Monte Carlo Simulation of Boron Implantation into (100) Germanium

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Abstract—We present a Monte Carlo simulation study for introducing Boron ions into Ge in the energy range from 5 to 40keV. The successful calibration of our ion implantation simulator for crystalline Ge is demonstrated by comparing the predicted Boron profiles with SIMS measurements. The generation of point defects are calculated with a modified Kinchin-Pease damage model. An implanted Boron profile in Ge is shallower than in Si for any given energy due to the larger nuclear and electronic stopping power of Ge atoms. We found that the higher displacement energy in Ge, the stronger backscattering effect, and the smaller energy transfer from the ion to the primary recoil of a collision cascade are mainly responsible for the significantly reduced damage in Ge.

I. INTRODUCTION

Germanium has regained attention in the semiconductor industry for optoelectronic devices that can be integrated on a Silicon chip as well as a potential device material for high-speed CMOS applications in the future. In recent years deep-submicron Ge MOSFET devices with a three times mobility improvement in comparison to Silicon devices were processed using an HfO2 based high-k dielectric on 200mm bulk Ge wafers [1], [2]. The junction leakage current was found to be about four decades higher for Ge than for Si at a typical operation temperature of 110°C. The reduction of the extremely high diode leakage will therefore be a key issue for Ge technology to obtain devices with a low off-current. Ge and high Ge content $Si_{1-x}Ge_x$ alloys (x > 80%) have been recognized as promising materials for photodetectors in optical transmission systems due to the high optical absorption coefficient for an operation at a wavelength of $1.3\mu m$ in the near infrared (NIR) regime [3], [4]. Epitaxial Ge-on-Si technology allows the integration of interdigitated Ge pinphotodiodes with CMOS circuitry on a Silicon chip to build optical communication receivers with low fabrication costs. While ion-implanted dopant profiles are well studied in Silicon for various dopant species and implantation conditions, dopant profiles are scarce in SiGe alloys as well as in pure Ge. However, an accurate and multi-dimensional simulation of ion implantation processes is required for this wide class of materials to optimize the dopant profiles and estimate the generated crystal damage for implantation applications.

II. MODELING OF IMPLANTATION IN GERMANIUM

The Monte Carlo ion implantation simulator MCIMPL-II is based on a BCA method and uses the universal ZBL potential [5]. The BCA model contains no tunable parameters and can be applied to all materials. Fig. 1 shows the surface plot of the data table for the center-of-mass scattering angle Θ using a bicubic spline interpolation. Lattice vibrations are considered by the Debye model with a Debye temperature of 450K. An empirical electronic stopping model [6] is applied and the damage accumulation is calculated by the modified Kinchin-Pease model [7] together with a model for point defect recombination. The simulator can handle complex threedimensional device structures consisting of various amorphous materials and crystalline Silicon.

We extended the target materials of the simulator from crystalline Silicon to the class of $Si_{1-x}Ge_x$ alloys and Ge by adjusting the lattice parameter a(x) of the crystalline model as a function of the Ge fraction x according to

$$a(x) = 0.02733 x^{2} + 0.1992 x + 5.431$$
 (Å) (1)

which approximates experimental data with a maximum deviation of about 10^{-3} Å [8]. While the ion moves through the simulation domain, a local crystal model (as shown in Fig. 2) is built up around the actual ion position for searching the



Figure 1: Tabulated scattering angle as a function of the reduced impact parameter and the reduced energy.



Figure 2: Local crystal model used for the simulation of Si, $Si_{1-x}Ge_x$ alloys of arbitrary Ge content, and Ge $(0 \le x \le 1)$.

next collision partner. The selection of the target atom species for $Si_{1-x}Ge_x$ alloys is defined by probability x for Ge and (1-x) for Si, respectively. In a screened Coulomb collision the energy loss of the ion, ΔE , is equal to the transferred energy to the recoil atom,

$$\Delta E = \frac{4 M_1 M_2}{(M_1 + M_2)^2} \cdot \sin^2 \frac{\Theta}{2} \cdot E_0$$
 (2)

where M_1 and M_2 are the masses of ion and target atom, Θ is the transformed scattering angle in the center-of-mass coordinates, and E_0 is the kinetic energy of the ion before the collision event [9]. From this equation it can be derived that a smaller energy loss ΔE occurs in nuclear collisions in Ge targets due to the different masses between ion and atom. The transferred energy ΔE from a Boron ion to a Ge atom is approximately the half (0.568-fold) compared to ΔE in Si at a given scattering angle. Note that the difference in masses between Boron and Ge leads also to a stronger backscattering effect which produces shallower profiles. The modified Kinchin-Pease model assumes that the number of displaced atoms (Frenkel pairs) in a recoil cascade is a function of the transferred energy ΔE from the ion to the primary recoil atom. A displacement energy E_d of 15eV has become widely accepted for Silicon. We fitted a value of $E_d = 30 \text{eV}$ for Ge by comparison of simulated Boron profiles with SIMS data. The used value for the displacement energy in Ge is in good agreement with $E_d = 31 \text{eV}$ which was deduced for Ge in [10]. The larger E_d value is responsible for a significantly reduced damage production in Ge compared to Si. Fig. 3 shows the number of produced point defects for a damage cascade, calculated with the modified Kinchin-Pease model. We calibrated the Lindhard correction parameter k_L of the empirical electronic stopping model to adopt the strength of



Figure 3: Number of Frenkel pairs generated by a primary knockon atom in Si and in Ge, assuming $E_d = 15$ eV and 30eV.



Figure 4: Monte Carlo simulation of 10 Boron trajectories in Si and in Ge using an energy of 10keV and a tilt of 7° .

the electronic stopping process which increases with the Ge content in the alloy [11]. We used the parameter $k_L = 1.75$ for Si and a value of 1.9 for Ge.

The Monte Carlo method is based on computing a large number of individual ion trajectories in the simulation domain by using appropriately scaled random numbers. After performing the Monte Carlo calculation, the dopant and damage data are both stored in histogram cells aligned on an orthogonal grid. The Monte Carlo result is then smoothed and translated from the internal orthogonal grid to an unstructured destination grid suitable for the subsequent simulation of the annealing process. We performed the simulation of one-dimensional profiles with at least 10^6 trajectories. Fig. 4 shows ten arbitrarily selected Boron trajectories in Si and in Ge. This comparison demonstrates that the stronger backscattering of Boron ions in Ge typically reduces the trajectory length.



Figure 5: Simulated 20keV Boron implantations in amorphous Ge and in (100) Ge using a dose of $6 \cdot 10^{14} \text{cm}^{-2}$ and a tilt of 7° compared to SIMS measurements.



Figure 6: Simulated 5keV Boron implantation in (100) Ge using a dose of $3 \cdot 10^{13} \text{ cm}^{-2}$ and a tilt of 7° compared to SIMS.

III. SIMULATION RESULTS AND DISCUSSION

Ge has a larger nuclear and electronic stopping power for ion-implanted dopants due to heavier atomic nuclei and their surrounding charge. Therefore the projected range R_p of an implanted dopant profile in Ge is shallower than in Si for any given energy. We found the R_p of the 20keV Boron implantation in Ge at 55nm and in Si at 80nm using the same conditions. Fig. 5 compares the Monte Carlo results performed with our calibrated ion implantation simulator to SIMS measurements. The pre-amorphization was performed by an implantation of ⁷²Ge with an energy of 200keV and a dose of 10^{15} cm⁻². The Boron implantations into amorphous Ge and into crystalline Ge were performed with an energy of 20keV, a dose of $6 \cdot 10^{14}$ cm⁻², and a tilt of 7°. Fig. 6 shows a good agreement between the simulated and measured Boron profile at a lower energy of 5keV and a



Figure 7: Comparison of produced vacancies for 20keV Boron implantations in Si and in Ge using a dose of $6 \cdot 10^{14} \text{ cm}^{-2}$ and a tilt of 7°.



Figure 8: Simulated 40keV Boron implants in (100) Ge at doses of $5 \cdot 10^{13}$, $5 \cdot 10^{14}$, and $5 \cdot 10^{15} \text{cm}^{-2}$ using a tilt of 7° .

lower dose of $3 \cdot 10^{13} \text{ cm}^{-2}$. Fig. 7 compares the simulated vacancy concentration profiles in Si and in Ge associated with 20keV Boron implantations. The maximum of the vacancy concentration is not at the wafer surface, since the electronic stopping process dominates at the high initial energy of the ions, when they enter the crystal. A Boron ions enters most likely a channel at the surface and despite of the tilted incident direction it can stay at least a short distance inside a channel. The higher displacement energy of 30eV, the stronger backscattering for Boron ions in Ge, and the smaller energy transfer ΔE from the ion to the primary recoil of a cascade are mainly responsible for the significantly smaller damage in Ge. Consistent with experimental observations in [12], 100% of the implanted Boron ions in Ge are immediately active without annealing for using a relatively high dose of $10^{14} cm^{-2}$, since Boron implanted Ge remains crystalline. Fig. 8 illustrates the



Figure 9: Simulated point response for a 10keV high-dose implantation of Boron into crystalline silicon.



Figure 10: Simulated point response for a 10keV high-dose implantation of Boron into crystalline germanium.

dose dependence of 40keV Boron profiles in Ge, which are simulated with the Kinchin-Pease damage model.

The point responses in crystalline Si and Ge are compared in Fig. 9 and Fig. 10. The width of the implantation window in an impenetrable mask is 8nm. Boron is implanted with an energy of 10keV, a dose of $5 \cdot 10^{15} \text{ cm}^{-2}$, and the ion beam is 7° tilted in such a way that the lateral component of the incident direction is parallel to the direction of view (<010 > direction). Therefore the presented point responses are symmetric. Approximately 420000 simulated ions enter the substrate at the mask opening and contribute to the Boron distribution. While the lateral penetration depth of Boron ions is only slightly reduced, the vertical depth is strongly reduced in Ge. The channeling tail is closely centered around the <100> axis in both cases. This demonstrates that in (100) Si or Ge, axial channeling in the <100> direction dominates by far over channeling in other directions.

IV. CONCLUSION

Boron implantation, generation of point defects and channeling have been investigated in crystalline Ge by using a physics-based simulation approach and SIMS profiles. As demonstrated in this work, our Monte Carlo ion implantation simulator can accurately predict Boron profiles for different energies and doses. The simulator can estimate the produced vacancies in the Ge crystal, which are associated with a specific implanted Boron profile. We found that the produced damage in Ge is significantly reduced compared to Si, which is consistent with former experimental observations indicating that Boron implanted Ge remains essentially crystalline. The shown point responses as well as single trajectories indicate that the Boron distribution in Ge is significantly reduced in the vertical direction, while the lateral profile is quite similar in Si and Ge.

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