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APPLIED PHYSICS LETTERS **86**, 031908 (2005)

Role of silicon interstitials in boron cluster dissolution

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(Received 21 July 2004; accepted 18 November 2004; published online 11 January 2005)

We present kinetic nonlattice Monte Carlo atomistic simulations to investigate the role of Si interstitials in B cluster dissolution. We show that the presence of Si interstitials from an oxidizing anneal stabilize B clusters and slow down B cluster dissolution, compared to anneal in inert ambient. We have also analyzed the influence of injected Si interstitials from end of range defects, due to preamorphizing implants, on B deactivation and reactivation processes. We have observed that the B cluster evolution can be clearly correlated to the evolution of Si interstitial defects at the end of range. The minimum level of activation occurs when the Si interstitial supersaturation is low because the end of range defects have dissolved or reach very stable configurations, such as dislocation loops. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1852728]

Ion implantation is currently the preferred method for introducing dopants such as boron into silicon for the fabrication of integrated circuits. This process produces a large amount of defects in the lattice, which can degrade the device performance.[1] Moreover, after implantation, dopants generally reside in nonsubstitutional lattice positions, and therefore, are electrically inactive.[2] Postimplant annealing is used to remove the implant damage, and incorporate dopants onto substitutional positions to activate electrically. However, during the subsequent annealing, two undesired processes take place: transient enhanced diffusion (TED) of the implanted B,[1] and formation of stable boron-interstitial clusters that immobilize and deactivate the B atoms.[2,3]

Several studies reported the role of Si interstitials in B cluster formation. The formation of B clusters traps a significant fraction of the Si interstitials during the nucleation time.[4,5] However, the role of Si interstitials during B cluster dissolution is not clearly understood. In this letter, we analyze the influence of Si interstitials in B cluster dissolution for subamorphizing implants. We also study the influence of the end of range (EOR) defects resulting from B implants into preamorphized Si on the evolution of B profiles during additional annealing after the solid phase epitaxial (SPE) regrowth.

For this study we carried out atomistic simulations based on kinetic Monte Carlo modeling of dopant diffusion and defect interactions in Si.[6] A number of studies for B cluster formation and dissolution have been reported in the literature.[3,7,8] In most cases, relatively low B concentrations ($<10^{20}$ cm^{-3}) and intermediate annealing temperatures ($\sim$800 °C) were considered. A deeper insight into the B clustering model is necessary due to the new requirements for ultrashallow junction formation. We have extended the model by Pelaz *et al.*[3] to include the new requirements of high B concentration and high annealing temperatures,[9] while maintaining the validity for traditional conditions. This B clustering model includes a complex pathway for B/Si interstitial interactions leading to B_nI_m complexes responsible for B deactivation.

First, we analyze the role of Si interstitials in B cluster dissolution by comparing the B activation during annealing in inert and oxidizing ambient, since it is known that oxidation sets a Si interstitial supersaturation at the surface.[10] Radic *et al.*[11] investigated the B activation/reactivation in crystalline Si of a 20 keV, 4×10^{14} cm^{-2} B implant in crystalline Si, using a two step annealing process. The first step consisted of an annealing at 750 °C for 30 min in inert ambient, to form the B clusters, while the second anneal step was done at 850 °C for 60 min, in inert or oxidizing ambient, to analyze the influence of Si interstitials in B cluster dissolution. They observed a deceleration in the B reactivation process when annealing was performed in an oxidation ambient compared to anneal in an inert ambient. However, this result was apparently in contradiction with some existing B clustering models, which predicted that the additional Si interstitial supersaturation created by the oxidizing ambient would accelerate the B cluster dissolution through the capture of Si interstitials and the emission of interstitial B.[11] In our simulations, we have accounted for the oxidizing ambient by setting the Si interstitial supersaturation to 10 at the silicon surface, i.e., injection of 10× the equilibrium concentration of Si interstitials, which is a typical value for this temperature range.[12] Our simulations show similar behavior to experiments, as can be seen in Fig. 1. The results are compatible with the model proposed by Pelaz *et al.*[3] and theoretical calculations by other authors,[7,8] where B clusters with more Si interstitials have a lower total energy, and therefore, are more stable. The presence of additional Si interstitials favors the presence of stable B clusters with a high Si interstitial content. Thus, a longer time is needed to emit Si interstitials trapped in B clusters and to obtain B clusters with a low Si interstitial content, which can dissolve through a low interstitial content pathway.[3,9] These observations are also in accordance to experiments by Mannino *et al.* which

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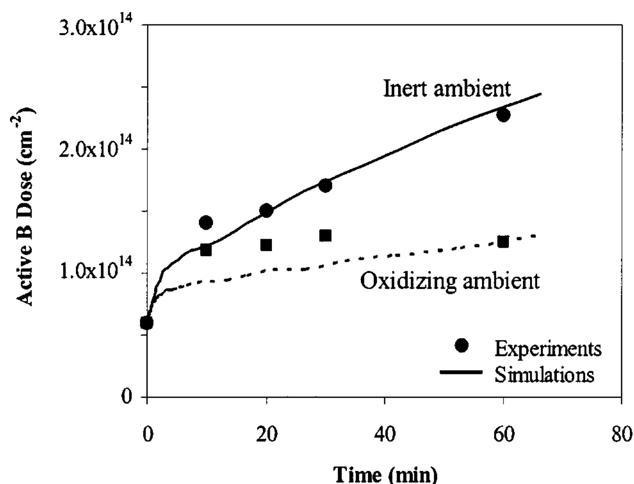

FIG. 1. Simulated and experimental (Ref. 11) time evolution of the active B dose during the second step anneal at 850 °C in inert and oxidizing ambient, for a 20 keV, 4×10^{14} cm^{-2} B implant.

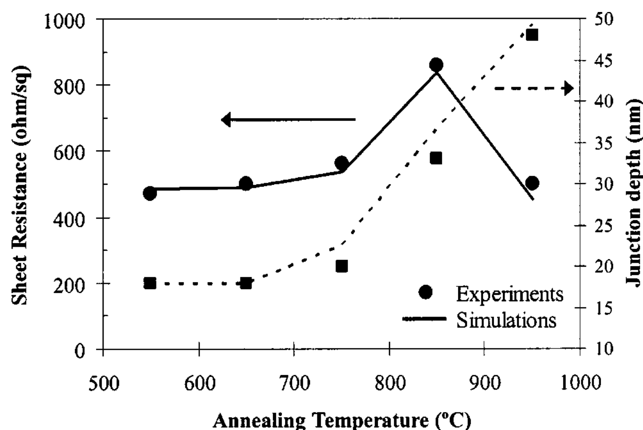

FIG. 2. Simulated and experimental (Ref. 16) sheet resistance and junction depth as a function of the annealing temperature for a 0.5 keV, 10^{15} cm^{-2} B implant in preamorphized silicon, after 10 s anneals performed after the regrowth of the amorphous layer.

suggested that increasing the Si interstitial supersaturation makes the B clusters more stable.[13]

The stabilization of B clusters by a Si interstitial supersaturation is also manifested in the evolution of the active B dose during annealing in the presence of Si interstitials injected from the EOR defects. There is experimental evidence that defects within the preamorphized layer are swept towards the surface during the regrowth of the amorphous layer, while defects beyond the amorphous/crystalline interface remain after regrowth.[14] For concentrations lower than 10^{20} cm^{-3} B is fully active after regrowth, but experiments[15–17] and theoretical calculations[18] evidence B clustering within the regrown layer for higher B concentrations. It has been also shown that in the cases of high B concentration additional thermal annealing after the SPE regrowth results in additional B deactivation.[16,17] In our simulations, we assume that only B concentrations up to $\sim 2\times10^{20}$ cm^{-3} are incorporated into substitutional positions during the regrowth,[15–17] and B concentrations above that value are in the form of small B clusters. Therefore, the initial simulation conditions for our study correspond to the situation immediately after the regrowth of the amorphous layer. We have analyzed the influence of the Si interstitials injected from the EOR defects on the B clusters during annealing after the SPE regrowth. For this purpose, we have simulated experiments reported by Jin *et al.*[16] consisting of a 0.5 keV, 10^{15} cm^{-2} B implant into silicon preamorphized by a 20 keV, 5×10^{14} cm^{-2} Si implant. The system was 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. Figure 2 shows the simulated and experimental values[16] for the sheet resistance and the junction depth after 10 s anneal.[19] The junction depth is derived from the simulated depth profiles, at a boron concentration of 3×10^{18} cm^{-3}, as in the experimental results of Jin *et al.* 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 our initial simulation conditions of active B concentration of 2×10^{20} cm^{-3}. However, for this high B concentration levels, even if the initial B concentration was considered fully active, similar deactivation value would be reached.[9] For annealing temperatures lower than 750 °C small B deactivation and minimal diffusion occur during the annealing after the regrowth. For the 850 °C anneal, significant B deactivation and diffusion are observed, while after the 950 °C anneal significant reactivation takes place at the same time that more B diffusion occurs.

To clarify the influence of the EOR defects on B deactivation and reactivation we plot in Fig. 3 the time evolution of the active B dose (approximately proportional to the inverse of the sheet resistance) and the Si interstitial dose held in defects for different annealing temperatures. The evolution of the Si interstitial dose stored in extended defects has been analyzed in a previous work.[20] Initially, the Si interstitial dose remains almost constant during a relatively long period of time, which is longer for lower annealing temperatures or deeper implants. It corresponds to the Si interstitial defect ripening, as very few Si interstitials are lost to the surface. When Si interstitial defects grow to larger sizes and the defect dose decreases the average distance among defects increases. Then, the loss of Si interstitials to the bulk becomes more significant, resulting in the quick defect dissolution, as can be seen in Fig. 3. We observe that during the time in which the Si interstitial dose remains approximately constant

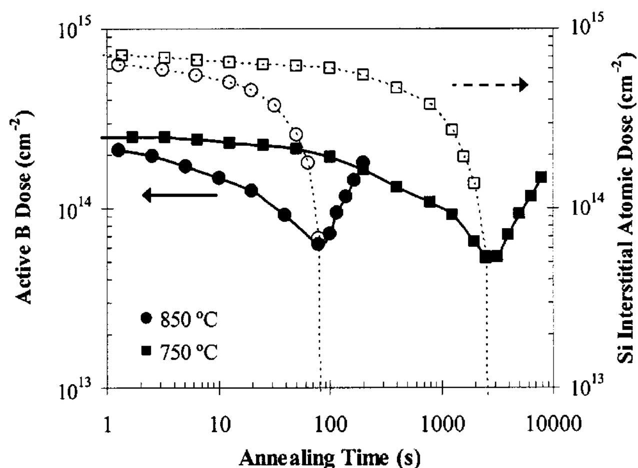

FIG. 3. Time evolution of the Si interstitial dose stored in EOR defects and the active B dose during annealing at 750 and 850 °C, for a 0.5 keV, 10^{15} cm^{-2} B implant in preamorphized silicon. The time to start B reactivation is correlated with the time for Si interstitial defect dissolution at the EOR damage region.

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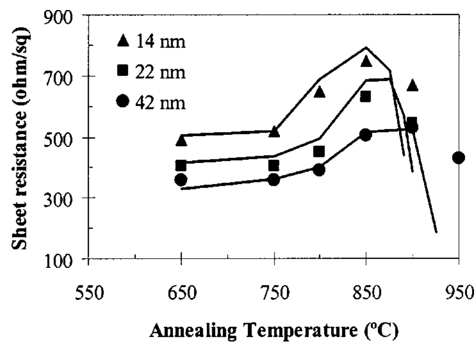

FIG. 4. Simulated and experimental (Ref. 17) values for the sheet resistance for a 1.5 keV, 3×10^{15} cm^{-2} B implants in preamorphized Si annealed at different temperatures for 1 min. The preamorphizing implants were 10^{15} cm^{-2} Ge at energies of 8, 12, and 25 keV, corresponding to amorphizing depths of 14, 22, and 42 nm, respectively.

the active B dose decreases slowly. Then, there is a faster deactivation, until the active B dose reaches a minimum. Afterwards, a reactivation process takes place. These processes occur faster at higher temperatures. We observe that the deactivation of the B profile takes place while a high Si interstitial supersaturation set by the EOR defects is present. The minimum level of activation occurs around the time of complete dissolution of defects at EOR, or when defects evolve to very stable configuration (such as dislocation loops) so that the free Si interstitial supersaturation is very small.

Since there exists a direct correlation between the Si interstitial defect dissolution and the distance of the defect band to the silicon surface,[21] it is expected that B deactivation and reactivation processes in the regrown layer are influenced by the preamorphizing depth, which determines the position of the EOR defects and the dissolution of these defects. We have studied that behavior based in some experiments of Pawlak *et al.*[17] consisting of 1.5 keV, 3×10^{15} cm^{-2} B implants in preamorphized Si annealed at different temperatures. The preamorphizing implants were 10^{15} cm^{-2} Ge at energies of 8, 12, and 25 keV, corresponding to amorphizing depths of 14, 22, and 42 nm, respectively. The simulated and experimental values for the sheet resistance at different annealing temperatures for 1 min and for the different preamorphizing depths are plotted in Fig. 4. Experiments and simulations show that the annealing temperature at which a maximum deactivation occurs for a given annealing time increases with preamorphization depth. This is reproduced in our simulations and can be explained in terms of the EOR defect evolution. As the distance of the Si interstitial defect band to the surface increases, higher temperatures are needed to anneal out the defects in a given time. Therefore, the temperature for maximum deactivation will increase with the preamorphization depth. Note, that the initial deactivation becomes higher as the EOR defects are closer to the B profile. Some overlapping between the tail of the B profile and the EOR defects causes a significant deactivation of the B in that region.

In summary, we have shown that the presence of Si interstitials stabilizes B clusters and slows down B cluster dissolution. For high concentration B profiles in preamorphized Si, the presence of Si interstitials at the EOR damage region leads to B deactivation during annealing after the SPE regrowth. The B cluster evolution is directly correlated to the evolution of Si interstitial defects at EOR. The minimum level of activation occurs when EOR defects are dissolved or reach such stable configurations so that the Si interstitial supersaturation is very low. Afterwards, B starts reactivating through the dissolution of B clusters.

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