Analytical model and Monte Carlo Simulations for Phosphorus implantation in Germanium including ion channeling

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***Abstract*—A Monte Carlo Simulator for dopant implantation (TaurusMC) was successfully calibrated for the implantation of Phosphorus in Germanium, based on both SIMS measurements and TEM. To avoid time-consuming Monte Carlo simulations, an analytical model was proposed based on the description of as-implanted profiles with a dual Pearson curve. This model covers a large range of energy (15-180 keV) and doses (10^{12}-10^{16} cm^{-2}), of interest to the ongoing scaling efforts of Ge MOSFETs.**

I. INTRODUCTION

Recently, there has been a renewed interest in germanium as a potential high mobility alternative to silicon for logic applications. Its low processing temperature also makes it compatible with advanced high-k and metal gates stack technology [1]. These properties propel recent research efforts in Ge MOSFETs. Various groups have reported on the fabrication of deep submicron Ge pMOSFETs: 125 nm devices have been produced on 1.5μm thick Germanium-on-Silicon layers [2] and on Germanium-on-Insulator (GOI) substrates [3], 60 nm Ge pMOSFETs with full NiGe source/drain regions have been reported in [4]. As this scaling continues, doping levels are expected to increase further while the need for shallower source/drain junctions arises. For pMOSFETs, phosphorus is the dominant n-type dopant (used for well and halo implants), although some research is being performed with Arsenic [5]. Phosphorus is also the most promising candidate among classical n-type dopants in Ge introduced by ion implantation (such as P, As, Sb), particularly in terms of electrical activity [6]. Accurate modeling of the dopant profiles is an important enabler for the continuing scaling effort. Unlike in Si processing, processing temperatures are typically limited to about 550°C [5]. At this temperature, P diffusion is very limited [6], increasing the need for accurate TCAD simulations of the as-implanted profiles. This paper addresses that need by calibrating a Monte Carlo simulator (TaurusMC, [7]) for P implantations into Ge substrates.

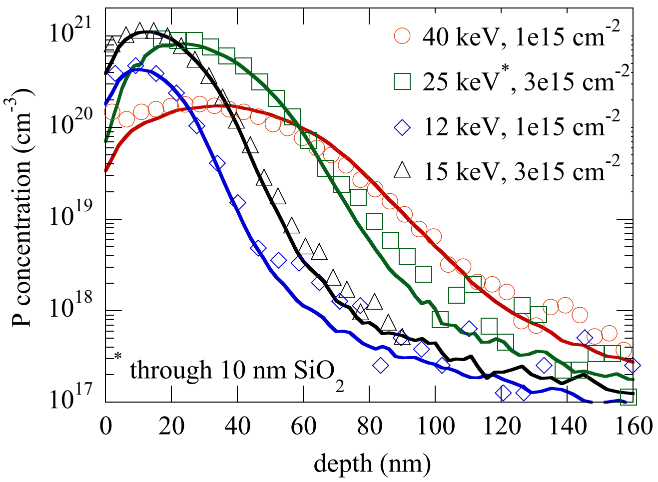

Fig. 1. SIMS measurements (symbols) and Monte Carlo simulation (lines) for various energies and doses of ion implanted Phosphorus in Germanium.

This paper is structured as follows: section II elaborates on the calibration of the Monte Carlo simulator, while in section III, an analytical model based on dual pearson distribution curves for P implantation in Ge is proposed in order to avoid the time consuming Monte Carlo simulations.

II. CALIBRATING THE MONTE CARLO SIMULATOR

A reliable calibration of TaurusMC for implantation of Phosphorus in Germanium does not exist. Although many of the required parameters are readily available (e.g. atomic mass, lattice constant, crystal structure etc.), accurate simulations of the channeling-related portion of the as-implanted profile must also consider damage accumulation in the Germanium lattice during the ion bombardment. As displaced atoms clutter the crystallographic channels in the substrate, the ion channeling process is reduced. This effect is known as damage-dechanneling [7] and is a function of the implanted dose as damage accumulation is a dynamic process during the ion implantation.

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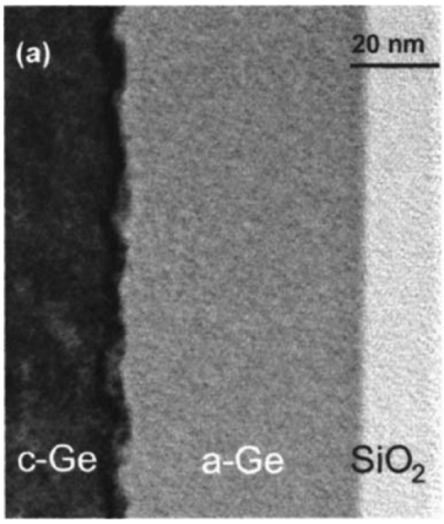

Fig. 2. TEM image of an as-implanted Ge sample, showing a ~50 nm amorphous top layer (from [8]).

The Monte Carlo simulator was calibrated in two steps. First, the simulated profiles were fitted to experimental data obtained from Secondary Ion Mass Spectroscopy (SIMS). Fig. 1 shows four such fits for different energies and doses. One of the experimental profiles included a 10 nm SiO_2 oxide layer on top of the Germanium (not shown), which was also included in the Monte Carlo Simulations. The fitting was performed by changing the parameters which control the damage evolution during implantation. Good fits were obtained with the experimental data, as can be seen from figure 1.

As fitting SIMS profiles is still an indirect way to check the damage evolution in the sample during the implant and susceptible to measurement noise in the channeling tail, a more direct approach to measure the damage evolution in the crystal lattice was taken in a second step. A TEM image from a P-implanted sample (Fig. 2) (25 keV, 3×10^{15} cm^{-2}, through 20 nm SiO_2) shows that the as-implanted sample has an amorphous top layer, which extends to a depth of about 50 nm. This amorphous layer is formed during the implant as a result of the ion bombardment. A Monte Carlo simulator, simulating the damage accumulation in the sample, should be able to estimate the extent of the amorphization. The calibrated TaurusMC simulator predicts this amorphous layer to be 49 nm thick. Considering the waviness of the amorphous-crystalline interface on the TEM picture, this result is certainly within error margins.

III. ANALYTICAL DESCRIPTION

A. *The as-implanted profiles*

Although the calibrated TaurusMC simulator produces good fits to experimental data, it suffers from the fact that the statistical noise inherent to Monte Carlo simulations can only be reduced by increasing the number of simulated particles. This has off course a detrimental effect on the simulation time. To address this problem, analytical functions such as the simple Gaussian or Pearson distribution curves have been used to describe dopant profiles. The tail resulting from ion channeling is often included by use of a second Pearson curve: the sum of the main and tail Pearson then represents the entire profile. This is illustrated in Fig. 3: A typical as-implanted profile from the simulator is fitted with a simple Gaussian, a Pearson and a dual Pearson curve. It can clearly be seen that the Gaussian nor the Pearson can include the channeling tail between 200 and 500 nm. The dual Pearson curve, which is the sum of two separate Pearson distributions for the main part and the tail, is able to fit the entire profile. The Pearson family of distribution curves contains 12 separately identifiable types (including the simple gaussian) and results from solving the differential equation [9]:

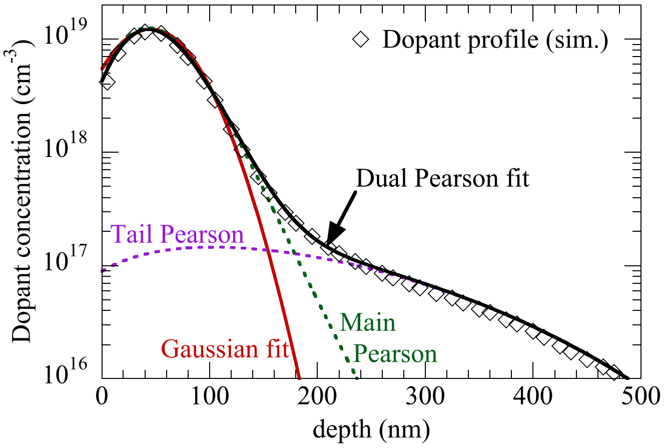

Fig. 3. Typical dopant profile (symbols) and various analytical fits: Gaussian, Pearson and Dual Pearson.

$$\frac{df(y)}{dy} = \frac{(y-a)\,f(y)}{b_0 + b_1 y + b_2 y^2} \tag{1}$$

The four parameters of Eq. 1 are related to the four moments of the Pearson distribution function: Range, straggle, skewness and kurtosis. In the remainder of this work, no restrictions are imposed on the type of the Pearson distributions and a general solution of the above equation is used. A dual Pearson curve requires thus 10 parameters: four moments (range R_p, straggle σ, skewness γ, kurtosisβ) and one normalization factor for each Pearson. In general, all these parameters can vary with both dose and energy.

B. *Analytical model*

Monte Carlo simulations of P implants were performed for energies from 15 to 180 keV and for doses ranging 10^{12}-10^{16} cm^{-2} (tilt 7°). This range covers the implant conditions used in present Ge pMOSFET research [10] as well as lower energy conditions which can be of use to future development of both n- and pMOSFETs. Based on these profiles, an analytical

TABLE I

ANALYTICAL MODEL FOR PHOSPHORUS IN GERMANIUM, USING 'DUAL PEARSON' CURVES.

	Main Pearson	Tail Pearson
Range R$_p$ (nm)	$0.84E$	$2.77E$
Straggle σ (nm)	$-0.00045E^2+0.516E+6.6046$	$-0.0035E^2+1.5E+47$
Skewness γ (-)	$-0.000023E^2+0.0007E-0.4009+1.1\left(1-\left(\frac{D}{D+2\times10^{14}}\right)^3\right)^3$	$0.000015E^2-0.005E+0.88$
Kurtosis β (-)	$0.0001018E^2-0.009883E+4.245$	$0.0000103E^2-0.00587E+3.36$
Dose D (cm^{-2})	$D_{main}=D-D_{tail}$	$D_{tail}=h_1(E)\left(\frac{D_T(E)}{D+D_T(E)}\right)^{1.7}+h_2(E)\left(\frac{D_T(E)}{D+D_T(E)}\right)^{1.7}$ $D_T(E)=a_TE^{b_T}$; $h_1(E)=e^{a_1ln(D)+b_1}$; $h_2(E)=e^{a_2ln(D)+b_2}$ $a_T=2.08\times10^{14}$; $a_T=2.08\times10^{14}$; $a_1=0.1$; $a_2=1$; $b_T=-0.745$; $b_1=1.29-388.81E^{-2.06}$; $b_2=26.3-0.0058E$
		E(keV)=implant energy ; D(cm^{-2})=implanted dose

model was constructed for each of the Pearson parameters, using a least-squares algorithm to fit each profile with a dual Pearson curve. This optimization procedure is necessary, as the moments (range, straggle, ...) calculated directly from the experimental or simulated data will not, in general, be sufficiently close to the real moments as they are inevitably calculated on semi-infinite profiles [9].

This analytical model is presented in Table I. Most of the Pearson moments can be described as a function of energy only, often with a second order polynomial. The dose of the channeling Pearson is a function of both energy and dose: for low-dose implants, the ratio of the ions that are contained in the channeling tail is constant; for high-dose implants the channeling ratio becomes smaller. This can be understood by considering that for very low doses, the ion channels remain intact during the entire implantation step. Every implanted ion has therefore an equal chance of channeling. On the other hand, high-dose implants damage these ion channels, eventually resulting in an amorphous top-layer as was the case in Fig. 2. This reduces the overall channeling ratio. Fig. 4 shows this dependence for the 100 keV implant: up to a total implanted dose of about 10^{13} cm^{-2}, the channeling tail contains ~25% of the implanted ions. For higher doses, this fraction drops significantly.

Fig. 5 and 6 show the Monte Carlo simulations and the analytical model for two energies (25 and 100 keV) and varying doses. A good agreement between the simulations and the analytical model could be obtained over the considered dose and energy ranges. Also, from these profiles, it is clear that the channeling dose (i.e. the tail in Fig. 5 and 6) saturates at a dose of about 4×10^{13}. While there is a clear increase in the dose of the main Pearson, the channeling tail remains almost identical for a total implanted dose of 10^{14} or above.

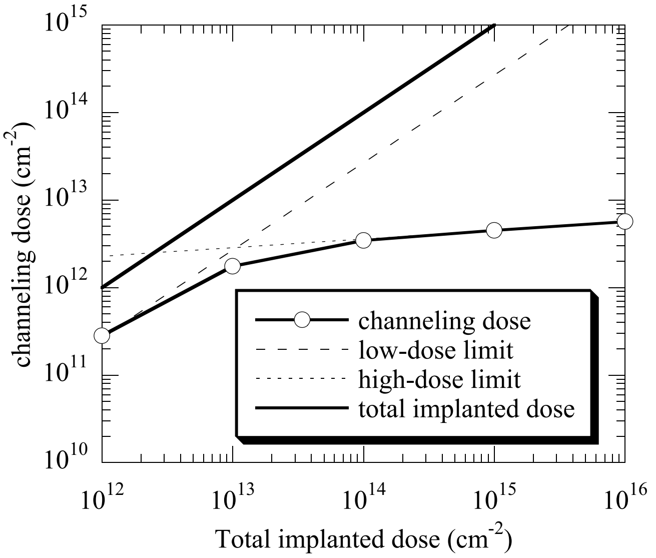

Fig. 4. Channeling dose as a function of total implanted dose for the 100 keV implant.

IV. CONCLUSION

The TaurusMC Monte Carlo simulator was calibrated for the implantation of Phosphorus in Germanium, based on experimental data from both SIMS measurements and TEM images. Based on this simulator, an analytical model was proposed based on the description of as-implanted profiles with a dual Pearson curve. This model covers a large range of energy (15-180 keV) and doses (10^{12}-10^{16} cm^{-2}) including those energy/dose combinations that are applicable in today's Ge MOSFET devices. The accurate description of P implantation steps in Ge will facilitate further scaling of Ge MOSFETs.

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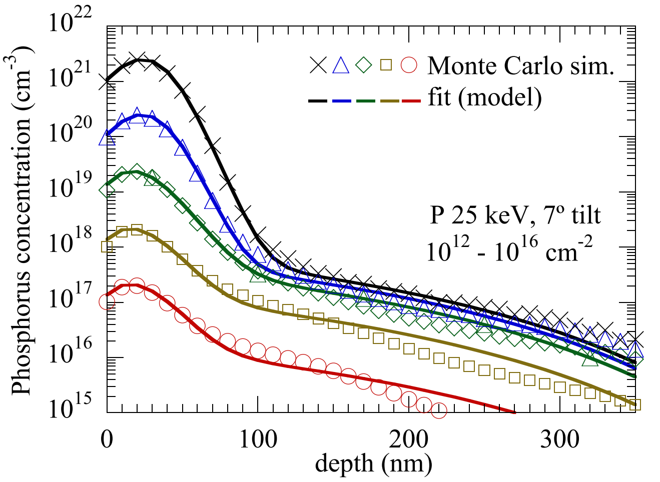

Fig. 5. Monte Carlo simulation (symbols) and analytical fit for a 25 keV implant and doses varying from 10^{12} to 10^{16}.

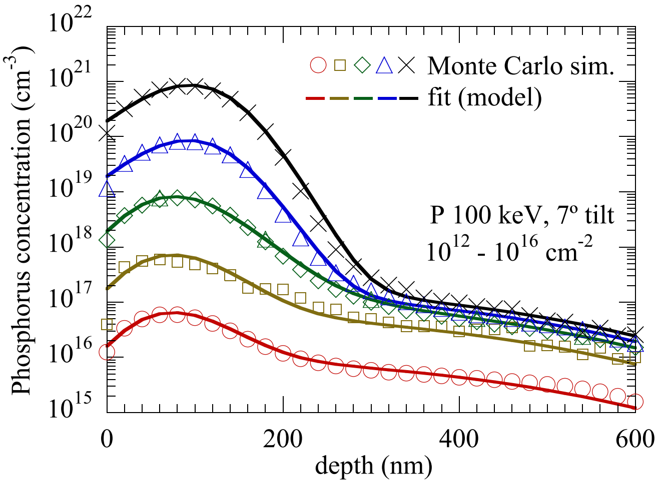

Fig. 6. Monte Carlo simulation (symbols) and analytical fit for a 100 keV implant and doses varying from 10^{12} to 10^{16}.

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