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Collaborative SIMS study and simulations of implanted dopants in Si

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Abstract

Implantation of doping elements is the main technique to achieve ultra-shallow source and drain junctions in semiconductor devices. For improving device performance, accurate determination of dopant profiles is important. They are typically measured using secondary ion mass spectrometry (SIMS). In this study, industrially important dopants F, P, Ge and As were implanted in single-crystalline Si(100) at 1 to 10 keV. The depth profiles of the dopants were measured using magnetic sector (MS), quadrupole and dual beam time-of-flight (ToF) SIMS and compared with the profiles calculated using molecular dynamics theory. It was found that the rising slope of calculated profiles coincide with ToF SIMS data, while the other techniques have significant surface transient effect. The falling slope coincides with MD SIMS data, while the slope in ToF SIMS data is delayed due to high energy analysis beam.

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1. Introduction

Implantation of doping elements has become the main technique to achieve ultra-shallow source and drain regions in semiconductor devices. The distribution of dopants affects electric field in the devices and, as device features shrink, it has macroscopic impact on device characteristics. Hence the accurate determination of depth profiles of low energy implanted dopants is important for improving the device performance. The distribution of implanted elements can be calculated using molecular dynamics (MD) theory. Physically, it is measured using secondary ion mass spectrometry (SIMS).

Four elements were implanted into Si(100) wafers for this work: they are light dopants F and P, and also heavy elements Ge and As, which play crucial roles in preamorphization, channel engineering and threshold voltage adjustment. The depth profiles of the implanted elements were measured in a Round Robin study by five teams using different SIMS instruments: magnetic sector (MS), quadrupole (Q) and dual beam time-of-flight (ToF). Comparison of their results allowed choosing appropriate profiles to compare with the results of MD simulation. A

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method is proposed to employ the ranges of coincidence between simulation and measurements to refine SIMS profiles to reduce the contribution of experimental artefacts.

2. Experimental

The doping elements F, P, Ge and As were implanted into Si(100) wafers in Axcelis Technologies. The energies and doses of the implantation are specified in Table 1. At each value of the energy, two wafers were implanted at different geometry of the ion beam: one at tilt = 0° and twist = 0°, the other at tilt = 45° and twist = 45°. The tilt angle is the angle between the incident ion beam and the normal of the wafer plane; the twist or azimuthal angle is measured with respect to the (100) plane in which the implants take place. The use of self-aligned (0° tilt) source-drain extension doping is common. Although tilt angles of 45° are not yet common in wafer fabrication process, a wafer orientation of 45° in the azimuthal direction, in addition to the 45° tilt angle, represents one of the worst scenarios in axial and planar channelling [9]. Such profiles should be hence be well calibrated.

Table 1.
Implantation conditions.

Element	Energies (keV)	Dose (atoms/cm^2)
Fluorine (F)	1, 2, 5	6×10^{13}
Phosphorous (P)	1, 2, 5	5×10^{13}
Germanium (Ge)	2, 3, 5	5×10^{13}
Arsenic (As)	2, 5, 10	5×10^{13}

The common condition of the Round Robin SIMS study was that Cs^+ was used as the sputtering ion and negative secondary ions were monitored. Other experimental parameters were set by each SIMS team for the best performance of their instruments.

For quadrupole SIMS analysis in Cascade Scientific Ltd, a Phi Adept 1010 SIMS instrument has been used. ; Cs 750 eV ion beam with 100 nA current was used at 60° incidence angle with the sample potential held at zero voltage.

The magnetic-sector SIMS data have been obtained in Chartered Semiconductor Manufacturing with a Cameca IMF Wf instrument with a 60° float column. A 10 nA Cs+ beam with net impact energy of 520 eV was used to bombard the sample biased at -3 kV at grazing 70° incidence angle. There was no voltage offset on the samples.

Time-of-flight SIMS was carried out at the Institute of Materials Research and Engineering with ION-TOF IV instrument. The sputtering beam was Cs 1 keV for depth profiles of P and F, and 3 keV for As and Ge with beam current 10 nA. The analysis beam was Ga 15 keV going in 1 ns pulses at 10 kHz with average beam current 2 pA. The incident angle of both beams was 45°.

3. Molecular dynamics simulation

The simulated profiles shown in this work have been obtained with the MD code, MDRANGE [1]. Nuclear effects have been treated with ion-target potentials obtained from density functional theory (DFT) calculations [2]. The Recoil Ion Approximation (RIA) has been employed, where only the ion-recoil interactions are considered. This is based on the assumption that the interactions between the ion and its nearest neighbors are much stronger than the lattice-lattice interactions. RIA has been shown to reduce the computational burden, with little effect on the final range profiles [1].

Electronic stopping affects the distribution of low energy doping ions, especially in high channelling directions such as those used in this study. The channelling of ions during the slowing down process has an important impact on the concentration profiles both in the vertical and lateral directions. In crystal channels, where the atomic and electronic densities are significantly lower than average, the importance of nuclear stopping is reduced relative to the electronic stopping and it is imperative that the electronic stopping model predict the ranges of the channelled ions accurately. A local electronic stopping model is adopted since a non-local model is not likely to work where the electron density in a channel is significantly lower than in other directions. This model is based on scattering phase shifts for Fermi-surface electrons [3]. The scattering phase shifts are determined within DFT for atoms embedded in a homogeneous electron gas [4] and are calculated in this work for F (Z=9), P (Z=15), Ge (Z=32) and As (Z=33). The anisotropy of the electron distribution is taken into account by using a 3D charge distribution of silicon [5].

In all the simulations, initially crystalline silicon was used as a target material. A native amorphous oxide layer on the surface was taken into account and measured experimentally to be 10±1Å in all cases. The surface temperature of the experiments, 300K was used and realistic atomic thermal displacements were obtained by setting the Debye temperature of

silicon to 519K [5]. The number of simulated ions used was 20,000, and deemed sufficient for good statistics. To determine the profiles over more than four decades of concentration, a version of Beardmore's rare-event algorithm [6] was implemented. An atom splitting scheme is employed so that at certain splitting depths the ion is split into two virtual ions with a statistical weight of half that of the unsplit ion [7]. This ensured accurate dopant profiles with good statistics and feasible computational overhead. The effect of damage build-up on range profiles is especially pronounced at low energies and is taken into account by changing the material structure in front of the path of the incoming ion [8].

4. Comparison of SIMS techniques

For a particular element and implantation energy, all measurements show similar descending slope on the depth profile, Fig.1, except for the following cases. Quadrupole SIMS is unable to mass resolve P from ^{30}SiH, hence the tails of the P profiles appears to have higher intensity. ToF SIMS uses Ga 25 keV as the analysis ion beam, which increases ion mixing, resulting in a delayed slope of the profiles. This effect is the most significant for Ge and As having atomic mass close to Ga, Fig. 2.

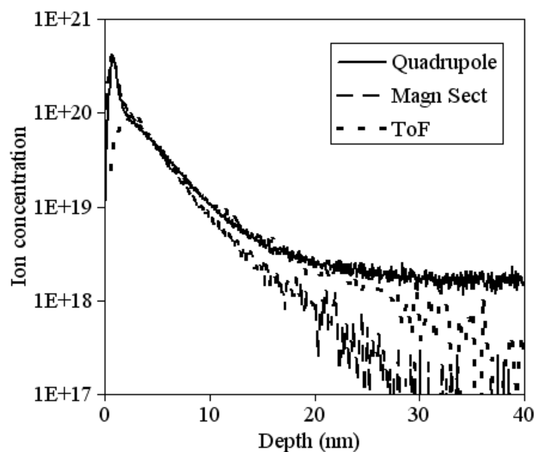

Fig. 1. Depth profiles of P implanted at 2 keV and normal incidence measured with various SIMS.

On the rising slope, the profiles from dynamic SIMS have a peak due to the surface transient effect, i.e. changes of sputtering rate and ion yield at the beginning of sputtering. This artefact peak is absent in ToF SIMS profiles, because the mass analysis and sputtering are done with different beams.

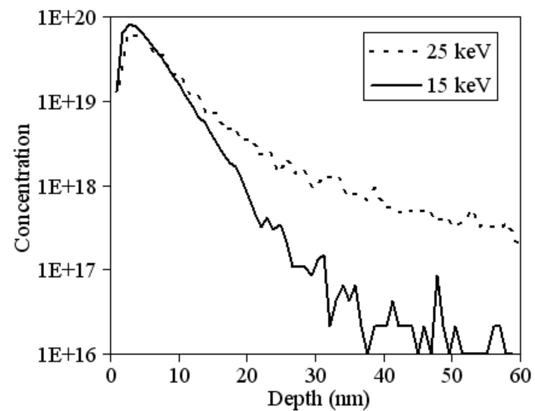

Fig. 2. ToF SIMS depth profiles of As implanted at 2 keV measured with Ga ions 15 and 25 keV.

5. Comparison of experiment and simulations

- Quadrupole SIMS (Q): It should be noted that at least part of the surface spike in the P profiles is SIMS artifact and merged into the actual peak, resulting in the high surface concentration. The poor agreement in the tail region of the N profiles can be attributed to the high detection limit of N. With the exception of N, good agreement of simulation with SIMS data is mainly seen in the trailing part of the profiles, even though channeling at such low energies is pronounced. The excellent agreement obtained with MD can be largely attributed to the local electronic model since electronic stopping dominates in channelling directions, where the phase shifts were *specifically* calculated for each target-projectile pair.
- Magnetic SIMS (MS): While the surface spike in the P profiles is still present indicative of ion mixing effects, MS-SIMS can better resolve the profiles at low atomic concentrations. As such, profiles measured by MS can span four decades of concentrations.
- Some examples shown below. Only P has both Q and MS SIMS. The rest consist of only Q SIMS.

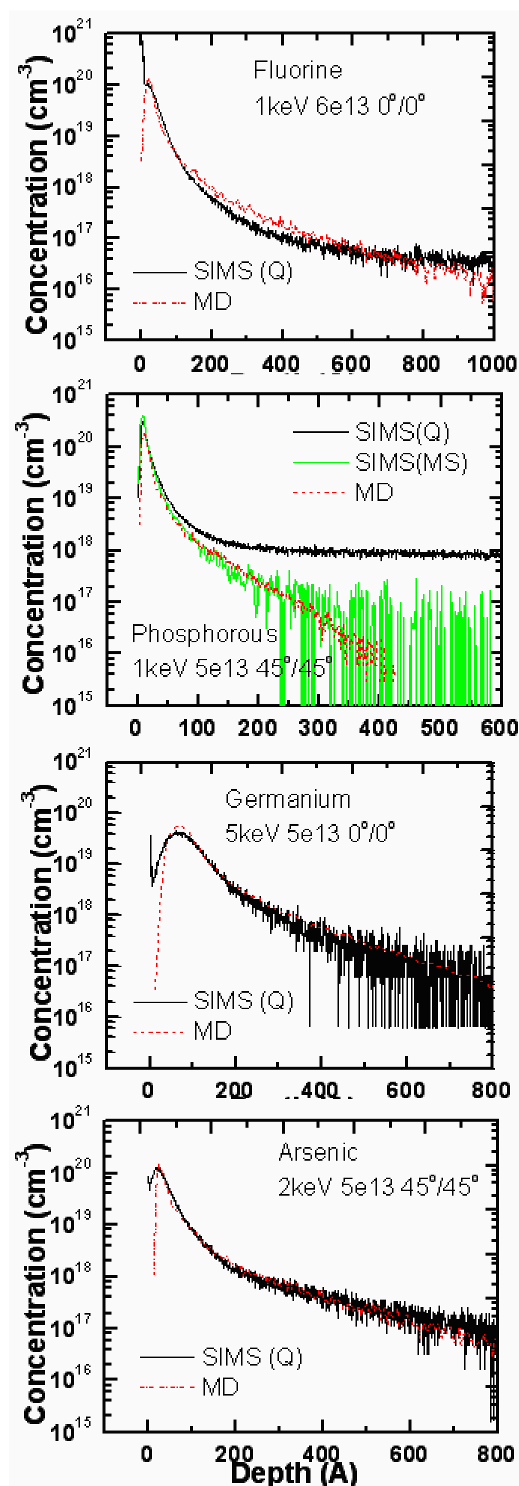

Fig. 4. SIMS depth profiles of F, P, Ge and As compared with the results of MD simulations.

6. Conclusions

Depth profiles of implanted dopants F, P, Ge and As were measured with dynamic (magnetic sector and quadrupole) SIMS and time-of-flight SIMS. On the rising slope of the dopant concentration, ToF SIMS gives more accurate result, while dynamic SIMS is more accurate on the descending slope.

The experimental SIMS profiles chosen in this way and the profiles simulated using MD coincide on the trailing slope of the implanted peak. On the rising slope, the agreement between SIMS and MD depends on how the native silicon oxide is taken into account in the calculation. Thus the ranges of coincidence between the measured and calculated profiles allowed us to refine SIMS data to reduce the contribution of experimental artefacts.

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