. Boulenc [a], A. Pakfar [a], C. Tavernier [a], F. Wacquant [a], C. Zechner [d], M. Juhel [a], J.L. Autran [e], F. Cristiano [b,c]

[a] STMicroelectronics, 850 rue Jean Monnet, F-38926 Crolles, France
[b] LAAS CNRS, 7 avenue du Colonel Roche, 31077 Toulouse, France
[c] Université de Toulouse, LAAS, F-31400 Toulouse, France
[d] Synopsys GmbH, Karl-Hammerschmidt-Str. 34, 85609 Aschheim, Germany
[e] IM2NP, Marseille, France

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The presence of capping materials during annealing (activation for example) can substantially impact the silicon junction profiles of Complementary Metal Oxide Semiconductor Field Effect Transistors (CMOSFET), depending on the nature of these layers. In this paper we specifically investigated the boron out-diffusion from a silicon junction into the silicon oxide in presence of a silicon oxide/silicon nitride capping bi-layer similar to the stacks used to form sidewall spacers. After 120 s anneal we observed with secondary ion mass spectrometry (SIMS) substantial boron dose loss in silicon and segregation at the silicon oxide interface related to oxide and nitride material properties, in particular to the hydrogen concentration. We then modeled the boron profiles in both silicon and oxide as a function of the hydrogen static and dynamic in the materials. The exponential-like boron diffusion profiles observed in oxide are reproduced by introducing a long hop mechanism mediated with hydrogen-related defects (HRDs).

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1. Introduction

Scaling transistor dimensions in complementary metal oxide semiconductor (CMOS) technologies implies an enhanced control of the physical dimensions and properties of ultra-shallow junctions (USJs) to manage device performances. In particular, the lightly doped drain (LDD) region under the sidewall spacer controls the serial resistance as well as the short channel effects (SCE) [1]. The need to limit the dopant diffusion and increase the activation in silicon, along with the introduction of new materials as well as the increased interface effects as the dimensions are reduced, have made the junction engineering a difficult challenge. In this frame, and according to the International Technology Roadmap for Semiconductors (ITRS) [2], the development of predictive models of segregation and dose loss are considered as key modeling and simulation challenges for the technology nodes after 14 nm.

Oxide nitride sidewall spacers have been introduced to control the overlap of the source-drain and LDD junctions with the gate oxide [3]. In the case of p-type metal oxide semiconductor (pMOS) transistors, several papers [4–7] have depicted the diffusion of boron from silicon to oxide during the thermal anneals performed subsequently to the sidewall spacer process steps. This effect, called out-diffusion, can lead to substantial boron dose loss from silicon into oxide, which may affect the electrical characteristics of pMOS transistors. Typically the resistance R_{ext} of the LDD extension and the threshold voltage V_t can be impacted. Fig. 1 shows a diagram of the materials and interfaces present in pMOS transistors. The boron out-diffusion phenomenon [1]highlighted with the red arrows in Fig. 1 is modulated by the diffusion mechanisms occurring in the LDD region, into the silicon and silicon oxide materials.

Several studies of out-diffusion of boron were initially carried out on thermally grown oxides aiming to evaluate the diffusion of boron from the doped polycrystalline gate through the gate oxide into the channel. It was shown [8] that boron diffusion in

* Corresponding authors at: Probion Analysis, 37 rue de Fontenay, 92220 Bagneux, France (Z. Essa).
E-mail addresses: zahi.essa@gmail.com (Z. Essa), pierre.morin@st.com (P. Morin).

[1] For interpretation of color in Fig. 1, the reader is referred to the web version of this article.

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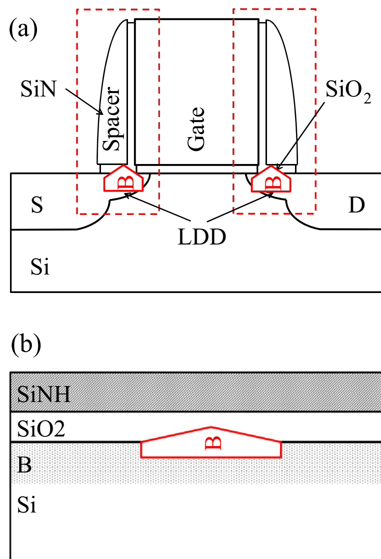

Fig. 1. (a) Materials (silicon, oxide and nitride) and structure of a pMOS CMOSFET. The lightly doped drain (LDD) and source/drain (SD) regions are doped with boron (B). The boron dose loss mechanism is expected to occur under the sidewall spacer between silicon and silicon oxide. (b) Equivalent blanket structure used for experiments.

oxide is modulated by the Si—O bonds, also called peroxy-linkage defects (PLDs). Several studies [8–10] have also shown the important role played by hydrogen during thermal anneals in a H_2 ambient. It has been postulated that O—H bonds called hydrogen-related defects (HRDs) also mediate boron diffusion in silicon oxide [8].

Since the advent of the 65 nm technology node, the oxide and nitride layers use for the sidewall spacer are formed at low temperatures to limit detrimental diffusion phenomena. Different types of chemical vapor deposition (CVD), plasma enhanced CVD, and more recently, atomic layer deposition (ALD) have been used as deposition techniques. As a result of the reduced temperature, these materials are hydrogen rich compared to the previous layer deposited at higher temperatures [11–13] and are expected to further impact the boron diffusion in Si and SiO_2. The content of hydrogen, and more specifically of HRDs in oxide depends on the process parameters. A boron diffusivity modulated by the concentration of OH bonds (or HRDs) was proposed to model the enhancement of boron diffusion in grown [10] and deposited [14] oxides. Although the boron diffusion depends on the initial OH concentration in the oxide, to our knowledge, the evolution of this concentration during post thermal anneal is not considered in any models. In addition to the oxide, the nitride top layer can influence the out-diffusion mechanism by injecting some hydrogen into oxide during thermal anneals subsequent to the spacer forming process, which modify the OH concentration in oxide. Moreover, the nitride can also act as a capping layer which results in substantial hydrogen retention into the pedestal oxide. Consequently, the boron diffusion in the oxide is increased [6]. Thus, to quantitatively study the boron out-diffusion mechanism in nitride/oxide/silicon spacer stacks during thermal treatment, we should monitor the physical characteristics and variation of the hydrogen-related species present in both the nitride and the oxide layers, in addition to the dependence of oxide boron diffusion with hydrogen-related species concentrations.

In this paper we have evaluated the boron out-diffusion and the corresponding dose loss mechanism modulated by the presence of different nitride/oxide capping bi-layers. To correlate the hydrogen-related species characteristics with the boron dose loss, we prepared a set of boron implanted and annealed silicon samples covered with different oxide/nitride blanket bi-layers, as described in Section 2. We used secondary ion mass spectrometry (SIMS) measurements to determine boron profiles in the multi-layer system presented in Section 3. The relationship between hydrogen content and boron diffusion and the statics and dynamics of the generation and diffusion of hydrogen in oxide and nitride are then presented in Sections 4.1 and 4.2. Based on these results, an improved boron out-diffusion model, which allowed for the reproduction of the different SIMS data, is presented in Section 4.3.

2. Experiments

We prepared five samples (S_1 to S_5) on (001)-oriented p-type silicon wafers according to the experimental plan presented in Table 1. We first performed a 1 keV $5 \cdot 10^{14}$ cm^{-3} BF_2 implantation step similar to the condition used for LDD in electrical lots. Four different material stacks were then deposited by combining two different oxides (OA and OB) and three different nitrides (NA, NB, and NC), which present different hydrogen characteristics.

Oxide OA was deposited at 625 °C by low pressure chemical vapor deposition (LPCVD) using a liquid tetraethyl orthosilicate (TEOS) precursor. Oxide OB is an un-doped silica glass (USG) film which was deposited at 400 °C by plasma-enhanced chemical vapor deposition (PECVD) using the reaction between SiH_4 and N_2O compounds. In addition, we determined the concentration of OH bonds in as-deposited OA and OB oxides with Fourier transform infrared (FTIR) spectroscopy [15].

NA and NC nitride layers were deposited by PECVD using a SiH_4/NH_3/N_2 chemistry at 480 °C and 400 °C, respectively. Nitride NB was obtained at 590 °C with LPCVD with hexachlorodisilane (HCD), ammonia (NH_3), and ethylene (C_2H_4) as precursors. NA, NB, and NC nitride densities were been determined by combining thickness measurement with ellipsometric spectroscopy and a high sensitivity weighing machine, resulting in an accuracy better than 2.5%. The initial hydrogen bond concentrations summarized in Table 2 were obtained with FTIR spectrometer using the methodology from Landford and Rand [16]. Hydrogen diffusion characteristics in silicon nitride were extracted with stress/TDS measurements and modeling methodology similar to those carried out by Morin et al. [17] and briefly described below. In silicon nitride films, hydrogen is incorporated by forming SiH or NH bonds [18] in the SiN lattice as a function of deposition process parameters. During a subsequent thermal anneal, hydrogen bonds can be broken, releasing free-diffusing hydrogen H atoms or di-hydrogen molecules according to various chemical mechanisms [19]. The released hydrogen species can then freely diffuse through the nitride film and eventually be transferred to adjacent materials or released in the annealing chamber atmosphere. The hydrogen release in the chamber depends not only on the kinetics of chemical hydrogen dissociation but also on the diffusion of released hydrogen through the layer. In addition, it has been shown that PECVD nitrides are mechanically meta-stable [17]. When submitted to post-thermal treatment, mechanical stress increases and hydrogen is released, as both mechanisms are related and follow similar kinetic behavior. Accordingly, measuring in parallel the hydrogen release and the stress variation on meta-stable PECVD silicon nitride layer subjected to a thermal cycle allows for a determination of hydrogen diffusion coefficients according to the following set of equations [18].

$$\frac{\partial H_{nit}}{\partial t} = D(H_{nit}) \frac{\partial^2 H_{nit}}{\partial x^2} + K(H_{nit}) SiNH \quad (1)$$

$$\frac{\partial SiNH}{\partial t} = -K(H_{nit}) SiNH \quad (2)$$

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