SIMULATION OF SEMICONDUCTOR PROCESSES AND DEVICES Vol. 12 Edited by T. Grasser and S. Selberherr - September 2007

# Modeling and Characterization of Advanced Phosphorus Ultra Shallow Junction Using Germanium and Carbon Coimplants

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#### Abstract

A continuum model of phosphorus diffusion with germanium and carbon coimplant has been proposed and calibrated based on secondary ion mass spectroscopy (SIMS) profiles aiming at ultra shallow junction (USJ) formation in advanced CMOS technologies. The phosphorus diffusion behaviors are well captured by our model under various implant and annealing conditions, representing a significant step towards advanced n-type USJ formation technique using phosphorus and carbon coimplant for aggressively scaled CMOS technologies.

## **1** Introduction

Modeling of carbon coimplant and its effects on dopant diffusion is of great interest since carbon suppresses interstitial-mediated dopant diffusion, known as transientenhanced diffusion (TED) for boron and phosphorus due to its interaction with free interstitials [1][2] [3][4][5], resulting in abrupt and shallower junction profiles that are essential for advanced CMOS technologies. Although a well calibrated carbon diffusion and carbon-interstitial reaction model has been developed [6], which satisfactorily describes the carbon diffusion behaviors, however, a well calibrated and CPU time effective continuum model for the phosphorus diffusion with germanium and carbon coimplants is still lacking for the advanced CMOS technology development. Phosphorus provides alternative solution to n-type USJ formation owing to its higher activation comparing to the commonly used n-type dopant arsenic, resulting in lower junction sheet resistance [8]. In this paper, we develop a continuum model in order to understand the underlying physics of carbon and phosphorus coimplant diffusion process. We implement our model into TSUPREM4 [7] and perform a series of numerical simulations in which we successfully reproduce phosphorus TED suppression caused by germanium and carbon coimplants. Our results quantitatively agree with the SIMS profiles reported earlier [1].

### 2 Experiments

The detailed wafer preparation and implant/annealing conditions have been reported elsewhere [1]. The coimplant conditions and associated junction characteristics are summarized in Table I.

## **3** Model Calibration and Discussion

#### **3.1** Carbon dopant defect cluster model

For carbon diffusion modeling, we begin with an introduction of modified carbon reactions in addition to the standard carbon cluster modeling [6], which provides useful insights into our SIMS data. Our modified carbon reactions are:

- $Cs + I \leftrightarrow Ci$  pairing and interstitial trapping (1)
- $Cs + Ci \leftrightarrow C2I$  CI trapping/emission (2)
- $C2I + Ci \leftrightarrow C3I2$  CI trapping /emission (3)

In reaction (1), Cs denotes a substitutional carbon, and Ci is a highly mobile carboninterstitial pair. Reaction (2) and (3) describe the Ci trapping/emission effect. In reaction (2), Cs forms Ci cluster C2I by trapping a Ci pair at the medium C concentration. The C<sub>2</sub>I cluster reaction has been well calibrated previously [2]. In reaction (3), C2I forms C3I2 by trapping Ci, which dominates at high C concentration. In our model, we assume that carbon is substitutional in the amorphous region as well as in the C3I2 clusters in the crystalline region during the beginning stage of annealing. In Fig. 1, we present our simulation results of the substitutional carbon Cs and carbon interstitial cluster C3I2 distribution before annealing according to (1) to (3); wherein the distinctive two-component character of the substitutional carbon distribution is uncovered. We note that the carbon distribution shown in Fig.1 plays a crucial role in the final simulated phosphorus TED suppression, without which the quantitative behaviors of phosphorus TED cannot be understood in our simulation. The carboninterstitial paring reaction rate R1 of reaction (1) can be written as follows [9]

$$R1 = \frac{\partial Ci}{\partial t} = D_C / (\lambda^2 \bullet I^*) (Cs \bullet I - (D_{Ci} / D_C)I^* \bullet Ci)$$

where  $D_C$  is the carbon diffusivity,  $D_{Ci}$  is the interstitial carbon diffusivity, I\* is the interstitial equilibrium concentration, and  $\lambda$  is the carbon-interstitial pair hopping distance. It is assumed that the reaction (2) and (3) are diffusion limited so their reaction rate can be written as

$$R2 = \frac{\partial C_2 I}{\partial t} = 4\pi a Dci \ (Cs \bullet CI - Kb_1 \bullet C_2 I)$$
  
$$R3 = \frac{\partial C_3 I_2}{\partial t} = 4\pi a Dci \ (C_2 I \bullet CI - Kb_2 \bullet C_3 I_2)$$

where a is the lattice spacing ,  $K_{b1}$  and  $K_{b2}$  are temperature dependent parameters given by the relationship:  $K_{b1}=5x10^{22}exp(-E_{b1}/kt)$  and  $K_{b2}=5x10^{22}exp(-E_{b2}/kt)$  where  $E_{b1}$  and  $E_{b2}$  are the binding energies extracted from the experiments [1].

#### 3.2 Phosphorus diffusion modeling

Regarding the phosphorus diffusion modeling, we include the following mechanisms in our model: (1) a 5-stream model for phosphorus diffusion, (2) a {311} self-interstitial clusters model proposed by C. S. Rafferty [10], and (3) a 3-phase segregation model for phosphorus dose loss at the silicon/oxide interface [7][11]. The parameters are calibrated according to experiment [1] based on the recommended values [7] as the initial one.

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#### 4 **Results and Discussion**

The phosphorus TED effect originates from the extra interstitials that are introduced into silicon by implants. The carbon is substitutionally introduced into the preamorphized region and forms an interstitial trapping layer. During the initial stage of spike annealing in which the solid-phase-epitaxial-regrowth (SPER) occurs, larger overlap of Ge PAI and carbon profiles would increase the amount of substitutional incorporation of carbon atoms in silicon, resulting in more carbon-interstitial pairing and hence greater phosphorus TED suppression. At the 4× Ge PAI implant energy, Ge profile completely covers the carbon profile, reaching maximum substitutional carbon concentration in the amorphous layer. This process can be well captured by our model as shown in Fig.2. It is worthy noting that at 4× Ge PAI implant energy, the end-of-range (EOR) effects reside deeper than the phosphorus junction, resulting in minimized defect-induced junction leakage. Our model is also able to precisely reproduce the carbon segregation at the amorphous/crystal interface created by the Ge PAI implant. Further reducing Ge PAI energy decreases amorphous layer thickness and substitutional carbon concentration and thus diminishes the phosphorus TED suppression. Fig 3 and 4 show the phosphorus profiles at the Ge PAI energy of  $2 \times$  and 1×, respectively, where the carbon-suppressed phosphorus TED becomes diminished according to our model. Our model also provides a quantitative understanding why Ponly and C+P implant exhibits typical TED behavior. Without Ge PAI, there are not enough substitutional carbon atoms to trap interstitials and phosphorus TED persists. In Fig. 5, we present our results for the P-only and C+P implants.

## 5 Conclusions

We propose a continuum model for phosphorus diffusion with germanium and carbon coimplants and obtain phosphorus and carbon profiles quantitatively agreed with the SIMS profiles. We analyze the mechanisms of phosphorus diffusion during the coimplant process, demonstrating the importance of the use of an amorphous layer to form a high concentration of substitutional carbon atoms in order to suppress the phosphorus TED. Our model provides essential ingredients for n-type USJ formation for 45 nm node CMOS technology and beyond.

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Germanium Carbon Phosphorus			Xj (a.u.)	thickness (a. u.)
		v	0.46	N/A
	v	v	0.43	N/A
v (1x energy)	v	v	0.31	0.15
v (2x energy)	v	v	0.21	0.21
v (4x energy)	v	v	0.19	0.34



Fig. 1 Simulated as-implanted

carbon profile using the modified carbon reactions (1),

(2), and (3). The arrow indicates the position of the a/c

1E21

interface.

P+C implant

P SIMS
P Simulation

Table 1. Summary of phosphorus junction characteristics using germanium and carbon coimplants after 1020°C spike anneal.





0 P SIMS

Δ

1E21

Fig. 2 Comparison of simulated and SIMS profiles of phosphorus diffusion with germanium of 4x energy and carbon coimplants after 1020°C spike anneal. The arrow indicates the position of the a/c interface.

1E21

1E20

Fig. 3 Comparison of simulated and SIMS profiles of phosphorus diffusion with germanium of 2x energy and carbon coimplants after 1020°C spike anneal. The arrow indicates the position of the a/c interface.



Fig. 4 Comparison of simulated and SIMS profiles of phosphorus diffusion with germanium of 1x energy and carbon coimplants after 1020°C spike anneal. The arrow indicates the position of the a/c interface.



P-only implant P SIMS
P Simula

Fig. 5 Comparison of simulated and SIMS profiles of phosphorus-only and phosphorus and carbon coimplant after 1020°C spike anneal.

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