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Materials Science and Engineering B 124–125 (2005) 392–396
MATERIALS SCIENCE & ENGINEERING B
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Dose loss and segregation of boron and arsenic at the Si/SiO_2 interface by atomistic kinetic Monte Carlo simulations

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Abstract

Continuum downscaling of MOSFET devices requires of ultra-shallow junction formation. Performance of the source and drain from B and As low energy implant and subsequent annealing is seriously affected by the presence of the $Si–SiO_2$ interface. Dopant loss due to segregation and dopant pileup at the interface during the transient enhanced diffusion (TED) are crucial phenomena for current and future CMOS devices. In this work we have implemented the Oh-Ward model [Y.-S. Oh, D.E. Ward, Tech. Dig. Int. Electron Devices Meet. 1998 (1998) 509] for the dopant behaviour at the interfaces integrated in an atomistic kinetic Monte Carlo simulator. Dopant traps at the interface can capture from or emit to either side of the interface. Furthermore, segregation of dopants and saturation of the interface by the presence of other species are also included. As a test of the model, low energy implants through a screen oxide have been simulated. When annealing these very shallow implants, a pileup at the interface is observed. The mechanisms involved in this process, as well as its dependence on the implant dose and energy are discussed.
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Keywords: Monte Carlo simulations; MOSFET; TED

1. Introduction

For the MOSFET technology nodes of 65 nm and beyond, the role of interfaces is becoming increasingly important. Ultra-shallow junctions at a depth of a few tens of nanometers are needed. Low energy implants are usually performed through very narrow oxides. Due to the low projected range, a fraction of the implanted dose does not reach the silicon. Furthermore, when annealing these low energy implants, additional dose losses in the silicon side have been observed due to the trapping at the Si/SiO_2 interface, either with the previous oxide or, if it had been removed, with the oxide formed during annealing. Experimental dose losses and segregation effects for typical dopants, arsenic, boron, phosphorus and antimony have been reported [1–9]. These dose loss effects and the segregation of the dopants at the interface seriously affect to the electrical performance of the MOSFETs. Sheet resistance increases [4,9] and threshold voltage variations [6] due to these dose losses have been reported.

This work addresses the role of the different mechanisms that affect to the pileup at the Si/SiO_2 interface, in order to be able to quantitatively predict the dose loss in different conditions through atomistic kinetic Monte Carlo (kMC) simulation.

2. Interface model

Several models for trapping and segregation of dopants at interfaces have been developed [6,10,11]. Oh and Ward [11] presented a model for the trapping of dopants at the interfaces during thermal annealing including the competition among different dopant species for trapping sites at the interface. They implemented the model in TSUPREM-4. In this model, the flux of a dopant into the interface from the silicon side as a function of time is given by

$$F(t) = h\left\{C_s(t)\left[1-\sum_{\text{species}}\left(\frac{\sigma_i(t)}{\sigma_{\max}}\right)+\left(\frac{e}{a}\right)\frac{\sigma_i(t)}{\sigma_{\max}}\right] - \left(\frac{e}{a}\right)\frac{C_{\text{solub}}\sigma_i(t)}{\sigma_{\max}}\right\} \quad (1)$$

where $\sigma_{\max}$ is the total trap density at the interface and C_{solub} the solid solubility limit of the dopant in silicon. a and e are the absorption and emission probabilities, and $h = a\sigma_{\max}$. Finally, C_s represents the volume concentration of the dopant at the interface in the material side and $\sigma_i(t)$ the density of trapped dopants at

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doi:10.1016/j.mseb.2005.08.030

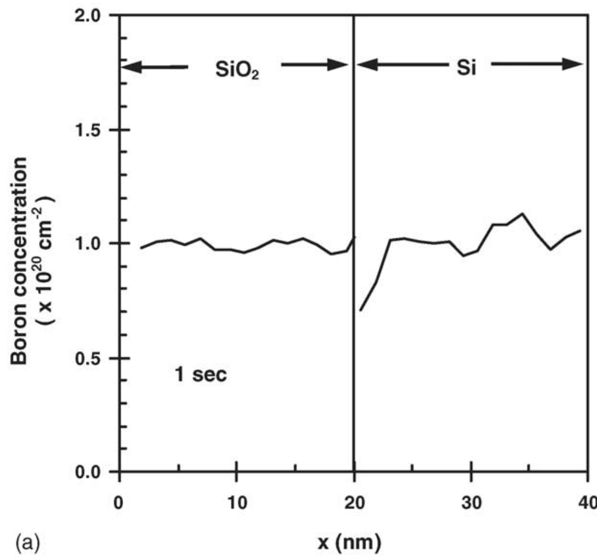
the interface. This expression for the flux represents the balance between trapping and detrapping rate. Oh and Ward calibrated the different parameters for B, P and As.

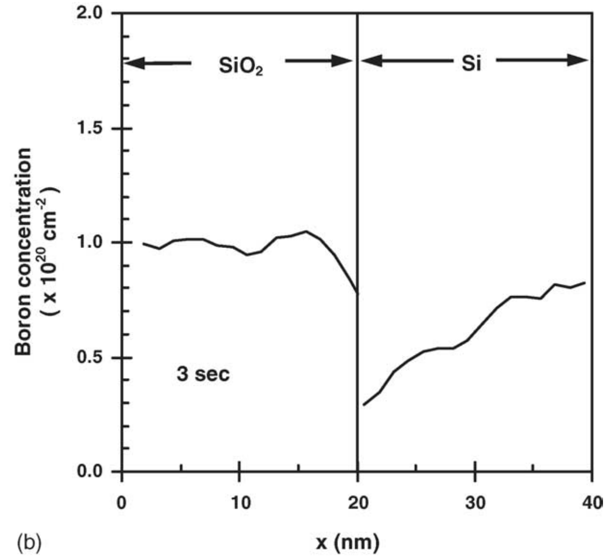
We have implemented this model in the atomistic kinetic Monte Carlo process simulator DADOS [12]. This simulator models individual particles (I, V, As, B, B_i, AsV, As_i, etc.), each of them jumping at a characteristic rate. When time goes by, some of these jumping particles can hit the interface. On average, the attempt frequency for this event is given by (DC_s/λ) where D is the effective diffusion coefficient and λ the jump distance. When a dopant hits the interface, it can be captured with a probability that can be identified from the above expression for $F(t)$ as:

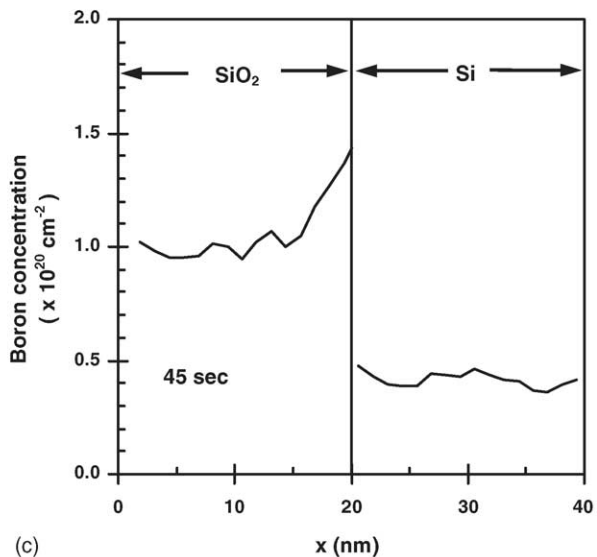
$$\text{Capture probabilty} = \frac{\lambda h}{D}\left\{1 - \frac{\sum \sigma_i}{\sigma_{\max}} + \left(\frac{e}{a}\right)\frac{\sigma_i}{\sigma_{\max}}\right\} \quad (2)$$

The product of the attempt frequency and the capture probability must give Oh-Ward expression for the capture flux at the interface. This capture flux is then dependent on both the near-surface dopant concentration and the density of empty traps. On the other hand, occupied traps can emit dopants. The emission rate is proportional to the solid solubility limit and to the density of occupied traps at the interface. For considering the oxide side, the segregation coefficient and the diffusivity of the dopant in oxide control the relative emission rate.

As a test of the model, we have simulated the boron segregation at the Si/SiO_2 interface. We start with an initial constant profile (Fig. 1a) that evolves at 1050 °C. Evolution of the boron concentration starting on that constant profile can be described as: trapping of boron mainly from the silicon (higher diffusion coefficient) and the subsequent decrease in the boron dose at that side (Fig. 1b); emission to the oxide and pileup of boron near the interface due to the low diffusivity (Fig. 1c); slow diffusion towards the bulk of the oxide until the profile finally becomes flat (Fig. 1d). At that time, the ratio between the concentrations at the two sides of the interface is equal to the segregation coefficient:







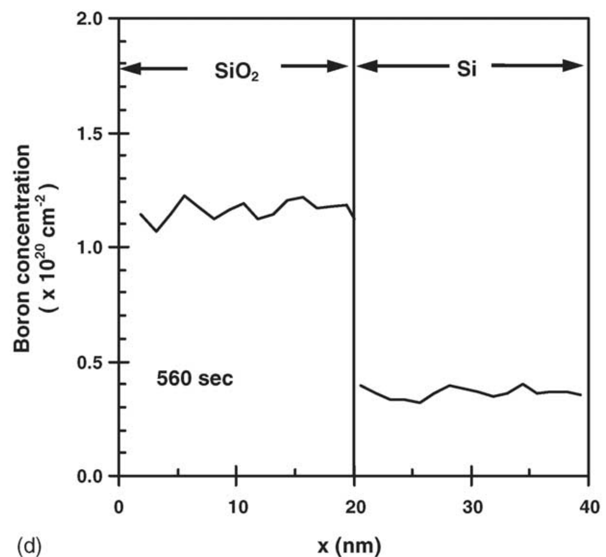


Fig. 1. Boron concentration profiles at 1050 °C at different times, starting on an initially constant boron profile of 10^{20} cm^{-3}.

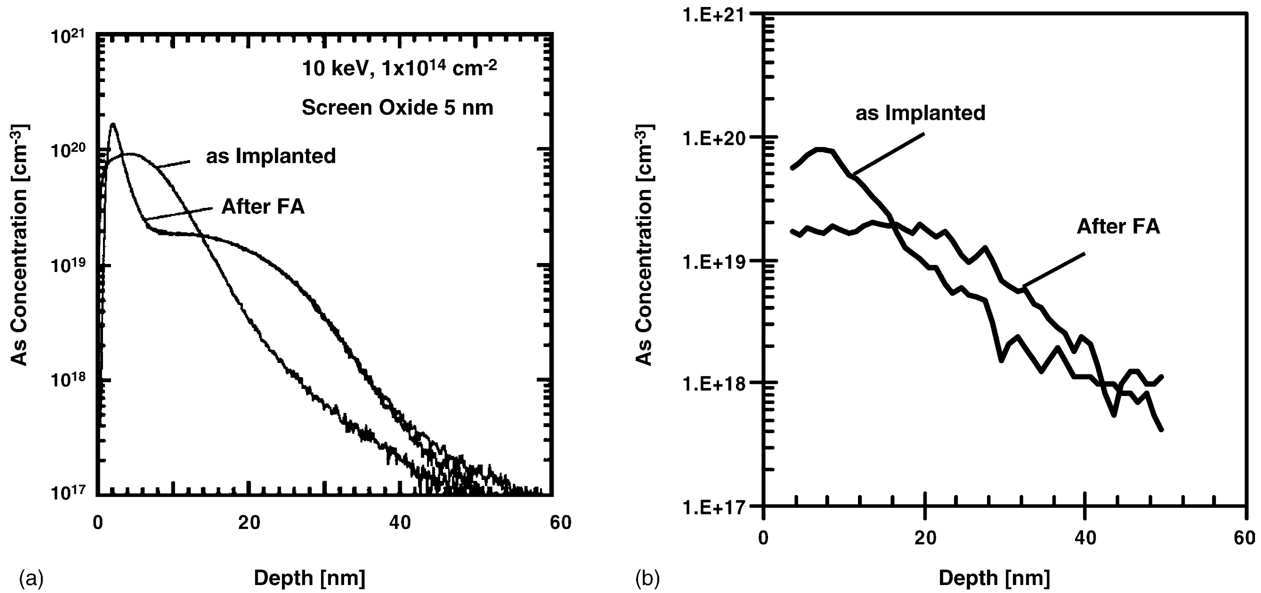


Fig. 2. SIMS (Ref. [9]) (a) and simulated (b) arsenic depth profiles before and after annealing. Implant energy and dose were 10 keV and 10^{14} cm^{-2}. Annealing was performed at 850 °C for 30 min.

$$\frac{C_{Ox}}{C_{Si}} \approx 3.3.$$

It should be pointed out that all the DADOS simulations presented in this paper include Fermi-level effects [13], clustering [14], damage build-up and amorphization/recrystallization [15].

3. Results

In order to study the dose loss due to the pileup at the Si/SiO_2 interface, we have reproduced the arsenic experimental results by Koh et al. [9], which we describe briefly. The experimental conditions roughly correspond to the fabrication of the source/drain (S/D) extensions for a MOSFET: (1) 1 keV arsenic implantation through a 5 nm screen oxide with a dose of 14^{14} cm^{-2}; (2) screen oxide removal; (3) furnace annealing (FA) at 850 °C for 30 min (during this anneal, a 2 nm oxide was formed). Two dose loss mechanisms were evaluated: (a) After step 2, arsenic atoms implanted in the screen oxide are lost; (b) during annealing, a fraction of the arsenic atoms are trapped at the interface. The interface kinetics and the dependence of this dose loss on the implant dose and energy were investigated. The pileup ratio γ_p is defined as the ratio of As loss by pileup, to the total amount of As implanted in Si. In our work, we focus on the dose loss due to the pileup at the interface.

Fig. 2a shows experimental profiles [9] of an arsenic implant at 10 keV and a dose of 10^{14} cm^{-2}, along with the profiles after a 30 min annealing at 850 °C. The reduction in the arsenic dose in Silicon is due to the trapping at the interface oxide–silicon, as can be seen in the interface peak, which is not present if the secondary ion mass spectroscopy (SIMS) analysis is performed after the 2 nm oxide has been removed. The experimental pileup ratio is 51%. Fig. 2b corresponds to the simulated profiles in the same conditions, in good agreement with the experiments and giving a pileup ratio of 48%. Notice that the depth scale in the simulation is not accurate due to discrepancy in the as-implanted profile. The simulated profiles (Fig. 2b) do not show the interface peak because they plot the arsenic concentration just in the silicon.

In order to investigate the interface kinetics, let us focus on the time evolution of the trapped dose. By comparing the near-surface trapped atoms peak for SIMS profiles at 5 and 30 min, the pileup is already formed at 5 min, and there is little variation between these times (Fig. 3a). Simulations for the time evolution of the trapped dose are in good agreement with experiments [9], as shown in Fig. 3a. Two regimes can be identified in the simulation. First, a short time regime (Fig. 3b), that corresponds to the dissolution time of the amorphous pockets generated by the implantation. As it is known, during the dissolution of amorphous pockets, point defects are released, giving rise to a transient enhanced diffusion (TED) that speeds up the As transport to the interface. We have tested that the characteristic time of this first mechanism does not depend on the parameters of the interface model, but on the implantation and annealing conditions. Once the initial transient has ended, a long-time regime was observed. It can be fitted by two interface parameters: the emission to absorption probability, e/a, and the density of interface traps, σ_{max}. Increasing e/a gives shorter long-time transients and reduces the density of trapped atoms. On the other hand, the final trapped dose at the interface can be adjusted through σ_{max}.

Experiments [9] show that lowering the implant dose decreases the pileup ratio at the interface. Simulations for 10^{13} and 10^{14} cm^{-2} show the same trend and also the agreement in quantitative values is good (Table 1). The corresponding time evolution of the pileup at the interface in our simulations is different for each dose. The lower dose implant produces less damage, so the amount of TED is less than for the higher dose and, consequently, the trapped dose due to this mechanism pileup is also smaller. The capture rate at the interface traps is proportional to the arsenic concentration close to the interface, which

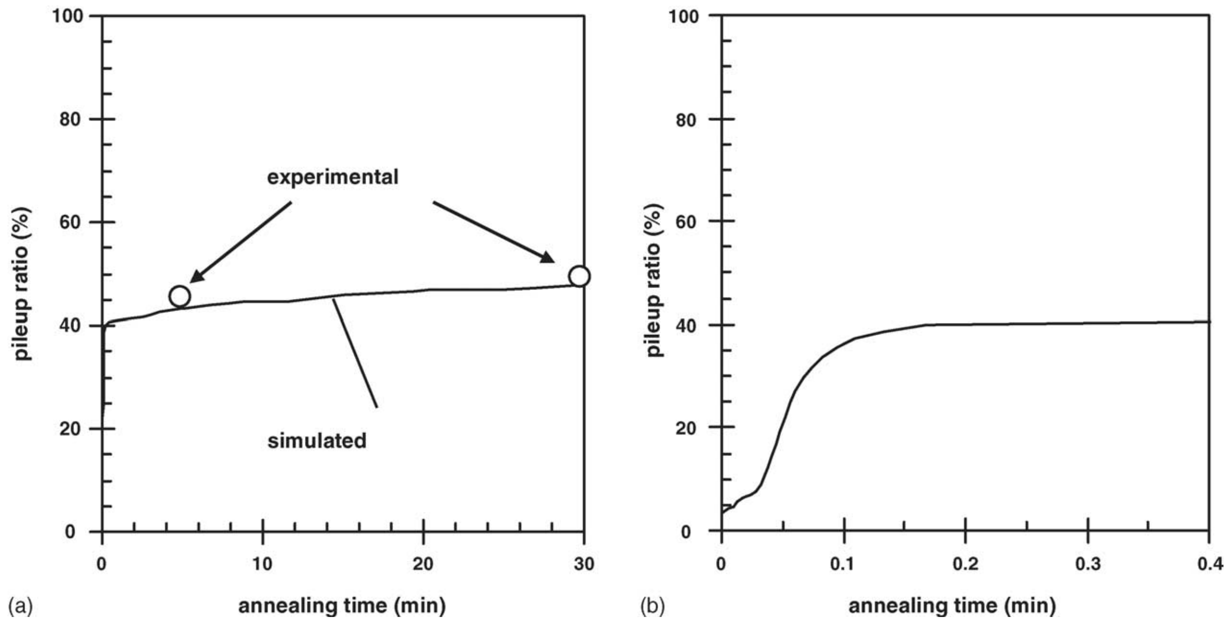


Fig. 3. (a) Experimental (Ref. [9]) (symbols) and simulated (lines) dependence of γ_p on annealing time at 850 °C for $e/a = 0.4$ and $\sigma_{max} = 3 \times 10^{14}$ cm^{-2}. (b) Detail of the initial stages of annealing.

Table 1
Experimental and simulated pileup ratio γ_p as a function of the total implanted dose

Implant dose (cm^{-2})	Experimental pileup ratio γ_p (%)	Simulated pileup ratio γ_p (%)
10^{13}	35	34
10^{14}	51	48

is lower for the 10^{13} dose. This lower capture rate gives rise to a slower evolution towards the steady state. As can be seen, this steady state has not been reached at 30 min (Fig. 4).

Finally, the dependence of the pileup with the implant energy has been investigated. In the experiments, implants at 5, 7 and 10 keV have been performed with a dose of 10^{14} cm^{-2} [9]. The annealing conditions are the same as before. Experiments indicate that the pileup ratio is lower for the smaller implant energies. Simulations also show the same trend, and similar quantitative values (Table 2). To understand this behaviour, it is necessary to keep in mind that the pileup ratio is defined as the ratio of the dopant loss to the implanted dose in silicon. Table 2 shows that the As dose trapped at the interface after annealing is about the same for the three energies. From Eq. (1) for only one dopant and

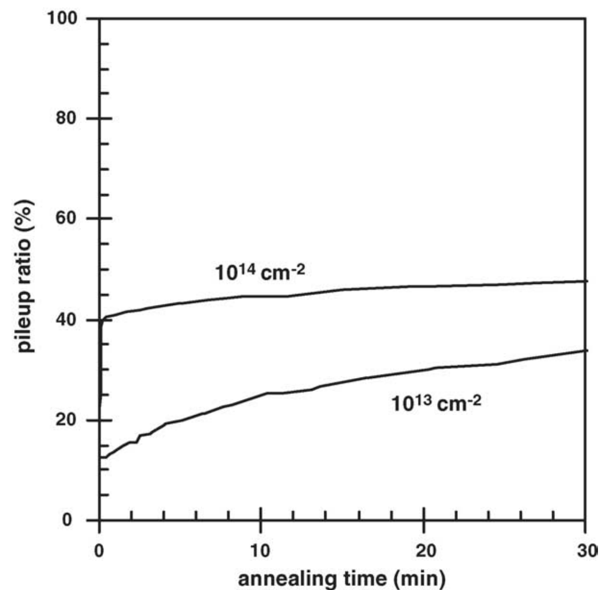


Fig. 4. Dependence of the pileup ratio γ_p on annealing time for 10 keV arsenic implants with 10^{13} and 10^{14} cm^{-2} doses.

Table 2
Experimental and simulated pileup ratio γ_p as a function of the implant energy

Implant energy (keV)	Experimental pileup ratio (%)	Simulated pileup ratio (%)	Initial implanted dose in Si (cm^{-2})	Final As dose trapped at interface (cm^{-2})
5	77	74	5.7×10^{13}	4.2×10^{13}
7	56	61	7.4×10^{13}	4.5×10^{13}
10	51	48	8.5×10^{13}	4.1×10^{13}

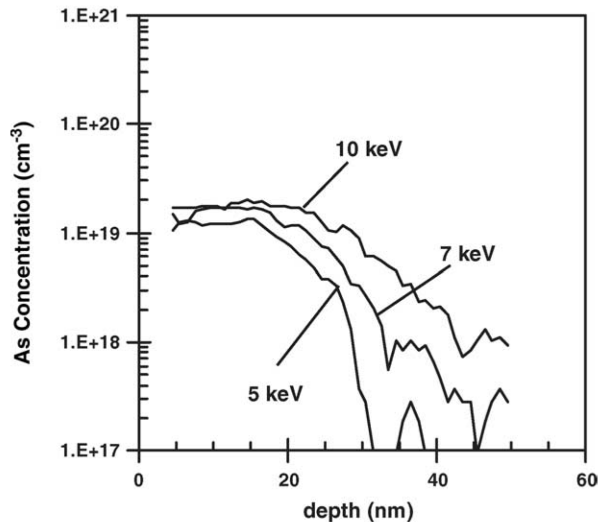


Fig. 5. Simulated arsenic depth concentration profiles after 30 min furnace annealing at 850 °C for different implant energies: 5, 7, 10 keV. The dose was 10^{14} cm^{-2} in all cases.

when the time is long enough for the dopant flux to vanish (steady state), the trapped dose is a function of the dopant concentration at the interface. Both experimental [9] and simulated concentration profiles show that, after annealing, this concentration is similar for the three implant energies (Fig. 5). So the difference in pileup ratio comes from the initial implanted dose in Si (Table 2): The total dose was the same for all the implant energies, but smaller energies have shorter projected range and, therefore, a larger fraction of the dose was implanted on the screen oxide, which was removed afterwards. So, when the annealing starts, the total amount of arsenic remaining in silicon is smaller for the lower energies.

4. Conclusions

In this work dopant dose loss and segregation at interfaces have been investigated by using the atomistic kinetic Monte Carlo process simulator DADOS. Time evolution of the concentration of an initially boron constant profile shows the proper segregation behaviour at the Si/SiO_2 interface.

Experiments reported in the literature of an arsenic-implanted and annealed silicon sample show a dose loss due to pileup of dopants at the interface. Our simulations show that the quantitative values for the trapped dose at the Si/SiO_2 interface, as well as its time evolution are in very good agreement with the experiments. The mechanisms related to the trapping/detrapping have been discussed. Furthermore, the simulated dependence of dose loss on the implant dose and energy given by our simulations are consistent with the experiments.

Acknowledgments

This work has been partially supported by the Spanish Government under project BFM2001-2250 and by the Castilla y Leon regional Government under project VA-010/02.

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