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Channeled MeV B, P and As Profiles in Si(100): Monte-Carlo Models and SIMS

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***Abstract*—Details of experimental (SIMS) channeled profiles in Si(100) for MeV dopants (B, P, and As) are compared with Monte-Carlo calculations (IMSIL and SRIM) for crystalline and amorphous Si in an ion energy range from 800 keV to 3.1 MeV. Effects of small angle off-axis ion incidence, implantation at elevated wafer temperatures and beam angle divergence are studied in some detail.**

Keywords—channeling, MeV dopant profiles, Monte-Carlo modeling, IMSIL, SRIM.

I. Introduction

Channeling of ions in crystalline solids has been linked to computer modeling of ion trajectories since the phenomenon was first discovered in simulations of neutron generated recoils in crystalline Cu in the early 1960's [1]. This led to a historic burst of global experimental and computational interest in the topic [2]. More than half a century later, intentionally channeled dopant ions are widely used to form deep junctions in memory and image sensor devices [3].

Experimental (SIMS) channeled profiles in Si(100) for MeV dopants (B, P, and As) are compared with Monte-Carlo calculations (IMSIL and SRIM) for crystalline and amorphous Si in an ion energy range from 800 keV to 3.1 MeV. Effects of small angle off-axis ion incidence, damage accumulation in Monte-Carlo modeling and implantation at elevated wafer temperatures are studied. Additional details are available in other papers in these proceedings describing SIMS results for implants at elevated temperatures [4] and results from other Monte Carlo simulations using a MARLOWE code [5].

II. Experimental Procedures

Implants were done with a S-UHE, a LINAC design with a high-charge state ion source, an 18 resonator RF acceleration stage and a folded beam line design allowing for a high degree of beam alignment and paralleism [6]. While the system is capable of implanting B, P and As ions at 5.0, 6.8, and 6.8 MeV, respectively, the implant conditions in this study were chosen to be similar to routine CMOS image sensor applications (see TABLE I).

Additional implants were done at various beam tilt and twist angles and at an elevated implantation temperature of 723 K.

Prior to implantation, the orientation of the axial direction of a lead wafer in the same production batch as the wafers used in this study was determined by V-curve methods described by Sano et al. [7]. Adjustments were made in the wafer tilt and twist directions to align the beam along the Si(100) axial direction for the test implants.

TABLE I: Implantation Conditions (300 K, 0 tilt).

Ion	Energy (MeV)	Beam current (e-uA)
^{11}B	1.5 ($^{11}B^{+}$)	78
	3.0 ($^{11}B^{2+}$)	63
^{31}P	0.8 ($^{31}P^{+}$)	50
	2.2 ($^{31}P^{2+}$)	100
^{75}As	1.4 ($^{75}As^{3+}$)	100
	3.1 ($^{75}As^{3+}$)	100

III. Monte-Carlo Simulations

Monte-Carlo simulations have been performed using SRIM [8] and IMSIL [9]. While SRIM is restricted to amorphous targets, in IMSIL the crystal structure and orientation can be taken into account. Under channeling conditions, ion ranges mainly depend on electronic stopping. We use a model composed of a nonlocal and a local part that is well calibrated for the cases studied [9]. Damage accumulation is estimated by the modified Kinchin-Pease model using a displacement energy of 15 eV and correction factors for the resulting number of Frenkel pairs ("damage recombination factors" [10]) of 0.3, 0.8, and 2 for B, P, and As ions, respectively. Temperature effects are taken into account using the Debye model with a Debye temperature of 490 K. The RMS vibration amplitudes for Si atoms used in the IMSIL simulations were 0.083 Å at 300 K and 0.125 Å at 723 K. The Si(100) axial channel diameter (at 0 K) is 2.716 Å. Beam divergence is implemented with a Gaussian distribution of angles with the stated divergence equal to the standard deviation.

IV. Results

A. Boron Profiles (0° tilt, 300 K)

SIMS, IMSIL and SRIM profiles for 1.5 and 3 MeV B aligned along Si(100) at an implantation temperature of 300 K are shown in Fig. 1. The ideal (0° off-axis alignment and divergence) IMSIL calculation shows a more pronounced deep channeled peak than the experimental SIMS profile. The depth of the deeply channeled profile edge is well aligned in the SIMS and IMSIL profiles. The depth of the shallower de-channeled ("random") peak in the SIMS data is well-aligned to the IMSIL profile and the amorphous Si calculations with SRIM.

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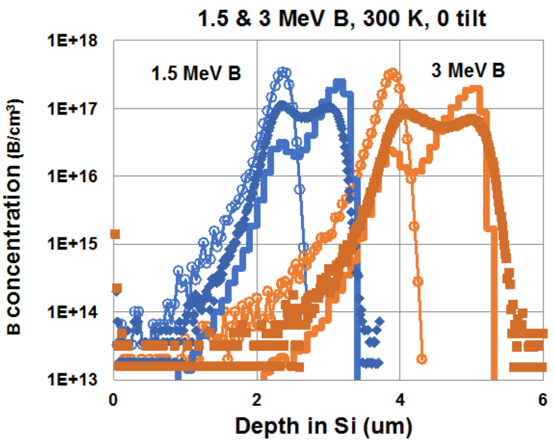

Fig. 1. 1.5 and 3 MeV Boron channeled profiles, SIMS (symbols), IMSIL (histograms), SRIM (open circles, amorphous Si). Dose = 1e13 B/cm^2.

B. Phosphorous Profiles (0° tilt, 300 K)

SIMS, IMSIL and SRIM profiles for 0.8 and 2.2 MeV P aligned along Si(100) at an implantation temperature of 300 K are shown in Fig. 2. The ideal (divergence-less) IMSIL calculation shows a more pronounced deep channeled peak than the experimental SIMS profile. The depth of the deeply channeled profile edge is well aligned in the SIMS and IMSIL profiles. The depth of the shallower de-channeled ("random") peak in the SIMS data is well-aligned to the IMSIL profile and the amorphous Si calculations with SRIM.

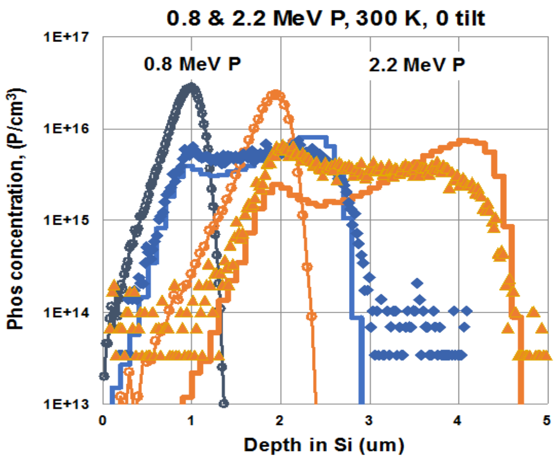

Fig. 2. 0.8 and 2.2 MeV Phosphorous channeled profiles, SIMS (symbols), IMSIL (histograms), SRIM (open circles, amorphous Si). Dose = 1e12 P/cm^2.

C. Arsenic Profiles (0° tilt, 300 K)

SIMS, IMSIL and SRIM profiles for 1.4 and 3.1 MeV As aligned along Si(100) at an implantation temperature of 300 K are shown in Fig. 3. The ideal (divergence-less) IMSIL calculation shows significantly deeper channeled profiles than the experimental SIMS profile. The peaks of the SIMS profiles are at similar depths as the "random" peaks and the experimental As profiles have extended channeled "tails", but not as deep as the IMSIL simulations.

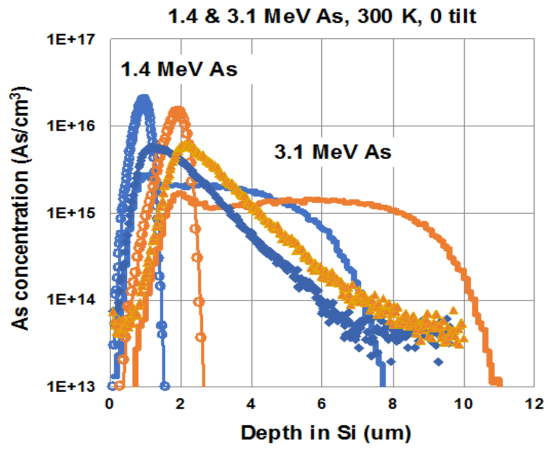

Fig. 3. 1.4 and 3.1 MeV Arsenic channeled profiles, SIMS (symbols), IMSIL (histograms), SRIM (open circles, amorphous Si). Dose = 1e12 As/cm^2.

D. Tilt Angle Effects

The effects of small angle off-axis tilts for 3 MeV B are shown in Fig. 4 for tilt angles of 0 to 0.1°. The effects of tilt angles up to 0.6° for 3.1 MeV As are showin in Fig. 5.

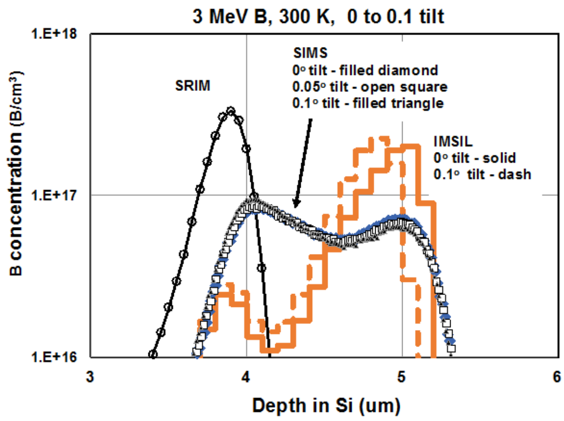

Fig. 4. 3 MeV B, tilt= 0, 0.05, 0.1°, SIMS (symbols), IMSIL (0, 0.1°, histograms) and SRIM (amorphous Si, circles). Dose = 1e13 B/cm^2.

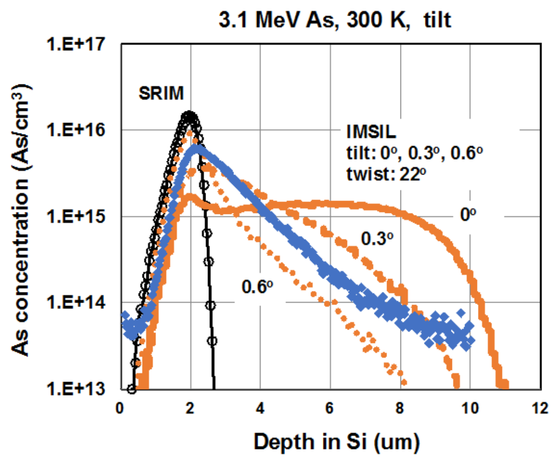

Fig. 5. 3.1 MeV Arsenic channeled profiles, (SIMS (at 0° tilt, symbols), IMSIL (0° 0.3° and 0.6° off axis, 22° degree twist, histograms), SRIM (open circles, amorphous Si). Dose = 1e12 As/cm^2.

E. Effect of Damage Accumulation

Removing the Kinchin-Pease damage accumulation had only a minor effect on the channeled profiles for all implant conditions. As an example, IMSIL profiles with and without damage are shown in Fig. 6 for 3.1 MeV As.

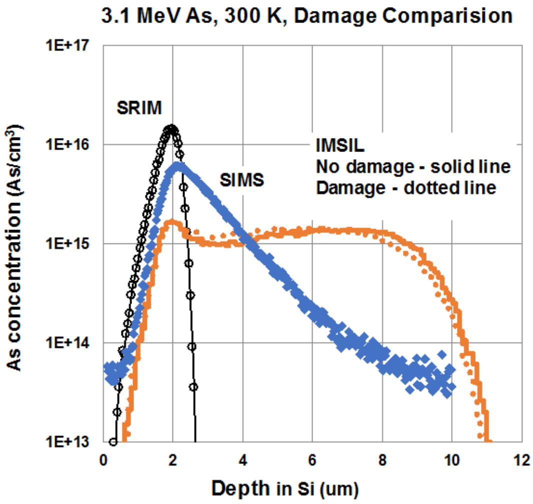

Fig. 6. 3.1 MeV Arsenic channeled profiles, SIMS (symbols), IMSIL with and without damage accumulation, (histograms), SRIM (open circles, amorphous Si). Dose= 1e12 As/cm^2

F. Effect of Wafer Temperature

Implantation at wafer temperatures of 300 and 723 K (450° C) for 1.5 MeV B is shown in Fig. 7. In both SIMS and IMSIL profiles the effect of elevated temperature is to decrease the deep channel peak and increase the de-channeled "random" peak, with a slightly shallower deep edge of the channeled distribution. More pronounced shifts to shallower channeled profiles and higher "random" peaks at elevated implant temperatures in both SIMS and IMSIL profiles are seen for 2.2 MeV P and 3.1 MeV As in Figs. 8 and 9.

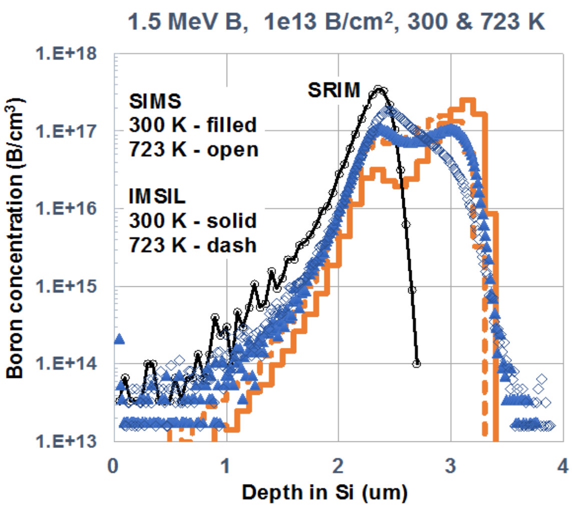

Fig. 7. 1.5 MeV Boron channeled SIMS profiles at wafer temperatures of 300 and 723 K (symbols), IMSIL (histograms) and SRIM (open circles) for amorphous Si target (no channeling). Dose = 1e13 B/cm^2.

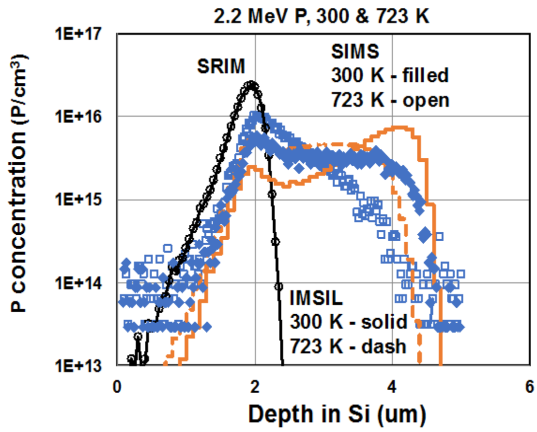

Fig. 8. 2.2 MeV Phosphorous channeled profiles at wafer temperatures of 300 and 723 K, SIMS (symbols), IMSIL (histograms), SRIM (open circles, amorphous Si). Dose = 1e12 P/cm^2.

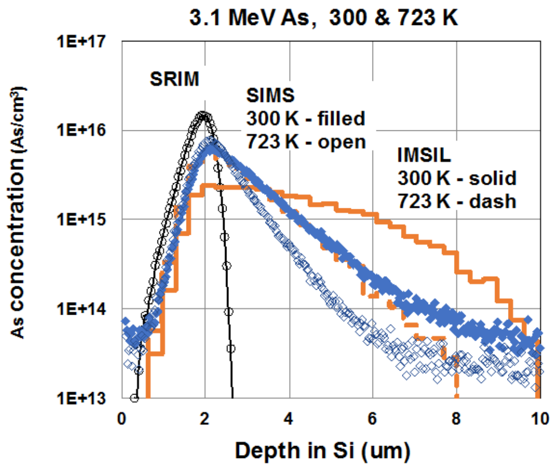

Fig. 9. 3.1 MeV Arsenic channeled profiles, SIMS (symbols, filled for 300 K, open for 723 K), IMSIL (histograms; solid line for 300 and dashed line for 723 K), TRIM (open circles, amorphous Si). Dose = 1e12 As/cm^2.

G. Effects of beam divergence

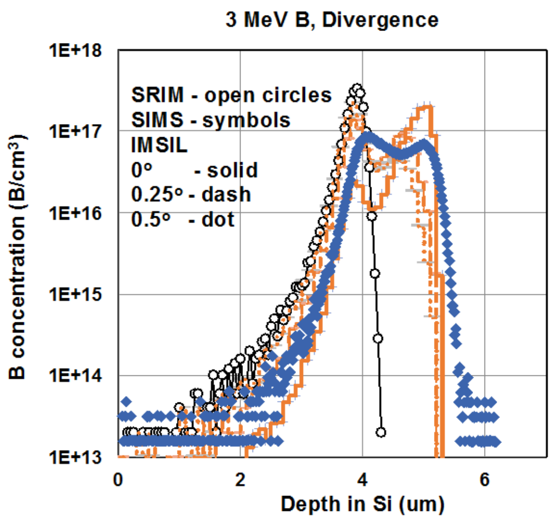

Fig. 10. 3 MeV Boron channeled profiles, SIMS (symbols), SRIM (open circles, amorphous Si), IMSIL (histograms). Dose = 1e13 B/cm^2. IMSIL divergence modeled at 0, 0.25 and 0.5 degrees.

Calculated effects of a Gaussian distribution of ion angles within the ion beam (divergence = 1 sigma) were similar to off-axis tilt and varied with ion types and energy. For 3 MeV B (Fig. 10), the apparent divergence angle, judged from the location and shape of the channeled B profile. was less than 0.25°.

For high-mass ions, such as 3.1 MeV As (Fig. 11), the apparent divergence value is ≈0.5°.

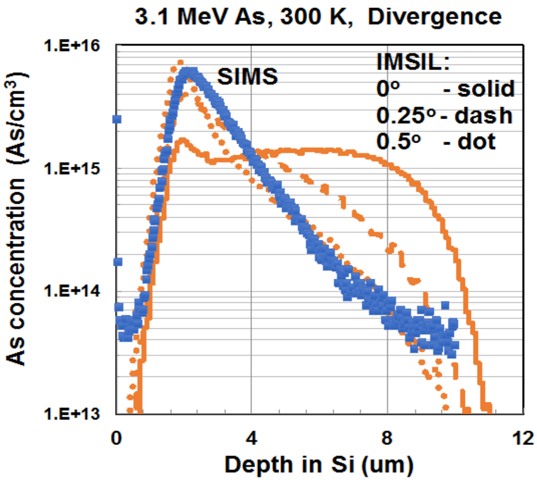

Fig. 11. 3.1 MeV Arsenic channeled profiles, SIMS (symbols), SRIM (open circles, amorphous Si), IMSIL (histograms). Dose = 1e12 B/cm^2. IMSIL divergence modeled at 0, 0.25 and 0.5 degrees.

The apparent ion divergence angles from this study vs. volume ion charge density, $Q_{charge\ state}$*n_{beam} (ions/cm^3), [11] (Fig. 12), implies that, at high ion densities, Coulomb repulsion effects are stronger and suggests that positive benefits can be obtained by improving space-charge balances in MeV dopant ion beams.

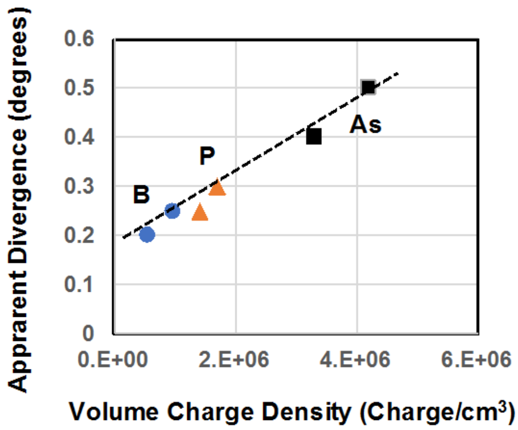

Fig. 12. Apparent ion beam divergence angles, as judged by channeled profile shape and location, for B, P and As ions in the energy range of 0.8 to 3.1 MeV, showing the effect of beam volume charge density.

V. SUMMARY

Actual channeled MeV dopant profiles, measured by SIMS, are not as highly channeled as the IMSIL Monte Carlo simulations (with ideal, 0° divergence beams and perfect alignment). This indicates that further improvements in deep channeled profiles are possible with advances in control of such beam properties as ion angle divergence. Operation of channeled implants at elevated temperatures at 450° C showed an increased degree of de-channeling, in both experimental and simulated profiles, with overall shallower dopant penetration for all dopants studied here. Effects of beam divergence were observed to be significant, especially for heavy, high charge state ions, such as As^{3+}.

REFERENCES

[1] M. Robinson, O. Oen, "Computer studies of the slowing down of energetic ions in crystals", Phys. Rev. 132 (1963) 1385.

[2] D.V. Morgan, "Channeling: Theory, Observations and Applications", Wiley (1973).

[3] N. Teranishi, Proc, IIT-2016 (IEEE: CFP1644Y), (2016) 21.

[4] M. Sano, H. Sasaki, Y. Kawasaki, M. Sugitani, "Change of depth profile for high temperature implantation in channeling condition", these proceedings (2018).

[5] H. Sasaki, S. Ninomiya, Y. Kawasaki, M. Sugitani, "MARLOWE simulation of high energy ions in single crystalline Silicon substrates", these proceedings, (2018).

[6] K. Watanabe, H. Sasaki, M. Kabasawa, M. Tsukihara,. K. Ueno, "Introduction of the S-UHE, a Single-Wafer Ultra-High Energy Ion Implanter", IIT14 (2014), 261-264.

[7] M. Sano, K. Tsukahara, S. Kawatsu, Y. Kawasaki, M. Koike, "Change in V-curve behavior depending on ion angle deviation in channeling condition", Proc. IIT2014, (2014) 96-99.

[8] J.F. Ziegler, J.P. Biersack, M.D. Ziegler, "SRIM The Stopping and Range of Ions in Matter", ISBN: 0-9654207-1-X (2008), program and tutorials at www.srim.org

[9] G. Hobler, "Monte Carlo simulation of two-dimensional implanted dopant distributions at mask edges", Nucl. Instrum. Meth. B 96 (1995) 155.

[10] G. Hobler and B. Murthy, "Towards a comprehensive model of electronic stopping in amorphous and crystalline silicon", Proc IIT2000, IEEE 00EX432 (2001) 209-212.

[11] M. Current "Perspectives on Low-Energy Ion (and Neutral) Implantation", International Workshop on Junction Technology, IWJT- 2017.