Improvement in the prediction of Boron diffusion during a Spike Annealing for Ultra-Shallow Junctions

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Abstract

The boron diffusion during a spike annealing involves complex phenomena that the simple Fick law cannot handle. Indeed, the diffusion mechanism of a dopant A in silicon implies the diffusion of at least 4 other species: AV, Al, I, V, where I and V are an Interstitial Si atom and a Vacancy, respectively. One of the most complete models, the pair diffusion model, takes these species into account. However, we will see that this model shows some limitations, and needs adequate modifications of default parameters used in the DIOS simulator, release 7.0 ISE commercial package. We show for the first time, using a step-by-step analysis, that the introduction of composite species in the pair diffusion model is mandatory to obtain at the same time a good profile shape and a realistic dopant activation.

1. Introduction

The ITRS roadmap requires accurate controlled channel dopant profiles and ultra-shallow junctions with low resistance. It is therefore necessary to use low energy ion implantation and to anneal at the highest possible temperature while limiting the total thermal budget (spike anneal). These short time anneals imply that the simulation of the transient phenomena, especially for boron diffusion, has to be more and more accurate. The first part of the paper shows the limitations of the up-to-date simulation model, and the second part show how this model can be modified to simulate more accurately the boron diffusion during a spike anneal.

2. Pair Diffusion model

The first and second Fick laws show some limitations towards boron diffusion modelling in silicon. In particular, the TED (Transient Enhanced Diffusion) is not accurately taken into account. The main approximation comes from the diffusivity D that depends upon B concentration, precipitations of species, and equilibrium between point defects in Si, i.e. vacancies and interstitials.

The pair diffusion model is the nowadays most complete approach to describe diffusion phenomena in silicon. Indeed, the point defect injection by oxidation or nitridation, the coupling effects between dopants by Si-interstitials (Emitter Push Effect), and TED (transient enhanced diffusion) can be perfectly reproduced.

Thus, many chemical reactions (paring, ionization, clustering) and diffusion mechanisms have been implemented in DIOS.

\[ A + V = AV \ , \ A + I = Al \] : pairing
\[ A = A_1 + V \] : Franck Turnbull,
\[ A + I = A_i \] : Kick out reaction,
where A, A_1, and A_i are substitutional and interstitial dopant atoms respectively.

Note also that the dopant-interstitial pairs can be ionised: A-I\_0, A-I\_1, A-I\_2...

Moreover, clustering reactions of Boron or Interstitial can also be used. For example, B_6 and I_4 clusters, considered as very stable species in Si, are implemented by default. However, immobile clusters such as B_6I_6 need to be defined by the user.

In summary, the physical laws [2],[3], implemented in DIOS are the following: a reaction rate R is defined for each reaction to take into account transient effects, the local conservation law, the Fick’s first law, the Maxwell-Gauss equation, and the mass, lattice sites, and charge balance equations. The default parameters implemented in the simulator are the most often encountered in literature, i.e. boron diffusivity for dopants, pairs and defects, solubility, segregation coefficients SiO2/Si, action mass law...

Regarding the implantation aspect, a “+1” model [4], [5] has been chosen for interstitial initial profile. Indeed, the “+1.4” profile, although more recent [6], gives less good result on fitting.

Moreover, the as-implanted SIMS profile has been fitted by an analytical function. Thus, the diffusion can be studied without being parasited by uncertainties on as-implanted simulated profile.

3. Simulation with default parameters

Figure 1 shows the SIMS depth profiling of Boron before and after anneal: dose=5e14 /cm², energy 1keV, spike anneal 1050°C. A triangular shape models the spike temperature profile. The ramp up is close to 250°C/s, the
temperature peak duration is about 0.5s, and the ramp down slope is 60°C/s.

Figure 1. Attempts to simulate the B dopant profiles after spike anneal with DIOS default parameters.

It appears that the tail diffusion for x>30nm is largely overestimated even after the first ramp up. This means that transient effects (TED) are not accurately taken into account. For x<30nm, the ramp up has almost no effect on diffusion, whereas the plateau (high temperature) and the ramp down (long time), show strong influence on this boron high concentration diffusion region. Finally, simulation is here unable to reproduce SIMS profile. Moreover, the active boron concentration is also not accurately modelled since the simulated sheet resistance Rs(simul) = 1300 Ohm/sq. is at least two times higher than the experimental one: Rs(exp) = 550 Ohm/sq.

The most advanced pair diffusion model describes correctly the diffusion in silicon in the majority of soak annealing. However, in the case of spike annealing where the interstitial oversaturation has a fast decreasing with time, and where composite species B3I6 are involved, the pair diffusion model shows some limits. Therefore, in the following simulations different hypothesis have been done, and parameter set changed in order to obtain a physically-based calibration.

4. Adequate fitting parameters

A better understanding of what happen during an RTA annealing is required to obtain a better simulation. However, in literature, only particular aspects of boron diffusion are treated and, according to us, no paper can nowadays give a global point of view of how the boron behave during a more complex thermal stress. Therefore, Figure 2 represents a step-by-step phenomenological synthesis of the spatial and time evolution of the crystalline defects oversaturation composed of Si-interstitials I and B3Si6 precipitates.


c) T ~ 800°C-900°C, {311} are formed, B3I6 dissolved --> B diffuses: the tail is formed. Then 2 possibilities for T > 950°C: d) Ef {311} ~ Ef (B3Si6), both species are dissolved, and B diffuses. e) Ef {311} < Ef (B3Si6), {311} are dissolved earlier, and B3Si6 after. Thus the oversaturation of I is lower, but final profile is the same: BED mechanism.

d) Dissolution

B3Si6 precipitates dissolution
B3 + 3I ↔ B3I6

e) Dissolution

B3Si6 precipitates dissolution
B3 + I ↔ B3I

Figure 2.a: t=0 after implantation. I2 precursors localised near Rp, Bl2 clusters further.
The modelling of boron diffusion with the introduction of BIC (Boron Interstitial Clusters) is still an on-going research work [7], [9], and not yet implemented in simulators.

It is useful to compare the literature synthesis of Figure 2 to what is implemented in the DIOS simulator with the same step-by-step approach (figures 3.a to d).

Thus the boron diffusion with the spike described in 3 has been simulated and “sampled” at different steps after the anneal beginning. We assumed (for a better fit) that the majority of boron is clusterized before the annealing starts. The main discrepancies between Figure 2 and simulated diffusion are highlighted in bold.

During the ramp-down, the active boron depth profiling continues to diffuse “normally”. The profiles remain quite the same as Figure 3.d except by a bump in the simulated part that may correspond to an excessive dissolution of $B_6$ clusters when temperature approaches the 1000°C zone.

5. SIMS vs. Simulation results

Figure 4 compares SIMS profiles before and after implantation to simulated profiles. A “+1” modelling of interstitial [4] [5] has been used, and standard diffusion parameters have been used taking into account transient clustering. Both simulated and SIMS profiles show some agreements except by a bump in the simulated part that may correspond to an excessive dissolution of $B_6$ Boron clusters.
Moreover, during the ramp up, only the tail of boron profile diffuses and then remains unchanged, as described in literature and in figure 2. Then in the apex and ramp down zones, a bump begins to form.

Figure 4. Comparison SIMS/simulation profiles.

The simulated sheet resistance is 700 Ohm/sq, whereas 550 is measured. The relative difference on the sheet resistance, is about 27%, and 13% on the junction position (for a 10^18 N doping type). These values are already satisfactorily compared to the uncertainties brought by USJ resistance measurement.

6. Corrections to “default DIOS” implementation

In order to reduce the bump in Fig. 4, and to be consistent to Figure 2, it is mandatory to introduce other crossed species like BnIm composed of Boron and interstitials. However it is not possible to implement all the reactions described in Fig. 2, for CPU time and algorithm convergence reasons. Therefore, only one composite specie has been implemented at a time.

The solid solubility and the equilibrium constant activation energies have been taken form literature [8] for each reaction BnIm = n.B + m.I (*), whereas constant terms have been fitted.

The best simulated profiles are drawn on Fig. 5.

Figure 5. B profiles simulated after anneal for different clusters implemented: BI4, B2I, B3I, B3I2, B4I.

First, the best fitting profiles are obtained for B3I and B4I clusters. This is consistent with the fact that these clusters are likely to have the lowest formation energy of each kind of BnIm cluster [8]. The junction position is obtain to less than 1% of relative difference but 36% for the 750 Ohm/sq simulated sheet resistance. Indeed some clusters are not dissolved after the spike.

Note also that the introduction of B1Im cluster with a large amount of I do not allow satisfying fitting. BI2, B1I, B1I2, and B1I3 introduction do not change the final profile. Indeed, Figure 3 shows that around 900°C the oversaturation of I starts decreasing. This creates an equilibrium move to the right in eq. (*) which results in BnIm clusters dissolution. And the more I included in BnIm, the more BnIm clusters dissolved. This might explain why the introduction of BI2, B1I, B1I2 and B1I3 has no effect on final simulated boron profile.

Trials have also been made on the Bn (de)-clustering rate and on the boron solid solubility (to increase the activation). But even with the optimum set of parameters the boron diffusion is still widely over-estimated.

7. Conclusion

The introduction of composite BnIm clusters allows to fit accurately the SIMS, however the sheet resistance is still slightly overestimated because of a large amount of clusters not dissolved by the reduced thermal budget of spike annealing.

The introduction of a “+1” model [4], [5], and making the assumption that all clusters are formed after implantation, allows to obtain less than 15% error on the junction depth and less than 30% on the sheet resistance. The introduction of composite species (BIC), such as B3I, results in a better fit, but a worst approximation of the sheet resistance. Despite all the trials, it seems not to be possible to obtain at the same time a good profile shape and very accurate dopant activation. Improvements concerning modelling still have to be done.

8. References