The role of silicon interstitials in the deactivation and reactivation of high concentration boron profiles

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Abstract

Boron cluster formation and dissolution in high concentration B profiles and the role of Si interstitials in these processes are analyzed by kinetic non-lattice Monte Carlo atomistic simulations. For this purpose, we use theoretical structures as simplifications of boron implants into preamorphized Si, followed by low-temperature solid phase epitaxial (SPE) regrowth or laser thermal annealing process. We observe that in the presence of high B concentrations (above $10^{20} \text{ cm}^{-3}$), significant deactivation occurs during high temperature anneal, even in the presence of only equilibrium Si interstitials. The presence of additional Si interstitials from an end of range (EOR) damage region accelerates the deactivation process and makes B deactivation slightly higher. We show that B deactivation and reactivation processes can be clearly correlated to the evolution of Si interstitial defects at the EOR. The minimum level of activation occurs when the Si interstitial defects at EOR dissolve or form very stable defects.

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1. Introduction

The formation of ultra-shallow junctions is crucial for the fabrication of MOS devices. As the lateral dimensions of the MOSFET channel are scaled down, the source/drain extension junction depth must be proportionately reduced in order to avoid short-channel effects. At the same time, the sheet resistance of the source/drain extension regions must be decreased so that they do not add significant resistance to the channel resistance. This means that even higher active dopant concentrations must be achieved in the ultra-shallow source/drain extension regions.

Boron implantation into preamorphized Si, followed by low-temperature solid phase epitaxial (SPE) regrowth is one of the techniques that are being investigated to meet the challenge. It has been observed experimentally that preamorphizing implants (PAI) enhances dopant activation during low-temperature SPE regrowth of the amorphous layer, with a minimal amount of dopant diffusion \cite{1,2}. It is generally assumed that B is incorporated into substitutional positions and becomes electrically active, and defects within the amorphous layer are swept towards the surface during the regrowth \cite{3,4}. Only defects beyond the amorphous/crystalline interface remain from the PAI. However, the activation achieved after SPE regrowth can only reach concentrations in the order of a few times $10^{20} \text{ cm}^{-3}$ \cite{1,5,6}. Laser annealing makes electrical activation up to levels $\sim 10^{21} \text{ cm}^{-3}$ possible \cite{7}. However, in the presence of high B concentrations, subsequent thermal treatments results in additional boron deactivation within the regrown layer \cite{1,5–7}.

In this work, we analyze the mechanisms for B deactivation and reactivation in high concentration B profiles, and the role of Si interstitials in these processes.
2. Simulation model

In order to analyze the deactivation and reactivation mechanisms for high concentration B profiles, we carried out atomistic simulations based on kinetic Monte Carlo modeling of dopant diffusion and defect interactions in Si [8]. For this study, we implement box-shaped dopant and damage profiles schematically representative of different process conditions. In other cases, we use a binary collision approximation code, MARLOWE [9], to generate coordinates of the displaced atoms in the lattice along with those of the implanted atom, in order to use more realistic profiles to compare with experimental data. The coordinates of the resulting dopants, Si self-interstitials and vacancies are transferred to the non-lattice kinetic Monte Carlo diffusion code DADOS. The energies used in Monte Carlo simulations are obtained from ab initio calculations or estimated by fitting experimental data. The migration and formation energies for Si self-interstitials are taken from Ref. [10]. For small Si interstitial clusters, we consider that boron diffuses by the interstitial binding energy of \( \{113\} \) defects and dislocation loops [11,12]. We consider that boron diffuses by the interstitial mechanism [13]. The B clustering model includes a complex pathway for B/\( \text{Si} \) interstitial interactions leading to \( \text{B}_n \text{I}_m \) complexes (\( \text{B}_n \text{I}_m \) represents a B cluster with \( n \) B atoms and \( m \) Si interstitials) responsible for B deactivation [14,15].

As in many proposed models [14,16,17], we consider that B clusters with a high Si interstitial content have a lower energy than B clusters poor in Si interstitials. The pathways for the B cluster formation and dissolution are determined by cluster energies and by B and Si interstitial concentrations. Two main pathways can be identified: a low Si interstitial content pathway and a high Si interstitial content pathway [14,15]. In the low interstitial content path, the B cluster formation occurs through the capture of mobile interstitial boron (\( \text{B}_1 \)) by the pre-existing clusters and the rapid release of Si interstitials (I), leaving B clusters with low interstitial content. In the high interstitial content path, Si interstitials are not emitted rapidly, resulting in B clusters rich in Si interstitials. Those interstitials are released later in the annealing, when the Si interstitial supersaturation decreases.

Recently, it has been presented an atomistic model of amorphization and recrystallization in Si [18]. However, to our knowledge there are no robust atomistic models in the literature for B interactions in amorphous Si. For low B concentrations, it is assumed that B is incorporated into substitutional positions. However, experiments [1,5,6] and theoretical calculations [19] evidence B clustering within the regrown layer for high B concentrations. We assume that only B concentrations up to \( \approx 2 \times 10^{20} \text{ cm}^{-3} \) [1,5,6] are incorporated into substitutional positions during the regrowth, and B concentrations above that value are in the form of small B clusters [20]. Therefore, the initial simulation conditions for our study correspond to the situation immediately after the regrowth of the amorphous layer.

3. Results and discussion

We have analyzed the deactivation and reactivation mechanisms for B clustering during annealing at 900 °C in different situations that may result from Si processes, by using different simplistic structures. Those consist of box-shaped B profiles, initially fully substitutional (electrically active), 20 nm wide, with concentrations of \( 10^{20} \text{ cm}^{-3} \) or \( 10^{21} \text{ cm}^{-3} \) (approximately corresponding to a low energy B implant to doses of \( 2 \times 10^{15} \text{ cm}^{-2} \) or \( 2 \times 10^{16} \text{ cm}^{-2} \), respectively) placed at the silicon surface. For Si interstitial and B profiles we have considered two different situations, which could be simplifications of real cases: (i) box-shaped B profiles that are initially fully active in the presence of only thermally generated equilibrium Si interstitials (as could correspond to laser annealed samples or B samples grown by molecular beam epitaxy (MBE)); and (ii) box-shaped B profiles that are initially fully or partially active up to \( 2 \times 10^{20} \text{ cm}^{-3} \), in the presence of box-shaped Si interstitial profiles, 10 nm wide, and separated 20 nm from the B profile (as could correspond to the end of range damage (EOR) resulting from preamorphizing implants or the damaged region that has not been melted during laser treatment or residual defects from an imperfect regrowth). The box-shaped Si interstitial profiles have a concentration of \( 5 \times 10^{20} \text{ cm}^{-3} \), corresponding to a dose of \( 5 \times 10^{15} \text{ cm}^{-2} \), which is in the order of Si interstitial doses obtained at EOR by preamorphization. To simplify, we call these cases as “equilibrium” and “EOR damage”, respectively.

Firstly, we have analyzed the B clustering behavior for the equilibrium case. The simulation results are shown in Fig. 1(a) which plots the time evolution of the active B fraction during annealing at 900 °C for B concentrations of \( 10^{20} \text{ cm}^{-3} \) and \( 10^{21} \text{ cm}^{-3} \) initially fully active. As can be seen, in the presence of only equilibrium Si interstitials, B does not deactivate during the annealing for the lower B concentration, but shows significant deactivation for the higher B concentration. Therefore, in the absence of any excess Si interstitials, the deactivation of B will only happen if the B concentration is high enough. Similar behavior is observed experimentally during thermal anneals of samples previously laser annealed [7]. B clustering in the presence of only equilibrium Si interstitials occurs because of the very high supersaturation of substitutional B that exists compared to the solubility. Since only the equilibrium interstitial concentration is present, the B deactivation can only take place through the low interstitial content path, by capturing interstitial boron and emitting some Si interstitials (\( \text{B}_n \text{I}_m \rightarrow \text{B}_n \text{I}_{m-1} \rightarrow \text{B}_n \text{I}_{m-1} + \text{I} \)). Initially, the reactions go towards the formation of B clusters and simultaneously, B diffusion occurs. Once the amount of B in clusters is high enough, the reactions are reversed because of the lost of \( \text{B}_1 \) and \( \text{B}_3 \) through diffusion, causing the B cluster dissolution through the reverse reactions in low interstitial content pathway.

The presence of a band of Si interstitials 20 nm deeper (EOR damage) makes the B deactivation process faster and
Fig. 1. Simulated time evolution of the active B fraction during annealing at 900 °C (including the time during the temperature ramp up at a rate of 50 °C/s) for theoretical box-shaped B profiles at concentrations of $10^{20}$ cm$^{-3}$ and $10^{21}$ cm$^{-3}$. (a) In the presence of only thermally generated equilibrium Si interstitials, B deactivation only occurs for very high B concentrations. (b) In the presence of Si interstitials coming from an EOR damage region, the behavior is quite similar, but B deactivation takes place faster. Even if the initial B profile is only partially active in the $10^{21}$ cm$^{-3}$ B concentration case, similar activation levels are observed. More severe, as can be observed in Fig. 1 (b). We also observe that similar deactivation is obtained if we consider an initial situation of partial B activation (initial active B dose of $2 \times 10^{20}$ cm$^{-3}$). The deactivation process occurs by the injection of Si interstitials from the EOR damage region. Therefore, the formation and dissolution of B clusters in the presence of EOR defects also takes place through a low Si interstitial content path. In all cases, B diffusion also plays a role in the reactivation process by lowering the concentration of substitutional B and additionally forcing the reactions toward the dissolution of B clusters.

Note that in all cases there is a faster deactivation first, which slightly starts during the ramping up of the temperature, followed by a slow reactivation process. A minimum level of activation is observed during the annealing process as a result of the initial deactivation followed by the slow reactivation. In Fig. 2, we have plotted that minimum active B fraction reached during annealing at 900 °C for initially fully active box-shaped B profiles with concentrations ranging from $10^{19}$ cm$^{-3}$ to $10^{21}$ cm$^{-3}$, and for the two different situations for the Si interstitial profiles: equilibrium and EOR damage. In the equilibrium case, when only the thermally generated equilibrium Si interstitials are present, B only deactivates if its concentration is significantly higher than $10^{20}$ cm$^{-3}$. The presence of Si interstitials from an EOR damage results in similar behavior to the equilibrium case, although the minimum active B fraction reached during annealing is slightly lower. This more pronounced deactivation in the presence of EOR Si interstitials is due to the fact that the additional Si interstitials increase the driving force towards the formation of B clusters.

To better understand the role of EOR Si interstitials in B deactivation and reactivation processes, we analyze the experimental data reported by Jin et al. [5] We have simulated a 0.5 keV, $10^{15}$ cm$^{-2}$ B implant in silicon preamorphized by a 20 keV, $5 \times 10^{14}$ cm$^{-2}$ Si implant, which amorphizes up to 32 nm. The samples were annealed at 550 °C for 40 min to regrow the amorphous layer, and followed by 10 s anneals at temperatures ranging from 550 to 950 °C. Fig. 3 shows the simulated and experimental values for the sheet resistance after 10 s anneals at different temperatures. As can be seen, there is a very good agreement between simulations and experimental data. We also plot the active B dose which is mostly proportional to the inverse of the calculated sheet resistance. The sheet resistance obtained at the lowest annealing temperatures corresponds to the activation resulting immediately after the regrowth of the amorphous layer. This corresponds to an active B concentration up to $2 \times 10^{20}$ cm$^{-3}$, which is considered in the initial conditions of our simulations. However, even if the initial concentration was considered fully active, similar deactivation value would be reached,
Fig. 3. Simulated and experimental [5] sheet resistance as a function of the annealing temperature for a 0.5 keV, $10^{15}$ cm$^{-2}$ B implant in preamorphized silicon, after 10 s anneals performed after the regrowth of the amorphous layer. The simulated active B dose is also plotted, which is mostly proportional to the inverse of the sheet resistance.

As we have seen previously. For annealing temperatures lower than 750 °C the sheet resistance is almost constant. For the 850 °C anneal, significant increase in the sheet resistance occurs due to B deactivation. And after the 950 °C anneal B reactivation takes place through B cluster dissolution, resulting in a decrease of the sheet resistance.

To clarify the influence of the EOR defects on B deactivation and reactivation we plot in Fig. 4 the time evolution of the active B dose and the Si interstitial dose during annealing at 850 °C for the previous experimental conditions. The evolution of the Si interstitial dose held in extended defects corresponds to the typical ripening and dissolution of Si interstitial defects, which has been analyzed in a previous work [21]. Initially, the Si interstitial dose remains almost constant during a relatively long period of time, which is longer for deeper implants (or lower annealing temperatures). The EOR damage region initially consists of a high density of many small defects. The average distance between these defects is small, and consequently, the Si interstitials emitted from defects are easily recapacitated by any of the surrounding defects. Thus, there is a minimal loss of the total number of Si interstitials during the initial ripening process. When Si interstitial defects grow to larger sizes and the defect dose decreases the average distance among defects increases. Then, the recapture of Si interstitials by other defects competes with the loss of Si interstitials to the bulk. More Si interstitials are lost as the defect dose decreases further, and finally results in the quick defect dissolution, as can be seen in Fig. 4. We observe that during the time in which the Si interstitial dose decreases slowly, the active B dose reaches a minimum. Afterwards, a reactivation process takes place.

It is known that Si interstitial defects dissolve faster as they are closer to the surface [22]. Trying to find a correlation between Si interstitial defects evolution and active B dose evolution, we have considered a different preamorphizing depth. To analyze the situation for a preamorphizing depth of 15 nm we have simulated a 0.5 keV, $10^{15}$ cm$^{-2}$ B implant in silicon preamorphized by a 6 keV, $5 \times 10^{14}$ cm$^{-2}$ Si implant, annealed at 550 °C for 40 min to regrown the amorphous layer.

The simulated time evolution of the active B dose and the Si interstitial dose held in defects for the 15 nm preamorphizing depth are also plotted in Fig. 4. The results show that there is a direct correlation between the Si interstitial defect evolution at EOR and the B deactivation and reactivation processes. It can be seen that Si interstitial defect dissolution and the initial B deactivation and subsequent reactivation take place faster as the distance from the EOR to the surface is decreased. As the distance from the EOR damage to the surface increases, the gradient of Si interstitials towards the surface decreases. Thus, the injection of Si interstitials is slower for deeper preamorphization depths. Therefore, the EOR defect dissolution is slower as well as the rate of B cluster formation. These observations are also in agreement with experiments of Pawlak et al. [6].

4. Conclusions

We have investigated the physical mechanisms for the B clustering formation and dissolution for ultra-shallow junction formation, and the role of Si interstitials in these processes. We have analyzed theoretical structures with fully or partially active box-shaped B profiles, as simplifications of the situation resulting after regrowth of preamorphized or laser annealed B implants. We showed that the deactivation
depends on the B and Si interstitial concentration. In the absence of excess Si interstitials, B deactivation only occurred for very high B concentrations. If there was a residual concentration of Si interstitials along with the B box, as EOR defects, the deactivation process was faster and more severe. We also observed that in the presence of EOR defects, the B cluster evolution was directly correlated to the evolution of Si interstitial defects at EOR. The minimum level of activation is reached when EOR defects dissolve. Afterwards, B starts reactivating through the dissolution of B clusters.

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References

[20] Because of the uncertainties existing in the status of B clusters resulting after the regrowth, we assume an initial condition of small B clusters with three B atoms. Our simulations show that the number of B atoms in these initial B clusters does not affect significantly to the posterior evolution of B clusters during annealing after the regrowth. No interstitials are included in these initial B clusters because otherwise a significant increase in TED is observed, contrary to experimental observations.