Atomistic simulations of extrinsic defects evolution and transient enhanced diffusion in silicon

F. Cristiano[1], B.Colombeau[2], C.Bonafos[2],
J.Aussoleil[2], G.Ben Assayag[2] and A.Claverie[2]
[1]LAAS/CNRS, 7 av. du Col. Roche, 31077 Toulouse, France
[2]CEMES/CNRS, 29 rue J. Marvig, 31055 Toulouse, France

Abstract

We present a "unified" model for the simulation of boron transient enhanced diffusion in both crystalline and preamorphised structures. The model describes the thermal evolution of a supersaturation of Si interstitial atoms in dynamical equilibrium with all types of extrinsic defects. We show some successful applications of our model to a variety of experimental conditions and give an example of its predictive capabilities at ultra low implantion energies.

1 Introducion

The transient enhanced diffusion (TED) of ion implanted boron in silicon is a major problem in advanced IC fabrication. It is driven by the excess Si interstitial atoms ($Si_{int}s$) generated by the ion implantation process. Early models aimed at the simulation of the basic experimental case of boron implanted into a crystalline substrate, where the dominant defects are typically the {113}s. These models assumed that a flux of $Si_{int}s$ (responsible for TED) originates from the continuous dissolution of the {113}s defects (Chao et al. 1996). More recently (Bonafos et al. 1997, Claverie et al. 2000), it has been proposed that TED is governed by the thermal evolution of a supersaturation of $Si_{int}s$ in dynamical equilibrium with all types of extrinsic defects formed after implantation (clusters, {113}s and dislocation loops (DLs)). Based on this description (Ostwald ripening), new models were proposed (Gencer and Dunham 1997) but often rely on many fitting parameters. While successfully fitting particular sets of experiments, they are not sufficiently accurate for predictive TCAD applications. Moreover, the increasing need to achieve ultra shallow junctions, has resulted today in the extensive use of preamorphised structures, where most of the extended defects formed after the implant are the DLs. Very few models have been proposed to simulate TED in presence of DLs (Chao et al. 1996). In addition, these models assume that DLs are perfect sinks for the interstitials, i.e. they behave in an opposite way to the {113}s.
In this paper, we present a "unified" model we have developed which describes the concomitant evolution of the defects and of the supersaturation of $Si_{int}s$ in both crystalline and preamorphised structures. Great effort has been put into the "physical" definition of the various parameters needed for the calculations, with the overall aim of reducing to a minimum the number of fitting parameters. We will present some applications of our model to a variety of experimental conditions and we will give an example of its predictive capabilities.

2 Simulation of defect growth and TED

Our model describes the concomitant time evolution of extrinsic defects and of the supersaturation of $Si_{int}s$ in the defect region, according to the Ostwald ripening theory. Each defect (of size n from 2 up to thousands of atoms) is characterised by its formation energy $E_f(n)$ (the energy required to add one extra atom to the defect) and capture efficiency A_n/R_{eff}. Both $E_f(n)$ and A_n/R_{eff} depend on the geometry of the defect (type and size), as recently described by Claverie et al. (2001). The growth of a given defect is calculated by the difference between its capture rate, F_n, and its emission rate, R_n. The capture rate F_n depends on the defect environment and is directly proportional to the mean interstitial supersaturation, S, in the defect region, while the emission rate R_n depends only on the defect formation energy $E_f(n)$. The evolution of the whole defect population is mathematically expressed as follows:

$$\frac{dN_n}{dt} = F_{n-1}N_{n-1} - F_n N_n + R_{n+1}N_{n+1} - R_n N_n \tag{1}$$

where N_n is the number of defects of size n, while the mean interstitial supersaturation (free $Si_{int}s$ in dynamical equilibrium with the defects) is given by

$$S = \frac{C_i}{C_i^*} = \frac{\sum_{n=2}^{\infty} \beta_n R_n N_n}{D_i C_i^* \left(\left(\sum_{n=2}^{\infty} \frac{A_n}{R_{eff}} N_n \right) + \frac{1}{L_{surf} + R_p} \right)} \tag{2}$$

β is the number of Si atoms released by the break-up of a cluster (β =2 for n=2, β =1 otherwise). R_p is the distance between the defect region and the surface, while the surface recombination length, L_{surf} is the only fitting parameter of the model.
The presence of an interstitial sink at the wafer surface (term $(L_{surf}+R_p)$ in eq. 2) imposes a "pinning" of the $Si_{int}s$ supersaturation that linearly decreases from the defect region towards the surface, as schematically shown in fig. 1a. This result implies that our model is equally applicable to both cases of crystalline and preamorphised substrates. In the first case, the defect region is generated by the boron implant itself and is located around the boron concentration peak. The boron diffusivity enhancement is therefore directly given by eq. 2. In the second case, the defect region is generated by the preamorphisation implant and can be much deeper than the boron profile. The boron diffusivity enhancement is therefore calculated by

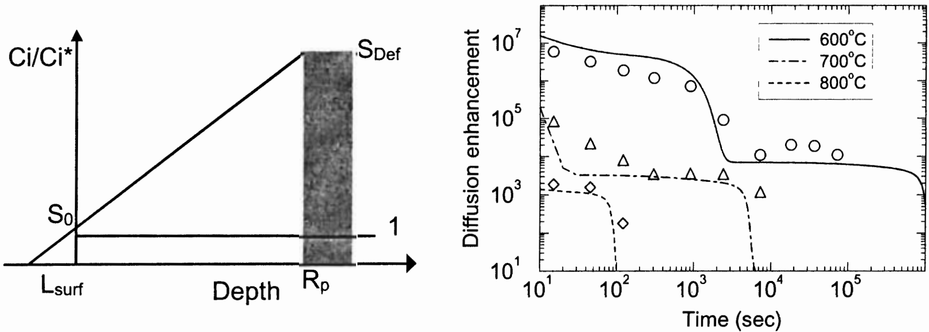

Fig. 1. *(a)* Depth variation of the amplitude of the $Si_{int}s$ supersaturation in the surface region. *(b)* Model validity test. TED of boron delta layers: comparison of measured diffusion enhancement (symbols) and simulated values (lines).

interpolating the $Si_{int}s$ supersaturation amplitude between the defect region (eq. 2) and the silicon surface, at the depth corresponding to the boron profile.

3 Results and Discussion

Typical results of our simulations are given in fig. 1b, where we have tested our model against the experimental study by Cowern et al. (1999), concerning the TED of CVD-grown boron delta layers after low dose Si^+ implantation. The measured evolution of the boron diffusivity enhancement, i.e. of the $Si_{int}s$ supersaturation, is well reproduced by the simulated curves, including the two "plateaus" associated to small stable clusters (size 4 and 8) and {113} defects observed at 600 °C. We have also been able to perfectly fit published data concerning the dissolution of {113} defects (Colombeau et al. 2001).

We now consider the case of direct boron implantation into a crystalline substrate. We have studied through computer simulations the effect of the implant energy in the range 1-25 keV, for a 10^{14} cm^{-2} boron implant. Fig. 2 shows the predicted evolution of the $Si_{int}s$ supersaturation in the defect region during a 950°C anneal. All implants show a sharp "peak" at very short times (when only small clusters exist), followed by a "plateau" associated with the ripening of {113} defects whose lifetime increases with increasing energy. This result demonstrates how the vicinity of the surface to the boron profile plays a crucial role in determining the TED decay time, especially at ultra low implantation energies. Indeed, these predictions are confirmed by the successful simulation of TED experiments of 2 keV implants (not shown).

We now present the application of our model to a typical case of boron TED in a preamorphised structure. Fig. 3a shows the SIMS profiles (symbols) measured after annealing at 950, 1000 and 1050°C for 10 sec of a series of samples implanted with 1 keV B^+ ions to a dose of $1x10^{14}$ ions/cm^2 into preamorphised silicon (150 keV Ge^+, $2x10^{15}$ ions/cm^2, a/c interface at 175 nm). The values of the average boron diffusion acceleration $<D_B/D_B^*>$ for the three samples are reported in the figure inset. They have been extracted by fitting the measured profiles using a commercially available process simulator and taking the boron diffusion coefficient as the fitting parameter (lines in fig. 3a). We have then used our model to calculate the average $Si_{int}s$ supersaturation in equilibrium with the defects (dislocation loops) for each of the three temperatures and the corresponding values in the region containing the boron

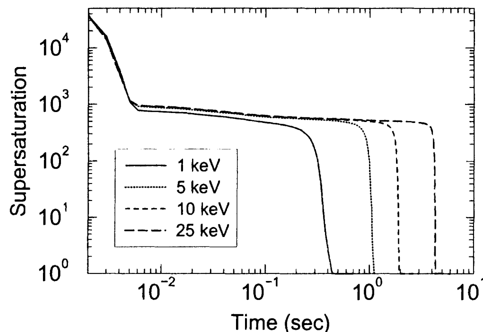

Fig. 2. Simulation of the $Si_{int}s$ supersaturation evolution for $1x10^{14}$ cm^{-2} boron implants in the 1-25 keV rage at an annealing temperature of 950°C.

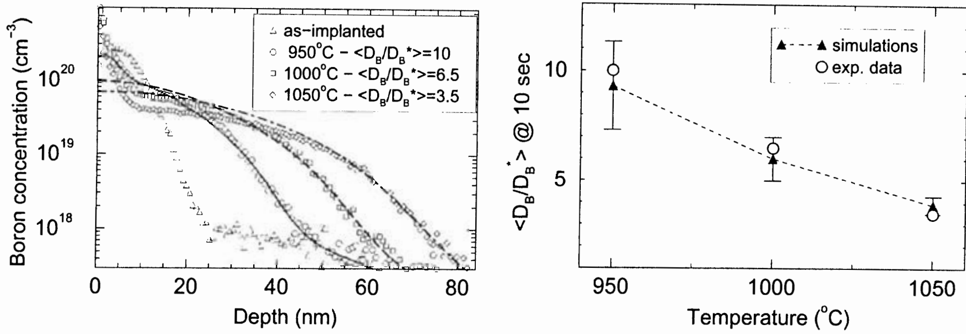

Fig. 3. *(a)* SIMS profiles (symbols) of 1 keV B^+ implants and acceleration coefficients (inset) extracted by a fitting procedure (lines). *(b)* Comparison between the simulated and measured values of the average acceleration coefficients for a 10 sec anneal.

profile, following the schematic description of fig. 1a. The calculated values are reported in fig. 3b (triangles) together with the measured ones (circles). An excellent agreement is obtained for all cases without changing any of the input parameters, except for the annealing temperature.

It is interesting to note that the low diffusivity enhancement in the preamorphised region is a "simple" consequence of the pinning of the $Si_{int}s$ supersaturation at the surface. There is therefore no need to describe the dislocation loops as a more or less efficient barrier against the the $Si_{int}s$ flux towards the surface.

4 Conclusions

We have developed an atomistic simulation of boron TED based on the Ostwald ripening of extrinsic defects occurring during annealing. The model applies to both crystalline and preamorphised structures. We have tested the model against some notorious experimental studies of TED and defect evolution. We have successfully applied our model to a variety of experimental conditions including ultra low energy implants. The strength of the model relies on the accurate physical description of the defects formation and evolution during annealing.

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