Lateral Range and Diffusion Simulation Capabilities for Ion Implantation in Compound Semiconductors

J.A. Turcaud

COHERENT - INNOViON, 2121 Zanker Rd, San Jose, CA 95131, USA - jeremy.turcaud@coherent.com

ABSTRACT – **New features and capabilities have been added to the ion implantation simulator called INNOViON coded on MATLAB software and using SRIM (Stopping and Range of Ions in Matter) simulated data. In addition to the existing automatic profile target optimization and channeling capabilities, a novel multiple implant diffusion simulation as well as lateral implantation and damage range modeling has been integrated. Examples, applications such as for processing of compound semiconductors, and prospects for these new features are introduced and discussed.**

INTRODUCTION

Since the 1980s, several codes, such as SRIM/TRIM [1] [2] [3] [4] [5], UT-MARLOWE [6], COSIPO [7], ACOCT [8], PEPPER [9], CrystalTRIM [10] [11], have been focusing on modeling ion ranges and damage distributions (created vacancies) in amorphous or crystalline targets, for ion implantation in semiconductors. These codes are either based on Monte Carlo (MC) atomistic modelling techniques, on molecular dynamics (MD) methods, or on combinations of both methods.

We previously introduced a simulator called INNOViON for simulation of ion implantation in compound semiconductors and silicon. It was designed on MATLAB which builds on SRIM simulated data and optimizes its modeling capability and computing speed. It allows for fast and highly accurate design of ion implantation sequences into semiconductor compound targets. This simulator also enables the heuristic modeling of channeling with temperature and dose, for substrates where diffusion is prevented.

We are now presenting two new capabilities which are multiple step diffusion simulation and lateral range modeling for both ion (dopant) and damage (vacancy) concentrations.

I. DIFFUSION MODELING CAPABILITY

Profiles are extracted from SRIM, for single and/or multiple steps. These dopant distribution profiles are analytically approached using a Monte-Carlo algorithm with sums of Gaussian functions. During annealing, these Gaussian expansions are evolving in relationship with the projected range R_p, the straggle σ_p, the intrinsic diffusion coefficient D_0, the temperature dependent diffusion coefficient D, the activation energy E_A, the ion dose Q_T, the temperature of annealing T, and the time of annealing t. See Equations 1 and 2.

Equation 1

$$n(x) = \frac{Q_T}{\sqrt{\sigma_p^2 + 2Dt}\sqrt{2\pi}} e^{\left(\frac{-(x-R_p)^2}{2\left(\sigma_p^2+2Dt\right)}\right)}$$

Equation 2

$$D = D_0 e^{-E_a/kT}$$

This is a powerful capability to design specific dopant profiles, such as constant dopant density with depth, using multiple-step implants and tailored annealing conditions. See Figure 1 for an example of Boron diffusion into Silicon after a 3-step implant and an annealing at 1300 °C for 5 minutes. The implant steps and the annealing steps are tailored together to achieve a desired target concentration across a specific depth.

II. LATERAL RANGE SIMULATION CAPABILITY

More applications in semiconductor compounds such as accurate area isolation are now requiring precise control of lateral implanted concentrations and damages [12]. We have developed a modeling capability for lateral range in ion implantation of semiconductor compounds based once again on SRIM extracted data. This time, 3D profiles are simulated and scanned over a matrix target while having part of it blocked by a mask. As such the lateral depth and range of implanted ions and damages under the mask can be assessed and precisely controlled using the species of the ions. the energy and dose, along with the angle of incidence of implantation. See Figure 2 for an example of an Xe implant designed for isolation into an InP stack.

It is highlighted in this figure that the lateral range of damage under the mask is strongly dependent on where one defines the damage threshold. As such, having a threshold at one standard deviation from the total peak concentration, as it is usually done, yields a lateral damage of maximum 600 A while using an arbitrary defined value of damage 9E19 vac/cm^3, consistent with significant electrical path annihilation, yields an apparent lateral damage range of 2000 A. This powerful capability enables precise control of how semiconductors are impacted by ion implantation under masked areas.

III. CONCLUSIONS

This article is presenting new simulation capabilities for ion implantation into compound semiconductor and silicon devices. Multi-step implants with diffusion and lateral damage range modellings, two key processes and parameters, can now be simulated using these new capabilities available in the INNOViON simulator.

The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request. The authors have no competing interests to declare that are relevant to the content of this article.

ACKNOWLEDGEMENT

The authors would like to thank J.F. Ziegler and J.P. Biersack for providing the SRIM simulation code.

Substrate: Si (Si, SiC)

Ions: B (B, P, As)

Temperature (C) 1300

Time (min) 5

MC 2e+04

Min range (A) 1

Concentration 1 (#/cm3) 1e+19

Mid range (A) 1000

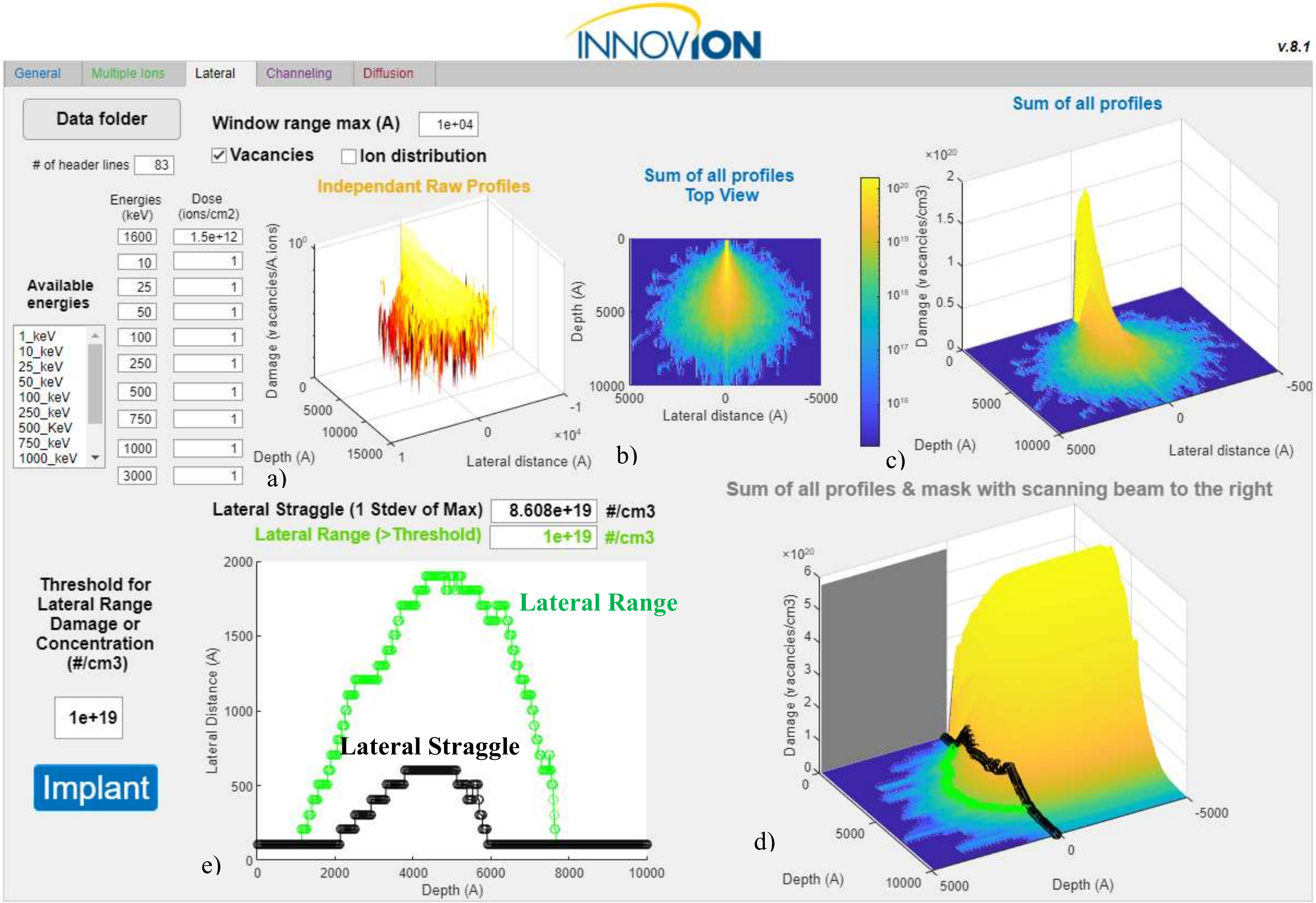
Concentration 2 (#/cm3) 1e+19

Max range (A) 1e+04

Window range max (A) 2e+04

Energy (keV)	Dose (ions/cm2)
500	1e+15
250	5e+14
50	1e+14
1	1
1	1
1	1
1	1
1	1
1	1
1	1

Figure 1. Example of diffused profile of Boron doped Silicon with 3 steps, 500 keV-1e15 ions/cm2, 250 keV-5e14 ions/cm2, and 50 keV-1e14 ions/cm2. The multi peak blue curve is simulated before annealing while the single peak red curve is simulated after annealing at 1300C for 5 min.



Window range max (A): 1e+04

☑ Vacancies ☐ Ion distribution

\# of header lines: 83

Available energies:
- 1_keV
- 10_keV
- 25_keV
- 50_keV
- 100_keV
- 250_keV
- 500_KeV
- 750_KeV
- 1000_keV

Energies (keV)	Dose (ions/cm2)
1600	1.5e+12
10	1
25	1
50	1
100	1
250	1
500	1
750	1
1000	1
3000	1

Lateral Straggle (1 Stdev of Max): 8.608e+19 #/cm3

Lateral Range (>Threshold): 1e+19 #/cm3

Threshold for Lateral Range Damage or Concentration (#/cm3): 1e+19

Figure 2. Example Xe implanted ions and damaged engineered to isolate some areas in an InP stack. Showing are the raw profile before any dose input (a), the 2D profile seen from above the point of impact (b), the 3D profile (c), the scanned-to-the-right profile with a mask on the left side blocking the line-of-sight incoming ions (d), two different lateral ranges as a function of depth depending on the definition of lateral threshold (e). (e) The upper green curve was obtained with the use of an arbitrary value of damage of 1e19 vac/cm3 for the threshold while in the lower black curve, we used one standard deviation from the maximum peak values. Both these curves are also shown on the 3D scanned graph (d)

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