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Boron diffusion and activation in polysilicon multilayer films for P^+ MOS structure: Characterization and modeling

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ABSTRACT

This work deals with in situ boron diffusion and activation in multilayer films: polysilicon (Poly1)/amorphous silicon (Poly2). These films are deposited by LPCVD technique. However, several heat treatments were carried in order to determine the optimal annealing conditions to suppress boron penetration from the gate to the substrate through the gate oxide in MOS structure. The boron concentration is monitored by secondary ion mass spectrometry (SIMS). To investigate SIMS profiles we proposed a model of boron diffusion into these multilayer structures. It is important to note that the parameter values of the studied films such as the diffusion coefficient, the activation percentage of boron as well as the acceleration rate of boron diffusion are deduced from adjustment of simulated profiles with experimental profiles. From these results, we inferred that the boron is electrically active and its distribution does not reach the oxide layer and consequently, the Poly2 may reduce the boron diffusion in optimal annealing conditions.

1. Introduction

The boron atoms used as dopant for the P^+ polysilicon gate penetrate easily through the gate oxide, which causes crucial problem of metal-oxide-semiconductor (MOS) devices. An intensive research activity is carried to improve the polysilicon gate, on one hand to satisfy the requirements of the miniaturization of the components, and on the other hand, to answer the good operating conditions of an MOS structure [1,2]. Among these conditions, it is necessary to be able to preserve the quality of the interface gate/oxide by preventing the doping impurities from penetrating the gate (strongly doped) towards insulator. To the deep diffusion of impurity (boron) up to the oxide coating several solutions can be planned: annealing with weak thermal budgets (low temperature and short duration of annealing) [3], co-doping with strong concentration boron–nitrogen where the N impurity type slows down the penetration of boron [4,5]. We are interested in a P^+ type polysilicon which could limit the boron diffusion through the structure and minimize the gate depletion while keeping the advantages related to polysilicon, such as self-alignment of the gate, source and drain zones, and a low resistivity. In the present study we have investigated a new structure formed with a multilayer based on silicon deposited in amorphous form at low temperature starting from disilane (Si_2H_6) and doped in situ from boron trichloride BCl_3.

2. Experimental procedure

Bi-layer films are deposited on oxidized monocrystalline silicon substrate (N type, 25 nm of thermal oxide SiO_2) in LPCVD furnace. The film consists of silicon amorphous un-doped layer (about 0.05 μm) obtained from disilane (Si_2H_6), onto which is deposited, from (Si_2H_6) and ammonia (NH_3), a layer of polysilicon boron doped in situ (thickness 0.13 μm). The weak heat treatment of this deposit should lead to a uniform doping in the gate and to negligible boron diffusion. Finally, thermal anneals were performed in a conventional furnace under nitrogen (N_2), in temperature range from 600 to 800 °C and times of 15 min to 8 h, to recrystallize the structure and to activate the doping impurity. To be noted that under such anneals, the amorphous layer is fully crystallized, giving a random oriented polysilicon (Poly2). On the contrary, the in situ doped polycrystalline layer (Poly1) is textured, ⟨110⟩ oriented, and do not rearrange significantly during the used annealing [6].

Experimental secondary ion mass spectrometry (SIMS) boron profiles are carried out using an ionic probe of type "CAMECA IMS4F6". The great sensitivity of detection and the good

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resolution in depth of this technique make it possible to inform about the localization of the impurities. On the basis of the obtained data, we can obtain the profiles which provide the concentration of the doping impurity as a function of the sample depth.

3. Model

From our model earlier established for the study of boron diffusion and its activation in doped monolayer polysilicon thin films under particular conditions [4], we undertake a new study of boron diffusivity and its activation in heavily doped multilayer Poly1/Poly2/SiO_2. We calculated the concentration SIMS profiles starting from an algorithm using an implicit method of finite differences, with specified boundary conditions and initial conditions. This equation is given by

$$\frac{\partial C}{\partial t} = \nabla\left\{ D_i \frac{(1+\beta f)}{(1+\beta)} \left(R + \frac{\alpha C}{\sqrt{(\alpha C)^2 + 4n_i^2}} \right) \nabla C \right\} \quad (1)$$

$$f = \frac{2n_i}{(-\alpha C) + \sqrt{(-\alpha C)^2 + 4n_i^2}} \quad (2)$$

where D_i is the boron intrinsic diffusion coefficient:

$$D_i = D_{i0} \exp\left(\frac{-E_a}{kT}\right) \quad (3)$$

where n_i is the intrinsic concentration, β is the ratio of the diffusivity induced by the charged vacancies and the global diffusivity induced by the neutral vacancies, C is the boron chemical concentration, α is the boron activation rate (α_1 in Poly1 layer, α_2 in Poly2 layer), and R is a term introduced into the model which consider diffusion complex phenomenon of the boron in amorphous silicon. This factor can be named the boron acceleration rate in the polycrystalline silicon (R_1 in Poly1 layer, R_2 in Poly2 layer), D_{i0} is the diffusion coefficient in the polysilicon, it is proportional to the diffusion coefficient for monosilicon and E_a is the activation energy.

The boron diffusion coefficient, which takes into account all the phenomena included in the model, is obtained from Eq. (1) using a method similar to that described in previous works [3,4].

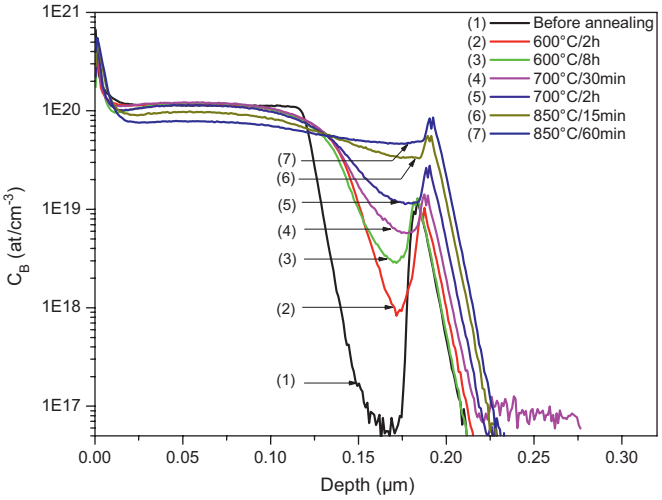

Fig. 1. Superposition of SIMS profiles before and after annealing.

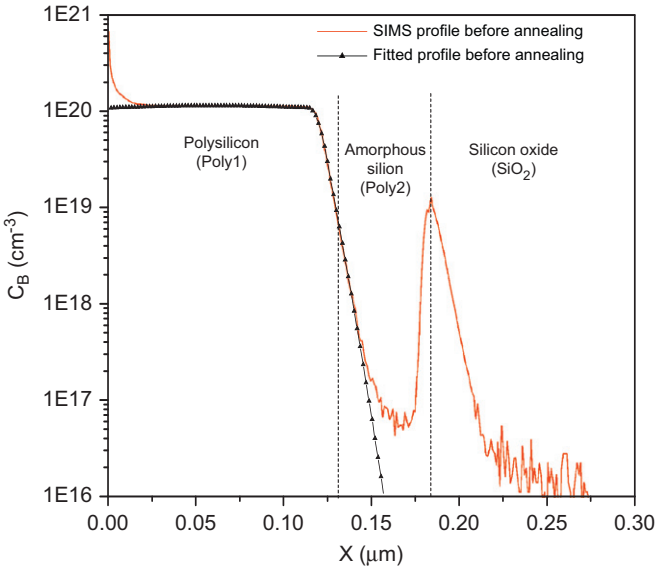

Fig. 2. Superposition of SIMS and simulated profiles before annealing.

4. Results and discussion

Fig. 1 shows the superposition of SIMS profiles before and after annealing. For a relatively low temperature of annealing of 600 °C, boron diffuses in the Poly2 layer but does not reach the oxide layer. Therefore, this layer could reduce the penetration of boron, it is worth noting that amorphous silicon is host of many defects and has tendency to capture the doping atoms to prevent them for reaching oxide layer. The increase of the annealing temperature up to 700 °C influences the redistribution of boron by more prolonged redistribution, but it always remains far from the interface Poly2/silicon oxide. In this case, the boron diffusion was also slowed down, due to the presence of Poly2 layer, because the defects found in Poly2 will disappear after thermal annealing at highest temperature. This can explain why at 850 °C, the boron reaches the interface Poly2/SiO_2 easily, which degrades the MOS structure reliability.

In this model, the simulation of the experimental profile obtained before annealing has been deduced by an analytical expression. Fig. 2 shows the superposition of SIMS and simulated profiles before annealing. This fitted curve will be introduced in the model as the boron initial concentration during the modeling steps.

Superposition of SIMS and simulated profiles after heat treatment at various temperatures and durations are illustrated in Fig. 3(a–f) where it is indicated that the simulated profiles by the proposed theoretical model fit very satisfactory with the experimental ones. Moreover, the fitting SIMS profiles and those calculated by our model allowed the deduction of the activation rate and the diffusion coefficient of the doping impurity, for the various durations and temperature of annealing.

The simulation of the profiles by our model enables us to obtain the order of magnitude of the adjustment factor β which we find equals to 0.13. This is in good agreement with those reported in the literature [7]. For the boron activation energy in the polysilicon films, we took the value of E_a: 3.42 eV, which is a default value for monocrystalline silicon [8].

The boron activation values are deferred in Table 1. In this table, the α_1 and α_2 values represent the boron activation