Activation and deactivation of implanted B in Si

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(Received 2 April 1999; accepted for publication 7 June 1999)

The temporal evolution of the electrically active B fraction has been measured experimentally on B implanted Si, and calculated using atomistic simulation. An implant of 40 keV, $2\times10^{14}\,\mathrm{cm}^{-2}$ B was examined during a postimplant anneal at 800 °C. The results show a low B activation (~25%) for short anneal times ($\leqslant$10 s) that slowly increases with time (up to 40% at 1000 s), in agreement with the model proposed by Pelaz *et al.* [Appl. Phys. Lett. **74**, 3657 (1999)]. Based on the results, we conclude that B clustering occurs in the presence of a high interstitial concentration, in the very early stages of the anneal. For this reason, B clustering is not avoided by a short or low-temperature anneal. The total dissolution of B clusters involves thermally generated Si interstitials, and therefore, requires long- or high-temperature anneals. [S0003-6951(99)01531-4]

Implantation of dopants is the standard technique for establishing dopant profiles, which in turn, determine the electrical characteristics of devices in integrated circuits. However, the implanted dopant is generally electrically inactive, and the energetic ions create a large concentration of defects that degrade the device characteristics. Postimplant thermal processing is required to anneal out the damage and to electrically activate the dopant. During this process, the presence of a high Si interstitial concentration causes transient enhanced diffusion (TED) of the dopant atoms[1,2] and their precipitation into clusters at a concentration well below the equilibrium solid solubility.[3,4] A large amount of research has been devoted to the understanding and modeling of dopant–defect interactions,[1–13] so that the final dopant profile could be accurately predicted for device design. B has received particular attention because it is a fast diffuser and the most common dopant used to form shallow *p*-type regions.

The enhancement of B diffusivity is understood and modeled in terms of the kick-out mechanism with Si interstitials.[5] The precipitation of B below the solubility limit is associated with the formation of immobile and electrically inactive B clusters.[3] Since B clustering is enhanced by the presence of a high concentration of Si interstitials,[2] and the amount of clustered Si interstitials decreases in the presence of high B concentration,[6] these clusters are believed to be complexes of B atoms and Si interstitials. However, controversy exists about the interactions that lead to the formation and dissolution of these clusters, which impact, in particular, the predicted evolution of the active fraction of B.[7–9] It has been proposed that a practically complete activation of B implanted Si can be achieved by annealing at 800 °C for very short times (<10 s).[9]

In this letter we present experimental results on the temporal evolution of the electrical activation of B implanted Si. We discuss the results on the basis of detailed dopant–defect interactions. We apply an atomistic model,[7,8] based on first principles[5] and molecular dynamics[10] calculations and diffusion experiments,[11] to explain and predict the experimental results from implanted B.

B diffusion and clustering is studied using *p*-type epi-Si wafers implanted with 40 keV B ions, to a dose of $2\times10^{14}\,\mathrm{cm}^{-2}$. Wafers were rapidly thermal annealed in nitrogen at 800 °C for ~0.1 (spike anneal), 1, 10, 100, or 1000 s, and the central part of each wafer was used for analysis. The electrically active B was determined from spreading resistance profilometry (SRP) in all five annealed samples. The total B concentration profile was determined by secondary ion mass spectrometry (SIMS) for an as-implanted sample and for samples annealed for 0.1 and 1000 s. Some of these profiles are shown in Fig. 1.

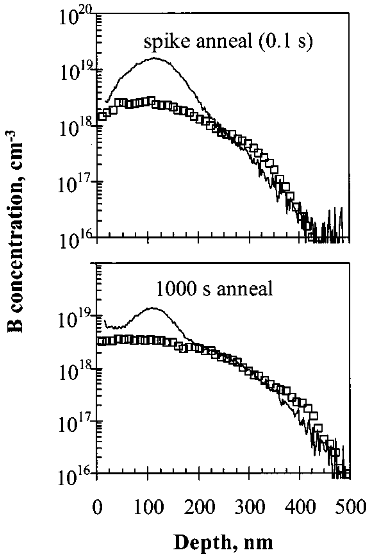

FIG. 1. SIMS (solid line) and SRP (squares) measurements of 40 keV, $2\times10^{14}\,\mathrm{cm}^{-2}$ B implanted into epi-Si, annealed at 800 °C.

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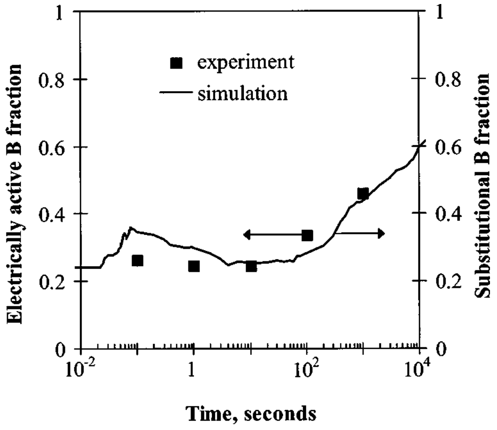

FIG. 2. The time evolution of the electrically active fraction of B during the postimplant anneal at 800 °C. Symbols correspond to the experimental data. The solid line corresponds to a simulation using the model reported in Ref. 8.

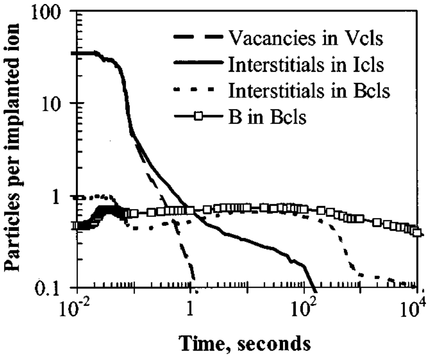

FIG. 3. Simulation of the time evolution during the postimplant anneal at 800 °C of the implant damage (Si interstitials and vacancies in clusters) and of the B atoms and Si interstitials in B clusters. The B atoms in clusters are not electrically active.

After implantation and annealing, the B profile shows a characteristic shape with an immobile part and a diffused tail, with a sharp transition between the two components at a concentration $\sim 3\times 10^{18}\,\mathrm{cm}^{-3}$ at 800 °C. The diffused tail of the B profile corresponds very well to the SRP profile, and therefore, to the electrically active B. The immobile part is electrically inactive and it is associated with B clusters. The electrically active fraction of B is extracted as the ratio of the active B dose, as determined by SRP, to the total amount of B in Si, as determined by SIMS. The temporal evolution of the fraction of electrically active B, presented in Fig. 2, indicates that (i) the active fraction of B is small, about 25%, for short annealing times ($\leqslant$10 s), and (ii) it slowly increases with time, up to 40% after 1000 s. These observations are in direct contradiction with the predictions of Ref. 9 for identical implant and anneal parameters.

The experimental results are in excellent agreement with the model for B clustering described in Ref. 8. This model was derived from a number of experiments on B diffusion and clustering in B-doping superlattices, grown by molecular beam epitaxy (MBE). The B marker layers diffuse normally and are electrically active in the presence of equilibrium Si interstitial concentrations or a small Si interstitial supersaturation during oxidizing anneals. However, a fraction of B atoms is immobilized and is electrically inactive when the damage produced by ion implantation overlaps with the B markers. In the simulations, all of the B atoms in the grown-in markers are assumed to be substitutional at the start. The implanted B atoms are assumed to be in interstitial positions. Transitions between substitutional B and interstitial B occur through the kick-out and kick-in mechanisms with Si interstitials.[5] The same mechanisms and parameters used to simulate B clusters in MBE grown B markers[8] are used in the simulation for B implants presented in this letter. We assume a ramp rate of 150 °C/s, as measured in the experiment.

According to the simulation model, several stages can be distinguished in the temporal evolution of damage and B clustering during the postimplant anneal, as shown in Fig. 3. (i) The formation of B clusters occurs at the very early stages of the anneal in the presence of a high concentration of vacancies and interstitials. The growth of B clusters takes place by adding mobile interstitial B to the pre-existing B clusters. In this model, the mobile B interstitial does not interact with vacancy clusters to produce substitutional B. Otherwise, the growth of B clusters would be inhibited and a high fraction of active B would persist while vacancies are present.[9] The initial B complexes have a high Si interstitial content (comparable number of Si interstitials and B atoms). (ii) As the anneal proceeds and the Si interstitial supersaturation decreases, B clusters emit Si interstitials, reducing their interstitial content. Also, some interstitial B atoms are emitted from the B clusters. The stable B clusters have a larger number of B atoms than Si interstitials (a ratio of approximately four B atoms per Si interstitial), and survive longer than the Si interstitial clusters (311's). (iii) The complete dissolution of the more stable B clusters takes place in a quasiequilibrium condition by the capture of thermally generated Si interstitials and then the release of an interstitial B. Therefore, long-time or high-temperature anneals are needed to activate the B completely, in agreement with experimental observations.[12]

The fraction of active B from the same implant as reported in Fig. 1, after annealing at a lower temperature of 700 °C, for 1, 10, or 100 s, was found to be only about 13%. These results are consistent with other experimental reports,[12,13] showing that the percentage of active B in crystalline Si is very low for a small thermal budget, increasing with temperature, from 600 to 1000 °C, and slowly with time. Low-temperature, long-time anneals exhibit the initial stages of the damage evolution and B clustering, in a similar fashion as during high-temperature, short-time anneals, although the kinetics of the reactions that drive B clustering varies with temperature. We conclude that a small thermal budget cannot avoid B clustering.

In summary, the electrically active fraction of 40 keV $2\times 10^{14}\,\mathrm{cm}^{-2}$ B implanted in Si is small, about 25%, within the first 10 s of annealing at 800 °C. During subsequent anneals B is slowly activated. In agreement with the model proposed by Pelaz *et al.*,[8] the results indicate that B clusters form during the early stages of annealing, in the presence of a high Si interstitial concentration. The dissolution of B clusters takes place very slowly with a quasiequilibrium Si interstitial concentration.

The authors would like to thank the Silicon Fabrication Research Laboratory staff at Bell Laboratories for their assistance with experiments.

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