Abstract

We have investigated and modeled the complex phenomenon of boron (B) redistribution process in strongly doped silicon bilayers structure. A one-dimensional two stream transfer model well adapted to the particular structure of bi-layers and to the effects of strong-concentrations has been developed. This model takes into account the instantaneous kinetics of B transfer, trapping, clustering and segregation during the thermal B activation annealing. The used silicon bi-layers have been obtained by low pressure chemical vapor deposition (LPCVD) method, using in-situ nitrogen-doped-silicon (NiDoS) layer and strongly B doped polycrystalline-silicon (P+) layer. To avoid long redistributions, thermal annealing was carried out at relatively low temperatures (600°C and 700 °C) for various times ranging between 30 minutes and 2 hours. The good adjustment of the simulated profiles with the experimental secondary ion mass spectroscopy (SIMS) profiles allowed a fundamental understanding about the instantaneous physical phenomena giving and disturbing the complex B redistribution profiles-shoulders kinetics.

Keywords: Boron, Nitrogen, Complex Redistribution, Silicon, Bi-layers, Annealing

1. Introduction

The strongly doped polycrystalline-silicon (P+ poly-Si) is a key element of today’s advanced very-large-scaleintegration (VLSI) technology. Boron (B) is the most widely used P-type dopant in recent integrated devices due its high solid solubility in Si. It is usually introduced into Si layers, followed by quick thermal annealing which electrically activates the B atoms. To continue scaling down P+ polysilicon gates of metal-oxide-semiconductor (MOS) integrated circuits, it is necessary to create very shallow junctions with strong-concentrations of electrically active boron (B). Two related processes limit the realization of this goal: (i) the enhanced redistribution of the B during the thermal dopant-activation annealing, which
causes B penetration through thin oxides from the P⁺ polysilicon gate into the underlying layers, and (ii) the formation of electrically inactive B clusters and B precipitates, which decreases the dopant activation rate. The use of low-energy doping methods, co-doping techniques, low thermal annealing temperatures, short annealing times, amorphous-silicon layers, and thin Nitrogen-Doped-Silicon (NiDoS) layers have been practiced to avoid the doping depletion of P⁺ polysilicon gate at the oxide interface. This last effect is one of the major performance limitations in the standard advanced MOS circuits.

Currently, significant research efforts are focused on improving the B activation; problem common to all the practiced methods and techniques. In this work, based on the approach of using thin bi-layers gate, we investigate NiDoS layers for reducing B enhanced redistribution or gate depletion and for improving B activation. Fast B transfer is reduced by increasing nitrogen atoms. The goal is to develop a fundamental understanding about the instantaneous kinetics of complex B transfer process into strongly in-situ doped P⁺ polysilicon/NiDoS bi-layers.

2. Experimental

The used simples, obtained in laboratory LAAS-CNRS of Toulouse (France), consist of two-layers (bi-layers) deposited at 480°C by thermal low-pressure chemical vapor deposition (LPCVD) method. The first layer, deposited on oxidized single-crystal silicon substrates with thermal oxide SiO₂ of 25 nm-thickness, consist of 200 nm thickness of nitrogen-doped-silicon (NiDoS); deposited with 1% of nitrogen content in disilane (Si₂H₆) and ammonia (NH₃) gases mixture. The second layer, deposited on the NiDoS layer, consist of about 110 nm-thickness of in-situ doped P⁺ polycrystalline silicon; deposited from Si₂H₆/BCl₃ gases mixture. Fig. 1 illustrates a schematic representation of the investigated samples structure.

![Fig. 1. Schematic representation of the investigated P⁺ doped poly-Si / NiDoS bi-layers structure.](image)

Fig. 2. Comparison between SIMS diffusion profiles before and after annealing for various temperatures and times.
In order to avoid long-range redistributions, thermal B activation anneals were carried out at relatively low temperatures (600°C and 700°C) for various periods ranging between 30 minutes and 2 hours. The experimental B

3. Model
The model parameters published in our previous work [3] and some other set of parameters have been used. To explain B redistribution in poly-Si/NiDoS bi-layers, the total B population is divided between the poly-Si region and NiDoS region, coupled together by effective B transfer or exchange between the two regions; named a two-stream transfer process. The B redistribution within poly-Si region differs to that within NiDoS region. Nitrogen (N) concentration in NiDoS region is almost uniform and so it is not necessary to use co-diffusion equations. The effect of N population on B redistribution has been only taken as a calibrating parameter. The B transfer is strongly affected by the kinetics of trapping, peak increasing, segregation, and solubility limit motion; since the solubility limit can be enhanced [4]. So, five transport mechanisms for B-atoms can be considered: (a) effective transfer in poly-Si region, (b) effective transfer in NiDoS region, (c) effective segregation near the interface poly-Si/NiDoS, (d) clustering effects in the two regions, and (e) peak concentration appearance and evolutions. Moreover, effects of strong B concentrations such as that of the internal electric field, the charged vacancies, and the solubility solid limit excess are also considered [3]. Fig. 3 illustrates the particular transfer kinetics in Si bi-layers structure during B activation annealing. B atoms diffuse with two effective diffusion coefficients in P+ doped-Si/NiDoS structure.

With a two-stream transfer process, the established model is given by the coupled continuity equations (1) and (2) for the two B populations in the Poly-Si region \( C_{BP} \) and the NiDoS region \( C_{BN} \).

\[
\frac{\partial C_{BP}}{\partial t} = \nabla \left( D_{BP}^{eff} \nabla C_{BP} \right) - T_{B}^{eff}
\]

\[
\frac{\partial C_{BN}}{\partial t} = \nabla \left( D_{BN}^{eff} \nabla C_{BN} \right) + T_{B}^{eff}
\]

\[
T_{B}^{eff} = k_{t}^{eff} \left( C_{int}^{BP} - \frac{C_{BN}^{int}}{k_{seg}^{eff}} \right)
\]

\( T_{B}^{eff} \) in equation (3) describes the effective transfer or exchange of B-atoms at the interface, between Poly-Si and NiDoS regions. It is obtained by use of effective transfer rate \( k_{t}^{eff} \) and effective B segregation
coefficient $k_{se}$ [3]. $D_{B_{poly}}$ and $D_{B_{NiDoS}}$ are respectively, the effective B redistribution coefficients in the Poly-Si region and NiDoS region.

As a result, the specified effective B redistribution coefficients in strongly doped Si bi-layers are modulated during annealing by the instantaneous concentrations and physical parameters.

4. Results and discussion

The experimental SIMS profiles after annealing have been simulated by using the initial profile before annealing as initial condition in redistribution model, and then calibrating independently values of six set of physical parameters; each of which has a clear physical meaning. Indeed, each of these parameters has a leading effect on a particular part of the redistribution profile where the associated physical phenomenon is dominating. So, each parameter affects the redistribution profile behaviour differently. The initial B concentration profile in Si bi-layers before annealing has been simulated without any difficulties by reproducing the experimental SIMS profile, using theoretical expressions and adjustment method. This first simulated profile has been used as initial condition during simulation of redistribution profiles after annealing. We have then deduced two individual B population profiles, according to the depth: B population in the poly-Si region $C_{B_{poly}}$ and B population in the NiDoS region $C_{B_{NiDoS}}$.

The simulation which reproduces very well the investigated SIMS profiles, shown in Fig. 4, illustrates the significant roles of the instantaneous kinetics of B transfer, clustering, clusters evolution, and that of B segregation for the precise reproduction of the redistribution profiles. The simulations accurately predict B redistribution in poly-Si region, transfer process within poly-Si/NiDoS interface, concentration peak evolutions, and redistribution within NiDoS region, with increasing annealing time and temperature.

**Fig. 4.** Simulated profiles (symbols) and SIMS profiles (lines) of B concentrations after annealing at: 600°C/2h, 700°C/30min, and 700°C/2h.

The effect of B-atoms interactions with charged vacancies, that enhances the B diffusivity, has been evaluated by varying the ratio of the intrinsic diffusivity induced by the positively charged vacancies on the global diffusivity induced by neutral vacancies $D_{i+/i0}$ [3]. The optimal value of this ratio obtained after best fitting is between 0.13 and 0.14, which is in good agreement with that reported by Mansour et al. [5]. The medium number of atoms to be trapped in formed small Si–B and B–B clusters in poly-Si region takes the value of 2. This value is similar to that obtained by Uematsu [6] for strongly doped single-crystal Si layers. However, the medium number of atoms to be trapped in formed small B–Si, B–B, N–Si, B–N, and B–N–B clusters in NiDoS region takes the value of 3; which lead to the best fitting for all the investigated profiles. Below the B solubility limit, strong-concentration B will lead to the formation of
small Si–B and B–B clusters that enhances the B diffusivity. This enhancement diminishes with the clusters evolution during annealing [3,6]. The B solubility limit has been found to be enhanced in our investigated bi-layers. The used expression given by Solmi et al. [7] was multiplied by a factor of about 4 to simulate the profiles inclinations or trend, which is in good agreement with the results in literature [4]. This means the excess of the produced complexes.

As shown in Fig. 5(a), near the bi-layers interface, the behavior of the instantaneous effective B diffusivity in poly-Si side is not very different to that in NiDoS side. It is transient because it firstly increases and then decreases with increasing annealing time. The B transient enhanced redistribution in NiDoS region is obviously related to that in poly-Si region. This can be explained by the effective B transfer process starting from the poly-Si region and the involvement of the same physical phenomena in the two regions (such as evolution of trapping, emission, clustering, and crystallization). The same effects have been observed for annealing at 700°C but they are only activated. The instantaneous contributions of the physical phenomena in the two regions are dependent on annealing temperature. Fig. 5(b) shows the instantaneous evolution of the B concentration in poly-Si region, for different depths before bilayers interface, for annealing at 600°C. We notice that the instantaneous B concentration is more and more influenced near the bi-layers interface. Its variation depends also on the annealing temperature.

![Image](image.png)

**Fig. 5.** The instantaneous evolutions of: (a) the effective B diffusivity in poly-Si side and NiDoS side, near the bi-layers interface, and (b) the B concentration in poly-Si region near the interface.

### 5. Conclusion

We have developed a redistribution model well adapted to the strong impurities-concentrations and to the particular structures of doped poly-Si/NiDoS bi-layers. This model takes into account technique of two-stream transfer via the interface, due to the dissimilar bi-layers. It has been revealed that B transient enhanced redistribution in NiDoS layer is almost related to that in poly-silicon layer. The formation of small B–Si and B–Si–N clusters enhances the diffusivity whereas the evolution of these clusters reduces this enhancement. We have concluded that B peak-concentration evolution dose not depend only on transfer kinetics from poly-Si region, but also on the trapping/segregation to the NiDoS region; under the effects of N concentrations and clustering kinetics.

### References


