Atomistic modeling of deactivation and reactivation mechanisms in high-concentration boron profiles

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We use kinetic nonlattice Monte Carlo atomistic simulations to investigate the physical mechanisms for boron cluster formation and dissolution at very high B concentrations, and the role of Si interstitials in these processes. For this purpose, high-dose, low-energy B implants and theoretical structures with fully active box shaped B profiles were analyzed. Along with the theoretical B profile, different Si interstitial profiles were included. These structures could be simplifications of the situation resulting from the regrowth of preamorphized or laser annealed B implants. While for B concentrations lower than 10^{20} cm^{-3}, B clusters are not formed unless a high Si interstitial concentration overlaps the B profile, our simulation results show that for higher B concentrations, B clusters can be formed even in the presence of only the equilibrium Si interstitial concentration. The existence of a residual concentration of Si interstitials along with the B boxes makes the deactivation faster and more severe. © *2003 American Institute of Physics.*
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Boron implantation is the most common process used for establishing p-type dopant profiles in silicon. However, the implanted ions generate a large concentration of defects that deteriorate the device performance,[1] and the implanted dopant is generally electrically inactive.[2] Postimplant thermal annealing is required to anneal out the damage and to electrically activate the dopant. The interaction between boron and silicon interstitials caused by the implant damage complicates the formation of ultrashallow, low resistivity junctions. During the regrowth of preamorphized and laser annealed implants the activation level of the samples is improved.[3–5] It is generally assumed that, during the solid-phase epitaxial (SPE) or liquid phase epitaxial (LPE) regrowth of an amorphous layer, boron is incorporated into substitutional positions and thus becomes electrically active. At the same time, the excess atoms existing in the amorphous layer are swept towards the surface during the regrowth, and thus, only the Si interstitials beyond the amorphous-crystalline interface remain. However, as devices are scaled down, higher carrier concentration levels are needed for ultrashallow junction formation. In the presence of high B concentrations the complete activation of B in amorphous layers is difficult.[4–5] The activation achieved during SPE regrowth hardly exceeds a threshold concentration in the order of $\sim 1-3\times 10^{20}$ cm^{-3}.[3–5] Laser annealing makes initial electrical activation up to levels $\sim 10^{21}$ cm^{-3} possible.[6] However, deactivation occurs during additional thermal treatments.[7]

Previous works[8–10] concluded that for medium B implant doses in crystalline Si, a pathway with a high interstitial content was driving the B cluster formation responsible for electrical deactivation. B atoms at concentrations in the order of 10^{19} cm^{-3} in delta doped marker layers (initially substitutional) formed clusters only when a high interstitial concentration overlapped the B profile. In this work, we analyze the scenario that arises for very high B concentrations, as those needed for the formation of ultrashallow junctions. We study the case of a simultaneous presence of high Si interstitial and B concentration (as corresponds to high dose B implants in crystalline Si) and also when the Si interstitial concentration is low and separated from the B profile (as corresponds to the end of range damage in regrown amorphous layers). For the latter case, we consider theoretical box shaped B profiles that are initially fully active in the presence of different Si interstitial profiles or with only thermally generated equilibrium Si interstitials.

To analyze the deactivation and reactivation mechanisms for high B concentration profiles we carried out atomistic simulations based on kinetic Monte Carlo modeling of dopant diffusion and defect interactions in Si.[11] Dynamic anneal during the implant and the ramp up in temperature until reaching the target temperature are included in the model. We consider that boron diffuses by the interstitialcy mechanism.[12,13] The B clustering model includes a complex pathway for B/Si interstitial interactions leading to B_nI_m complexes responsible for B deactivation.[8–10] We use the following expression for the total energies in electron-volts of the B_nI_m complexes, E_{tot}:

$$E_{tot}=-\left(0.98+\left(1.7-\frac{2.65}{\sqrt{\max(n_I,1)}}\right)\times\exp(-n_B)+\frac{[2.82\times\exp(-0.9\times|n_B-3.64|)]}{\{1+\exp[0.5\times(n_I-2\times n_B)]\}}\right)\times n_I-0.1\times n_B,$$

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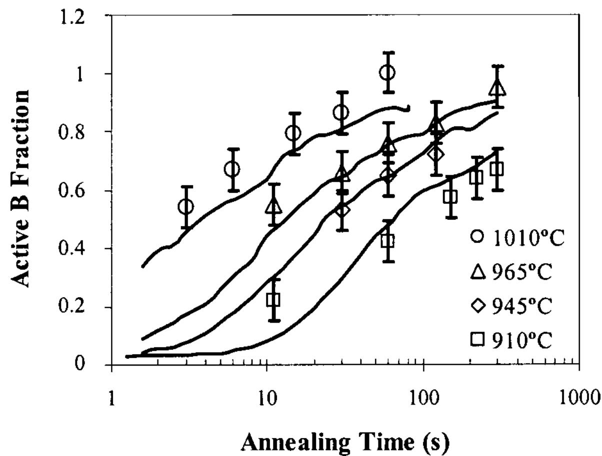

FIG. 1. Time evolution during annealing of the active B fraction for a 1 keV 10^{15} cm^{-2} B implant, annealed at temperatures from 910 to 1010 °C. Symbols correspond to experimental values obtained from Hall measurements. Lines correspond to simulated substitutional B.

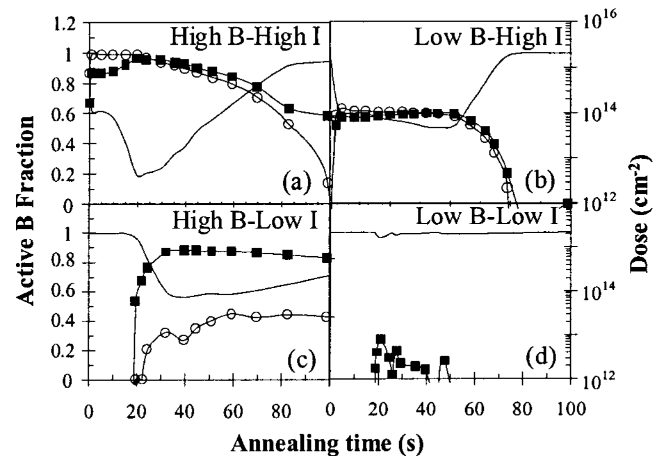

FIG. 2. Time evolution during annealing at 1000 °C (including the time during the temperature ramp up at a rate of 50 °C/s) of the active B fraction (solid line), and the dose of B (closed symbols) and Si interstitials (open symbols) stored in B_nI_m clusters. Different combinations of box shaped B and I profiles, 20 nm wide, are considered: (a) 10^{21} cm^{-3} B and I; (b) 10^{20} cm^{-3} B and I; (c) 10^{21} cm^{-3} B, no excess I; and (d) 10^{20} cm^{-3} B, no excess I. When a high Si interstitial concentration is present, overlapping the B profile, B clusters with an initial high content of Si interstitials are formed, both for high and low B concentrations. When the Si interstitial concentration is low, B clusters are only formed in the case of high B concentration, and the number of Si interstitials trapped in the B clusters is significantly smaller than the number of B atoms.

where n_B and n_I are the number of B and Si interstitial atoms in the B_nI_m clusters, respectively. This expression is consistent with the model proposed by Pelaz *et al.*[9] In that model, there are two different main pathways for the formation of the boron clusters. The predominance of a given pathway is determined by cluster energies and by B and Si interstitial concentrations. In the low interstitial content path, the B cluster formation occurs through the capture of mobile B_i by the pre-existing clusters and the rapid release of Si interstitials, 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 anneal when the Si interstitial supersaturation decreases.

First of all, we study the evolution of B activation of a 1 keV 1×10^{15} cm^{-2} B implant in crystalline Si, annealed at different temperatures ranging from 910 to 1010 °C. In Fig. 1 we compare the active fraction experimentally obtained from Hall measurements,[5] with the substitutional B resulting from our simulations. Simulation results are in very good agreement with the experimental data, which gives validity to the model. A detailed analysis of the evolution of B clusters indicates that the high interstitial content path dominates at the very early stages of the annealing, similar to the results observed for lower dose implants.[8–10] The experimental anneal temperatures and times correspond already to the reactivation process. This occurs through the low interstitial content path, by the capture of equilibrium Si interstitials and emission of mobile B interstitials, that can diffuse out of the B peak, and thus, lowering the B concentration.

The situation is quite different when B is implanted in preamorphized Si. For low B concentrations and a deep enough amorphous layer, B is electrically active and no excess interstitials overlap with the B profile after the regrowth. The Si interstitial supersaturation set by the end of range defects at the original amorphous-crystalline interface is not enough to deactivate the B atoms during additional anneals.[14] Nevertheless, it has been observed that in the presence of high B concentrations the activation during annealing is not complete. It has been suggested that some kind of precursors of B clusters could form during the regrowth process.[6] Other studies suggest that B is initially incorporated into substitutional positions but gets deactivated quickly, possibly by residual damage resulting from an imperfect regrowth or by interstititials injected from the end of range damage.[5]

Because of the uncertainties in the status resulting after the regrown process we have carried out simplified simulations that can approximate the real case. Those consist of box-shaped B profiles, initially fully substitutional, 20 nm wide, with concentrations ranging from 10^{19} to 10^{21} cm^{-3} (which correspond to implanted doses from 2×10^{13} to 2×10^{15} cm^{-2}), and placed 100 nm in depth to avoid surface effects. To better understand the deactivation and reactivation mechanisms, we have monitored in Fig. 2 the time evolution of the active and inactive boron dose, and the Si interstitial dose retained in boron clusters, corresponding to B profiles of 10^{21} cm^{-3} [Figs. 2(a) and 2(c)] and 10^{20} cm^{-3} [Figs. 2(b) and 2(d)]. Two cases are considered for the Si interstitials: Si interstitial profiles identical to the B dose [Figs. 2(a) and 2(b)], and no excess Si interstitials [Figs. 2(c) and 2(d)]. The simulation shows that when a high Si interstitial concentration is present overlapping the B profile, B clusters are formed, both for high and low B concentrations, and they initially trap many interstitials. Then, interstitials are released and the B profile slowly activates. When the Si interstitial concentration is low, B clusters are only formed in the case of high B concentration (above $1-3\times10^{20}$ cm^{-3}). This result is consistent with the experimental observation that for low B concentration, B activates during regrowth and does not deactivate with additional anneal. For the low Si interstitial concentration cases, the number of Si interstitials trapped in the B clusters is significantly smaller than the number of B atoms, indicating that B clusters are formed through the low interstitial content pathway. In all cases, there is a faster deactivation first, sometimes during the

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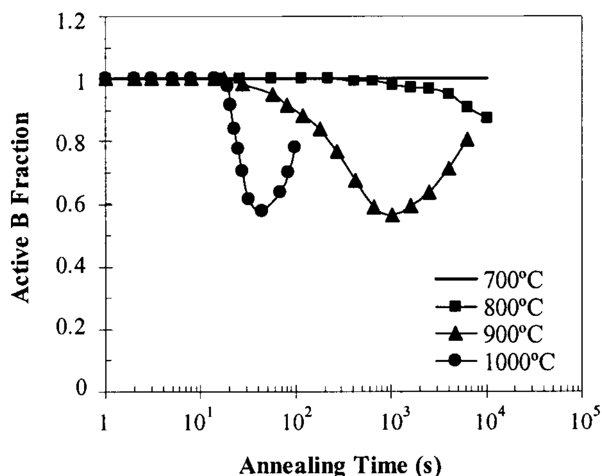

FIG. 3. Time evolution of the active B fraction for different annealing temperatures for a 20 nm wide box-shaped B profile with a concentration of 10^{21} cm^{-3}, and with no excess Si interstitials. At low temperatures the deactivation process is very slow.

ramping up of the temperature, and then, a slow reactivation process. A minimum level of activation is observed during the annealing process.

When only equilibrium Si interstitials are injected from the surface the kinetics of the deactivation process is very dependent on the anneal temperature, as can be seen in Fig. 3. It plots the time evolution during annealing at different temperatures of the active B fraction for a 20 nm wide box-shaped B profile of with a concentration of 10^{21} cm^{-3}. At temperatures below 900 °C the equilibrium Si interstitial concentration is so low that the deactivation process may take hours. The results are consistent with experimental observations in laser annealed samples with an initial high active B concentration, which show slow deactivation when an additional furnace anneal at low temperature is performed.[7]

The simulation results are obviously very dependent on the particular parameters used in the model. Theoretical calculations and empirical parameter extraction[8,15–17] indicate that B clusters with no Si interstitials are not energetically favorable ($E>0$), while B clusters with interstitials are more stable (compared to separated B and Si interstitials). In the presence of large concentrations of Si interstitials, the formation of these B clusters with high interstitial content becomes the preferred pathway. When no excess Si interstitials exists, the formation energy of the Si interstitials must be taken into account in the evaluation of the total energy. This evaluation process produces unfavorable results for the high interstitial content pathway. A bottleneck for the formation of B clusters through the low interstitial pathway must exist so that B clusters are not easily formed for medium B concentrations unless the Si interstitial concentration is high.[8–10] Theoretical calculations indicate that the energy of B_2 is quite high compared to that of Bi. Therefore B_2I is more likely to dissolve into B_s+B_i than to form B_2+I. Only when the initial B concentration is very high and the Si interstitial concentration is low, the reaction is driven towards the formation of B_2 and the release of a Si interstitial. Thus, B clusters can be formed through this pathway, with minimal intervention of Si interstitials.

In both cases, when the excess Si interstitials have been annihilated, the resulting B clusters have low interstitial content (in the case of high interstitial pathway, Si interstitials are released later on). The boron reactivation (cluster breakup) is through the capture of equilibrium interstitials and release of B_i leading from larger clusters to smaller clusters and eventually substitutional boron.

In summary, we have shown that the deactivation mechanism for B implants in crystalline Si takes place through a high interstitial content path, and it occurs even for low B doses. However, for the initially fully active B profiles, the deactivation mechanism depends on the B and Si interstitial concentration. In the absence of excess Si interstitials, B deactivation only occurs for very high B concentrations. If a residual concentration of Si interstitials exists overlapping the B profile, the deactivation takes place rapidly even at low temperatures. The reactivation mechanism takes place in all cases through a low interstitial content path, by the capture of native Si interstitial defects and the emission of B interstitials.

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