Physical insight into ultra-shallow junction formation through atomistic modeling

L. Pelaz *, M. Aboy, P. Lopez, L.A. Marques, I. Santos

Campus Miguel Delibes, University of Valladolid, 47011 Valladolid, Spain

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Abstract

We use atomistic simulations to gain physical understanding of relevant dopant–defect interactions involved in junction formation. The analysis of the energetics of B–Si interstitial clusters (BICs) indicates that a high Si interstitial supersaturation is necessary to nucleate BICs in crystalline Si, but only a Si interstitial supersaturation slightly larger than that set by BICs is enough to cause the stabilization and growth of preexisting BICs. We have analyzed the mechanisms associated to B uphill diffusion and deactivation in preamorphized Si upon subsequent annealing. Both phenomena occur simultaneously and they are the result of the trapping of B atoms by preexisting B clusters in the high concentration region.

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1. Introduction

The shrinking of Si device dimensions has revealed material and process limits that make the fabrication of integrated circuits very complex. In the field of doping technology for planar bulk CMOS devices, one of the most challenging requirements concerns to the achievement of doping profiles in the source/drain extension regions with shallower junction depths for the control of short-channel effects (~10 nm), while simultaneously optimizing the sheet resistance (~500 Ω/sq) and doping abruptness at the extension-channel junction [1].

Modeling has become an essential step for the understanding of physical mechanisms involved in junction formation and for process evaluation and optimization. Important and challenging issues in the area of the front-end process modelling are the diffusion and interactions of dopants and defects [1]. These processes are highly transient, and its dynamics needs to be captured by models in order to define the optimum processes that provide maximal dopant activation with minimal diffusion. Predictive process simulation has stimulated the development of detailed models about dopant diffusion, evolution of extended defects, and formation and dissolution of dopant–defect clusters [2–4]. Although continuum models are the mainstay in process simulators used in the semiconductor industry, atomistic process models are very helpful to extract relevant parameters (diffusivity, binding energies, etc.), to improve the understanding of physical interactions and even to perform full process simulations that can be directly compared to experimental results [3].

We focus on the case of B because it is one of the most common dopants used for the formation of p-type regions due its high solid solubility in Si. However, transient enhanced diffusion (TED) and formation of B–Si interstitial clusters (BICs) make the formation of ultra-shallow low-resistivity junctions difficult. When B is implanted in crystalline Si, BICs are formed rapidly [3]. Their
dissolution requires high thermal budgets and the process is accompanied by significant diffusion, which poses a trade-off between little diffusion and high activation. Because of the larger activation energy for BIC dissolution compared to that for B diffusion, improved junction depth/sheet resistance specs can be achieved by high-temperature short-time anneals (spike, flash, sub-melt laser) rather than by lower-temperature longer-time processes [5].

A method to reduce the formation of BICs is the preamorphization of the Si layer. During low-temperature solid-phase epitaxial regrowth (SPER) damage is swept towards the surface at the same time that most B atoms are incorporated into substitutional positions resulting in high activation levels with minimal diffusion. Activation levels up to the surface at the same time that most B atoms are incor-

vation. We analyze the mechanisms associated to B activation and redistribution in Si.

2. Simulation model

In our model we simulate ion implantation using the binary collision approximation, and the kinetics and interactions of dopants and defects through a non-lattice kinetic Monte Carlo code. In this model reactions are described through their reaction rate probability instead of formulating a complex set of coupled partial differential equations. The interest of this model to solve complex problems with relevance for junction formation has been demonstrated for the case of the B–Si interstitial clusters [3].

Ab initio, tight-binding and classical molecular dynamics calculations provide the energetics of B–Si interstitial complexes [7–11]. Also, some values have been extracted by parameter fitting from experiments [3,4]. Although there are some differences in the particular numbers obtained by different authors, they agree on the overall description of the system. B clusters with no interstitials have a larger energy. The energy decreases when a Si interstitial is added and also as the number of B atoms in the complex increases, at least up to size 4. In Fig. 1 we represent the energetics of relevant BICs using the perfect lattice and substitutional B as a reference level. We also include the energy of free Si interstitials, and Si interstitials in {113} defects and dislocation loops. There are a number of consequences that can be extracted from this energy diagram:

(a) BICs are easily nucleated (BI$_m$, B$_2$I$_m$ complexes are easily formed) in the presence of a high free Si interstitial concentration (for instance, in the implanted region). However, Si interstitials released from {113} defects are not likely to nucleate BICs since small BICs (1 or 2 B atoms) have a higher energy than Si interstitials in 113’ s. This explains why BICs are formed in the zone that overlaps with the implant damage, where free Si interstitials are initially available, but not in other regions, that are only reached by Si interstitials slowly injected from the defects generated in the implanted regions [3].

(b) BICs and {113} defects compete for Si interstitials generated during implantation since their formation reduces the energy of the system. If the B concentration is large enough to form BICs with 3 or 4 B atoms, Si interstitials are preferably trapped in BICs (they have lower energy than in 113’ s). Therefore, the formation of BICs may inhibit the formation of {113} defects, as it has been experimentally demonstrated [12].

(c) BICs are stabilized in the presence of Si interstitials injected from {113} defects or from other Si interstitial sources that set a Si interstitial supersaturation higher than that set by BICs [13]. However, BICs can dissolve in the presence of dislocation loops (the energy level of Si interstitials in loops is lower than that in BICs).

(d) When B concentration is very high and B atoms are likely to be nearby, BICs can be formed even with low Si interstitial concentration [4]. B complexes with only substitutional B atoms are not energetically favourable, and the energy significantly decreases by adding a Si interstitial.

The modelling of B in amorphous Si is more complex and the energetics may not be the same as in crystalline Si. SPER eliminate the excess Si interstitials, and leave the B atoms in substitutional positions up to $\sim 2 \times 10^{20}$ cm$^{-3}$. Above this concentration, several B atoms are likely to be together and it is energetically more favourable to form B$_3$I than to leave three neighboring B atoms [10]. Thus, during SPER B atoms are left substitutional, but some BICs are formed in the high B concentration region.
3. Uphill diffusion and deactivation in high concentration preamorphized B implants

SPER requires small thermal budgets but the regrowth temperature is not enough to remove the EOR damage of the preamorphizing implant. After SPER, BICs and substitutional B atoms in the regrown layer coexist with the EOR defects formed beyond the a/c interface. Upon an additional annealing, Si interstitials are injected from these defects and they interact with B atoms in the regrown layer.

B uphill diffusion is observed at the early stages of annealing after SPER. This means that B atoms are displaced towards regions of higher B concentration, against the B gradient. This effect was observed when high B fluences were implanted in preamorphized Si but it was not observed when B was implanted in crystalline Si [14], as we illustrate in Fig. 2. In the case of crystalline Si, a large fraction of B atoms are immobilized in BICs and therefore they are not able to diffuse. Only B atoms in the tail diffuse a little bit. In the case of preamorphized Si, only concentrations above $2 \times 10^{20} \text{ cm}^{-3}$ are in BICs and the rest are substitutional B. Those B atoms may interact with Si interstitials injected from the EOR defects and diffuse upon annealing.

In order to clarify the causes of uphill diffusion we have tested several possibilities in our simulations, which are illustrated in Fig. 3. The initial B profile is taken from [15] just after the SPER anneal. A Ge implant of 30 keV $10^{15} \text{ cm}^{-2}$ was used to preamorphize up to $\sim 55$ nm. Then, 0.5 keV $10^{15} \text{ cm}^{-2}$ B was implanted and annealed at 650 °C during 5 s for SPER. We show the evolution of the B profile during additional annealing at 800 °C. In the simulation with the complete model (Fig. 3(a)) we observe the progressive displacement of the B profile towards the surface in the region of intermediate B concentrations for increased annealing times, 10, 30, 60 and 120 s at 800 °C. If we remove EOR defects (Fig. 3(b)) we observe down-hill diffusion of B atoms that were initially substitutional. Then, we can conclude that Si interstitial defects are...
necessary for uphill diffusion. To elucidate whether a Si interstitial gradient is necessary or a flat Si interstitial supersaturation is enough to cause B uphill diffusion, we have set a flat Si interstitial background. In this case we observe uphill diffusion (Fig. 3(c)), similar to that observed in our reference simulation (Fig. 3(a)). This indicates that the gradient of Si interstitials towards the surface may help B uphill diffusion, but it is not necessary. In our last test we have included the EOR damage but we have inhibited the formation of BICs in our simulations. In this case no uphill diffusion appears (Fig. 3(d)). Only downhill diffusion of B atoms in all the B profile is observed. We conclude that BICs are also necessary to observe uphill diffusion.

In Fig. 4 we plot the evolution of the active (substitutional) B atoms and Si interstitials stored in {113} defects at the EOR, during 800 °C annealing of a 0.5 keV, $10^{15}$ cm$^{-2}$ B implant into a 50 nm preamorphized Si layer. Experimental data are extracted from [15].

In Fig. 5 we compare B deactivation during 60 s annealing at 800 °C subsequent to SPER. We observe that during the time in which uphill diffusion is observed (~120 s), B deactivation occurs. This happens also while EOR defects are dissolving by the emission of Si interstitials. The Si interstitial supersaturation set by the EOR defects stabilizes BICs which trap diffusing B atoms. This causes apparent uphill diffusion and simultaneous B deactivation. When the Si interstitial supersaturation decreases because EOR dissolve or evolve towards more stable configurations such as loops, BICs cannot longer be maintained and they dissolve. Then, the amount of substitutional B increases and normal downhill occurs.

4. Effect of the EOR distance to the surface

Since Si interstitial defects emitted from EOR defects in preamorphized implants play a relevant role in B diffusion and deactivation, we have analyzed the influence of the position of the EOR defects. In Fig. 5 we compare B deactivation during 60 s annealing at different temperatures for two different amorphization depths. The simulations correspond to the experimental conditions reported in [16]: a 0.5 keV $2 \times 10^{15}$ cm$^{-2}$ B implant into preamorphized Si with 8 keV or 20 keV $10^{15}$ cm$^{-2}$ Ge implants resulting in amorphous layers of ~19 nm or ~38 nm thick respectively.
Note that in the shallower pre-amorphizing implant, B deactivation is more intense and the temperature for maximum deactivation is lower.

In Fig. 6(a) we plot the average Si interstitial supersaturation versus depth at 800 °C. We observe that, for the shallower preamorphizing implant, the Si interstitial gradient is steeper, and the Si interstitial supersaturation in the near surface region (where B profile is located) is higher. This explains the more intense B deactivation. In Fig. 6(b) we plot the evolution of Si interstitials in [113] defects at the EOR. They dissolve faster in the case of the shallower implant and consequently B reactivation also start faster.

5. Conclusions

We have used atomistic simulations to gain insight into the mechanisms involved in junction formation. Through the analysis of the energetics of BICs we can conclude that although a very high Si interstitial supersaturation is necessary to nucleate BICs in crystalline Si, only a Si interstitial supersaturation slightly larger than that set by larger BICs is enough to cause the stabilization and growth of preexisting BICs.

We have analyzed the mechanisms associated to B uphill diffusion and deactivation in preamorphized Si upon subsequent annealing to SPER. We have concluded that both phenomena are correlated and they are the result of the trapping of mobile interstitial B by pre-existing BICs in the high B concentration region. This is possible because of the Si interstitial supersaturation set by the EOR defects beyond the a/c interface. When this supersaturation decreases, BICs dissolve and B diffuses down-hill. The closer the EOR defects are to the surface, the larger the Si interstitial gradient is. Also, the Si interstitial supersaturation in the near surface region, where B atoms are located, is higher. As a result the B deactivation is stronger and occurs faster.

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References