Ion Implantation Simulation and Optimization in Semiconductor Compounds

J.A. Turcaud*, J. Schuur, and R. Pong

*II-VI Incorporated, 2121 Zanker Rd, San Jose, CA 95131, USA - *jeremy.turcaud@ii-vi.com, +1 (669) 287-9506*

KEYWORDS: Implantation, Simulation, Isolation, Channeling, SiC, INNOViON

ABSTRACT – An ion implantation simulator called INNOViON coded on MATLAB software and using SRIM (Stopping and Range of Ions in Matter) simulated data is introduced. Using this application, ion and vacancy distributions in a target for multiple implant energies can be generated. In addition, inherent SRIM limitations and mitigation techniques embedded inside INNOViON are discussed. A Monte-Carlo profile matching optimization principle, a very useful feature for isolation ion implantation processing, is discussed. Finally, a heuristic channeling simulation capability based on multiple profiles found in the literature is described.

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, in term of created vacancies, in amorphous or crystalline targets. They are either based on Monte Carlo (MC) atomistic modelling techniques or on molecular dynamics (MD) methods or on combinations of both methods. Briefly, the first method consists of estimating the trajectory of the ions by sampling from a true or hypothetical distribution of energy loss by independent electronic and nuclear stopping powers. The second approach, MD, on the other hand, focuses on solving the many-body Newton's mechanics [12] equation. This paper presents a modeling expansion application coded on MATLAB and based on SRIM data which extrapolates to calculate distributions for all energies of interest, cleans up inherently noisy SRIM-generated data, automatically optimizes the energy, dose, and number of steps required to create a target profile, and finally models channeling effects.

I. COMPARISONS AND OPTIMIZATION OF SRIM SIMULATED PROFILES USING FILTERING PROCESSING

I.1. QUICK CALCULATION *VS.* MONOLAYER COLLISION MODES

The SRIM code is based on the binary collision approximation. This method assumes that the incoming ion loses energy gradually from the electronic stopping power of the target and then collides elastically with the nuclei. After collision, solving the classical scattering integral yields the scattering angle and the energy lost from the ion and thus transmitted to the nuclei. Between collisions, this approximation considers a straight flight path between nuclei.

SRIM offers several simulation modes. The first one is called the quick calculation mode. It is based on rapid statistical estimates derived from the Kinchin-Pease formalism which uses an energy displacement approximation. This is briefly outlined in Equation 1. For a deeper explanation please refer to Ziegler *et al.* [4].

The number of point defects or vacancies N_d created inside a target is determined by whether the amplitude of the energy from collision with the primary knock-on (PKO), E_ν, is larger than the displacement energy, E_d, required to remove an atom from a site. E_d is approximated from tabulated values.

$$N_d = \begin{cases} 0 & \text{for } E_\nu < E_d \\ 1 & \text{for } E_d \leq E_\nu < \dfrac{2\ E_d}{0.8} \\ \dfrac{0.8\ E_\nu}{2\ E_d} & \text{for } E_\nu \geq \dfrac{2\ E_d}{0.8} \end{cases}$$

Equation 1

We emphasize that this SRIM mode utilizes a free flight approximation to save computing power resources. As such only collisions occurring after a fixed distance into the target are examined.

A SRIM mode that requires more computing resources is called the monolayer collision mode. In this mode every single nucleus in the path of the incoming ions is examined for potential path change depending on the energy of the incoming ions. Since this mode does not use any free flight approximation, every collision is computed using calculations of surface binding energies between atoms. As such, for typical compound semiconductor substrate thicknesses used, the calculation time dramatically increases and can range between 2 to 20 times longer depending on the thickness of the target.

Figure 1 shows a comparison between the two modes for hydrogen ions incoming at 90 keV into a target made of three layers of InP with the same density and a GaAs

layer with a 20% higher density. As illustrated, for the quick calculation mode, non-physical peaks are appearing at the interfaces between the InP layers even though the density and atomic composition are kept constant between layers. We believe this is an artificial aberration induced by the free flight approximation and boundary conditions, probably because of having a new layer, even though of same density, might reset the free flight clock and induce nonlinear effects in the output ion PKO calculations.

It is also important to mention that SRIM does not consider any crystallographic orientation. It only uses amorphous input layers. Consequently, the peaks seen at interfaces with the same density on either side cannot be attributed to a mismatch in the crystallographic orientations between layers.

When using the monolayer collision mode, such nonphysical peaks disappear and only differences in density as seen between the layer InP #3 and the GaAs layer induce a slope change in the vacancy profile.

Finally, the projected range, depth at maximum concentration is slightly shifted to deeper values with the monolayer collision mode.

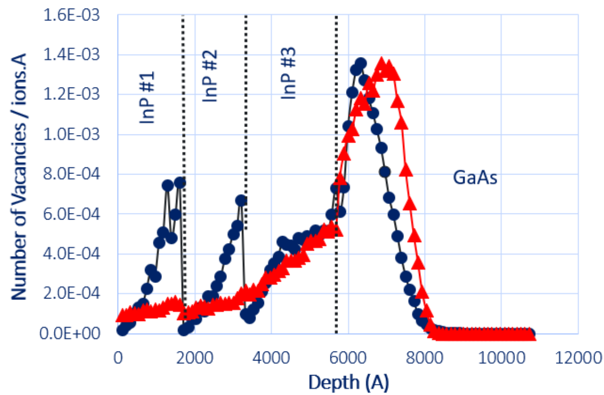


Figure 1. Comparison of simulated ion implantation vacancies, normalized per ion dose, using SRIM between the quick calculation mode in blue circles and the monolayer collision mode in red triangles.

I.2. High frequency smoothening of quick calculation parasitic peaks

To take advantage of the high-speed calculation and remove these non-physical parasitic peaks induced in the quick calculation mode, we implemented a Fourier smoothing approach which removes these high frequency variations from the profile. As shown in Figure 2.a, we simulated with SRIM, the profile vacancies obtained by ion isolation on a hypothetical GaAs target made of multiple layers of same densities as it can often be designed in opto-electronic devices. As you can see on Figure 2.b, a high frequency depth spectrum is generated using INNOViON then it is removed from the original profile to yield a clean and smoothed profile (Figure 2.c).

This smoothing treatment is nearly instantaneous and combined with the quick calculation method keeps the total calculation time far shorter than what the monolayer collision mode requires.

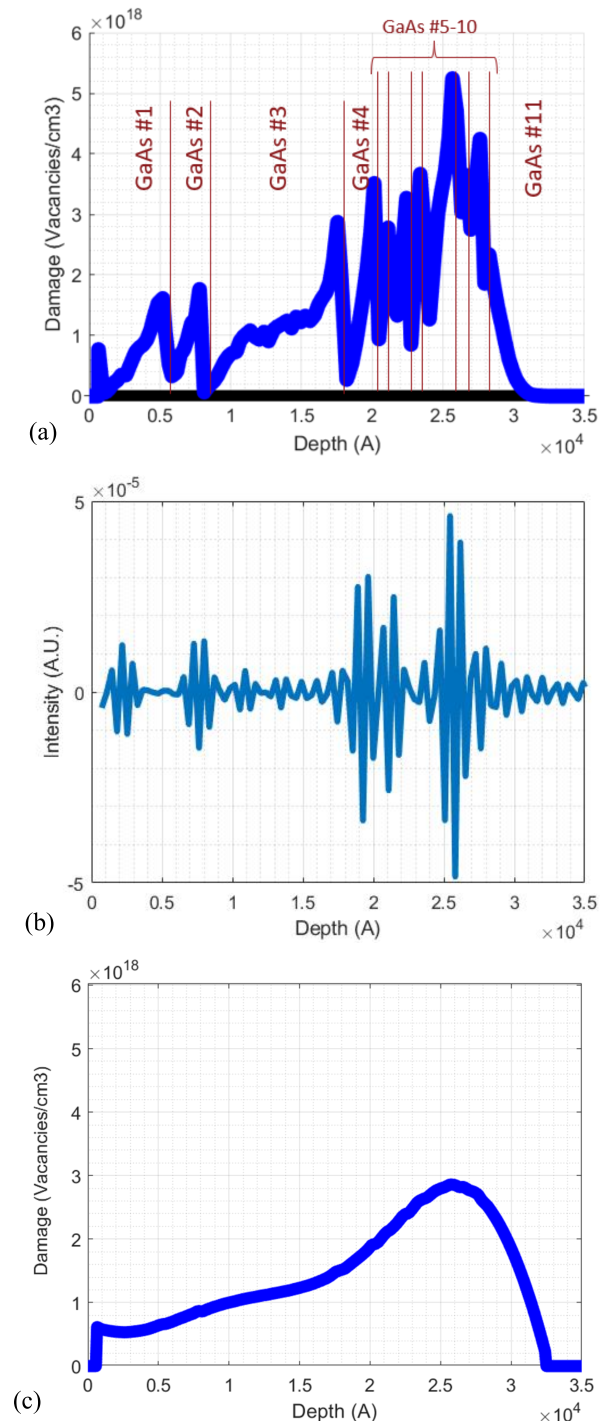


Figure 2. (a) Example of vacancy density induced by a 320 keV hydrogen ion profile being dramatically degraded by non-physical parasitic peaks emerging at the interfaces between GaAs layers despite having the same density. (b) High frequency peaks extracted from the profile illustrated in (a). (c) Corrected profile after removal of high frequency peaks.

II. EXTRAPOLATION OF ENTIRE DEPTH PROFILE FROM SRIM SIMULATIONS

The SRIM code generates implanted layer profiles using a single energy value input. While this is efficient, it can be rather time consuming if one wants to simulate profiles for several ion energies.

We have developed an extrapolation technique that generates profiles for the entire energy using referenced ion distributions based on any fixed energy window size. As shown in Figure 3, the extrapolated ion distribution, at every 1 keV for a hydrogen implantation into a GaAs substrate, matches very well the initial SRIM modeled profiles.

For the sake of clarity, the modeling is done into a single layered substrate, but this method yields similarly highly accurate modeling on multilayered targets.

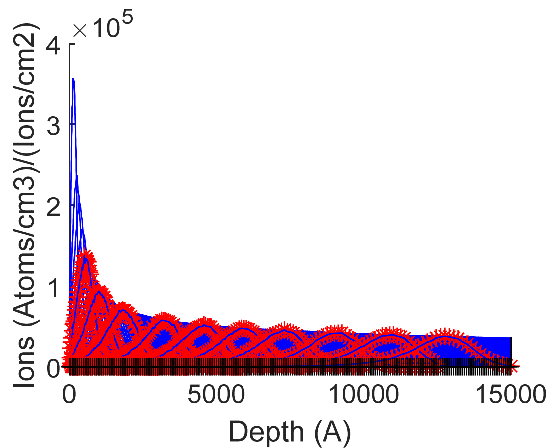


Figure 3. Simulated ion distribution of hydrogen into GaAs with implant energies of 5 to 175 keV in 17 keV steps in red, compared with values of ion distributions extrapolated at a 1 keV energy frequency in thin blue lines (b). Being very closely distributed, the blue lines resemble a continuous thick blue exponentially decreasing curve, except at low energies where we can discern a few individual curves.

The extrapolation technique, which is imbedded in INNOViON, is based on a change of basis vectors from the SRIM simulated ones for which the coordinates in the 2D planes are transposed into an alternative vector space which basis vectors are the projected range and the longitudinal straggle.

III. AUTOMATIC MONTE-CARLO PROFILE MATCHING OPTIMIZATION

Building on the extrapolation feature described previously, we implemented a Monte-Carlo optimization technique which matches as many energy/dose combination steps as desired to either an implanted ion or vacancy distribution profile target.

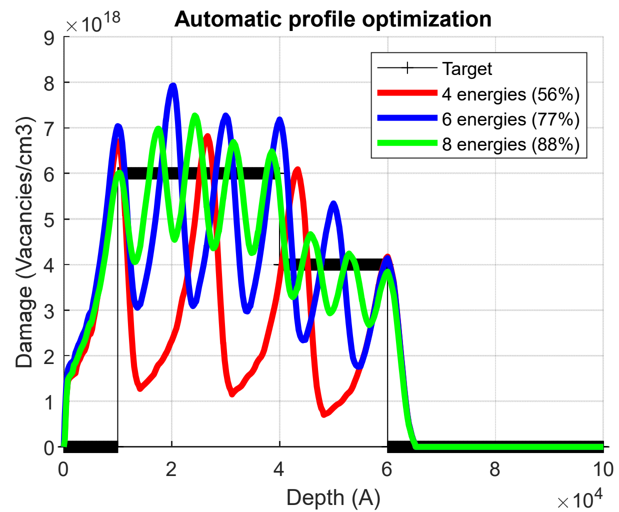
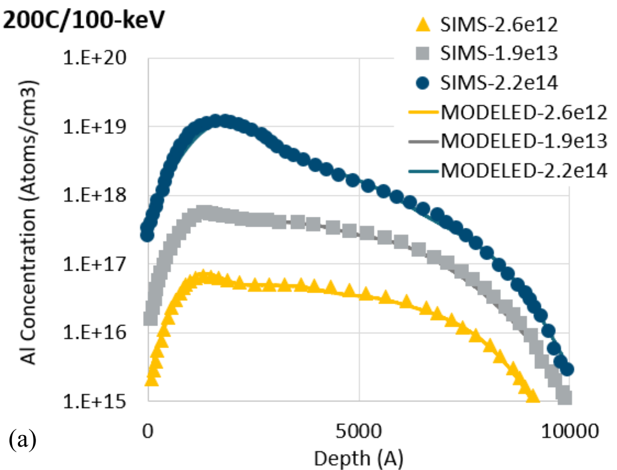
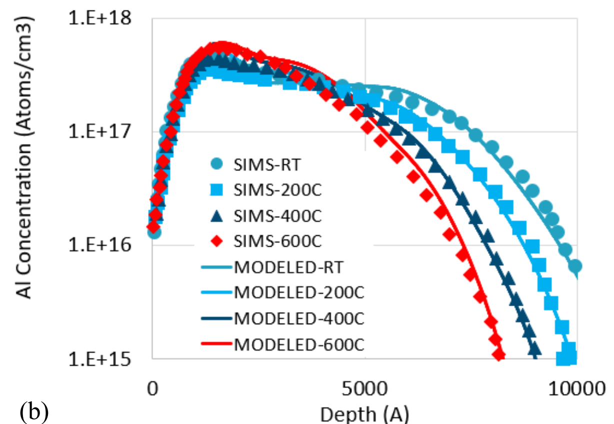


Figure 4. Automatic profile generated for hydrogen implants into an InP substrate with the target profile in thick straight black lines. Increasing the number of energy/dose steps leads to a higher matching ratio, defined as the percentage of one minus the difference between the target and simulated profiles, as listed in the figure.



(a)



(b)

Figure 5. Comparison between SIMS profiles and simulations for Aluminum implants into the 4H-SiC [0001] channel with dependence on dose (a) and temperature (b).

Shown in Figure 4 is the increasing accuracy as a function of the number of steps used between the damage distribution and the target profile. This feature enables a high accuracy in designing implantation sequences into any semiconductor compound target.

IV. Channeling capability

For SiC applications, since the diffusion of dopants is nearly nonexistent, the channeling effect is often being used to implant a "box profile" into the substrate. We developed a heuristic method based on a Taylor-Young expansion into Gaussian functions of channeled ion curves extracted from Secondary-Ion Mass Spectroscopy (SIMS) profiles found in the literature [13] [14]. By determining the evolution of the Gaussian function with energy, dose, and temperature the simulator can recreate the channeled curves. See Figure 5 for the case of Aluminum into the [0001] main channel of 4H-SiC and the profile channeling dependence on dose and temperature. The simulator based on SIMS data accurately reproduces the experimental results.

V. Conclusions

In this paper, we introduced an ion implantation simulator called INNOViON designed on MATLAB. It builds on SRIM simulated data and optimizes its modeling capability and computing speed. It allows for fast and high accuracy design of ion implantation sequences into semiconductor compound targets. Finally, this simulator enables the heuristic modeling of channeling with temperature and dose, for substrates where diffusion is prevented.

Acknowledgement

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

Acronyms

SRIM: Stopping and Range of Ions in Matter
MC: Monte Carlo
MD: Molecular Dynamics
PKO: Primary Knock-On
SIMS: Secondary Ion Mass Spectroscopy

References

[1] J. Ziegler, "The calculation of low energy He ion stopping powers," *Nucl. Instrum. Meth. A,* vol. 149, pp. 129-135, 1978.

[2] J. Ziegler, J. Biersack and U. Littmark, The Stopping and Range of Ions in Solids, New York: Pergamon Press, 1985.

[3] J. Ziegler, The stopping and ranges of ions in matter. Handbook of stopping cross-sections for energetic ions in all elements, vol. 5, New York: Pergamon, 1980.

[4] J. Ziegler, Handbook of Ion Implantation Technology, Amsterdam: Elsevier Science Ltd., 1992.

[5] M. Hautala, "Channeling of B and As near the silicon (001) axis.," *Nucl. Instrum. Meth. B,,* vol. 15, pp. 75-77, 1986.

[6] B. Mulvaney, W. Richardson and T. Crandle, "PEPPER - A process simulator for VLSI.," *IEEE Trans. Comp. Aid. Des.,* vol. 8, pp. 336-349, 1989.

[7] M. Posselt and J. Biersack, "Computer simulation of ion implantation into crystalline silicon.," *Nucl. Instrum. Meth. B,* vol. 64, pp. 706-710, 1992.

[8] M. Posselt, C. Schmidt, T. Feudakl and N. Strecker, "Atomistic simulation of ion implantation and its application in Si technology," *Mat. Sci. Eng. B,* vol. 71, pp. 128-136, 2000.

[9] Y. Yamamura and W. Takeuchi, "Monocrystal sputtering by the computer simulation code ACOST," *Nucl. Instrum. Meth. B,* vol. 29, pp. 461-470, 1987.

[10] B. Obradovic, G. Wang, Y. Chen, D. Li, C. Snell and A. Tasch, UT-MARLOWE Version 5.0 Manual, 1999.

[11] J. Ziegler and J. Biersack, SRIM textbook, 2008.

[12] G. Hobler, K. Nordlund, M. Current and W. Schustereder, "Simulation Study of Al Channeling in 4H-SiC," *22nd International Conference on Ion Implantation Technology (IIT) - Material Science,* vol. IEEE, 2018.

[13] M. Linnarsson, A. Hallen, L. Vines and B. Svensson, "Channeled Implantations of p-Type Dopants into 4H-SiC at Different temperatures," *Materials Science Forum ,* vol. 963, no. 1662-9752, pp. 382-385.

[14] K. Nordlund and A. Kuronen, "Molecular dynamics simulation of ion ranges at keV energies," *Nuclear Instruments and Methods in Physics Research B,* vol. 115, pp. 528-531, 1996.