DEVELOPING STUDENTS COMPETENCES BY MEANS OF SIMULATION: USE OF A RESEARCH TOOL FOR UNDERSTANDING ION-MATTER INTERACTION IN SOLID STATE PHYSICS

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1. Introduction

Science and technology define the degree of development and potential progress of a modern society and researchers and engineers are stimulated to search for new materials and methods to improve and renew technological artifacts. Physics education plays a fundamental role in the education system and it cannot undervalue the importance and urgency of integrating and updating the curricula with modern physics and technology.

The introduction of modern physics in secondary school and university must be relevant and needs correlation to the actual technological world. However, the understanding of the laws and the rules that govern the phenomena in the modern fields of physics often requires a background knowledge of quantum mechanics, statistical physics and mathematical methods that make very hard or impossible an approach to students.

In this paper a possible way to introduce fundamental aspects of ion-matter interaction is presented. The aim is pursued through the use of a program, SRIM: the Stopping and Range of Ions in Matter, for the simulation of ion implantation, a widely used technique, in particular, in materials research and industry. The background knowledge can be very essential and coincides with subjects which are normally introduced in secondary school, such as the atomic structure of matter, the periodic table of the elements, neutral and ionized atoms, the charge interactions and the collision physics. This activity is then suitable for first level university students as well as for students of secondary school especially with materials science specialization. School teachers could not have the needed attainments and a materials science training course is recommended.

SRIM calculates the stopping and ranges of ions in the kinetic energy range 10 eV – 2 GeV per amu into matter and simulates an ion implantation using full quantum-mechanical treatment of ion-atom collisions. It supplies as output complete numerical tables as well as 3D plot distributions of the ions with target damage, sputtering, ionization and phonon production. Each ion track and target atom cascade are followed in detail and presented in animated plots. Students experiment with the use of an advanced research instrument and are allowed to understand and learn new physical phenomena such ion diffusion, target atom recoiling, atom cascade and surface sputtering, as well as statistical concepts such projected range, straggling, electron and nuclear stopping power and radiation damage.

2. SRIM simulation for physics education

Ion implantation technology is widely used for electronic materials and recently is more and more often mentioned and treated in books or in scientific documentary films. Besides, the phenomena involved in this process such ion production, acceleration and interaction with matter are common to many scientific fields. Few emblematic examples: ion beams are employed in medicine for irradiation of cancerous cells with high efficiency and spatial resolution; natural radioactivity and fast charged particles coming from space, in some cases, can be thought of as ionized atoms interacting with the atmosphere, with the earth or the skin and the organs; the problem of the nuclear waste storage since the walls of the container are affected by alpha particles (helium ions) implantation coming from the nuclear decays.

It is very important that a physics course gives students the opportunity of moments of direct contact with the research and technology world, just treating particular topics which involve arguments transversal to many fields of science [1].

The problems often encountered introducing modern technology in physics teaching are: i) high technical instrumentation required to obtain reliable and significant experimental data; ii) prohibitive and expensive costs; iii) particular environmental conditions needed (e.g. powder particle concentration, humidity and temperature); iv) health hazard for the use of high voltages, toxic gases and substances; v) long period of specialization training to acquire competencies in the use of instrumentation, machines and processes.

The use of a simulator, a technique also adopted in formation courses for technician and researchers, overcomes all these technical difficulties making easier the students reaching the results and learning physics. Moreover students are not required to know the numerical and analytical methods, often overcomplicated, which are necessary to solve the physical equations.

An other important advantage coming from the use of a simulator in a learning activity is the possibility of trying situations not easily realizable or absolutely unrealistic and purely theoretical to investigate the influence of the input parameters. This is perhaps the major motivation that justifies an activity exclusively employing simulations as this.

SRIM simulates the ion implantation process starting from few input parameters about the beam and the target and makes Montecarlo calculations of the ion trajectories which can be displayed singularly with details and synthesized into distribution graphs and synthetic statistic quantities.

Simulation and modeling in physics education are didactic strategies widely experimented and adopted, and various research papers have been published on these topics [2,3]. An important point is that students could have difficulties to distinguish model and reality [3]. Working with SRIM, students are precluded to have any direct contact with the phenomena under investigation and the teacher has to guard the students (and himself) against confusion. The activity with SRIM should be preceded by an introduction about the role of modeling in the knowledge of the physical world. An important topic to be submitted to the students and discussed is the Montecarlo method employed by SRIM. The simulation is made by solving the equation of motion of each ion singularly. The calculation of a particular ion trajectory is obtained using random numbers to quantify the stochastic quantities involved in the collisions, e.g. the collision probability, the collision parameter and the degree of energy loss. The final product, as it happens in an actual implantation process, is the result of the superimposition of all the single ions events.

Taking into account the above observations, we propose an activity employing SRIM designed according to the following points:

i) qualitative exploration of the ion motion into matter;
ii) analysis of the influence of the input parameters;
iii) search for physical phenomena occurring in the implantation process;
iv) identification of quantities typical of the ion-matter interaction physics;
v) problem solving activities aimed to the evaluation of these quantities by elaboration of the simulated data.

3. What is SRIM?

SRIM is a free simulation program that can be downloaded from the internet address www.srim.org and runs on personal computers. It results from the original work by J.P.Biersack [4] on range algorithms and the work by J.F.Ziegler on stopping theory [5].

SRIM is used in research to plan ion implantation processes to fit the desired ion depth profile and target damage. SRIM calculates the stopping and range of ions (10 eV – 2 GeV/amu) into matter and simulates an ion implantation using a full quantum mechanical treatment of ion-atom collisions. This calculation is made very efficient by the use of statistical algorithms which allow the ion to make jumps between calculated collisions and then averaging the collision results over the intervening gap. During the collisions, the ion and atom have a screened Coulomb collision, including exchange and correlation interactions between the overlapping electron shells. The ion has long range interactions creating electron excitations and plasmons within the target. These are described by including a description of the target collective electronic structure and interatomic bond structure when the calculation is setup. The charge state of the ion within the target is described using the concept of effective charge, which includes a velocity dependent charge state and long range screening due to the collective electron sea of the target. A full description of the calculation is found in the tutorial book [6]. This book presents the physics of ion penetration of solids in a tutorial manner, then presents the source code for SRIM with a full explanation of its physics. Further chapters document the accuracy of SRIM and show various applications.

SRIM accepts complex targets made of compound materials with up to eight layers, each of different materials. It calculates both the final 3D distribution of the ions and also all kinetic phenomena associated with the ion energy loss: target damage, sputtering, ionization, and phonon production. All target atom cascades in the target are followed in detail. Plots of the calculation is made in real time, moreover they can be saved and displayed when needed. On request, numerical tables of the stopping of ions as well as of the ions and displaced target atoms trajectories and energies can be compiled and saved for elaboration purpose.

Figure 1 shows the window of input parameters for stopping calculation of hydrogen ions into silicon. The parameters to be supplied are: the ion type and its mass, the energy range of stopping power calculation, the target composition, the units. Table for frequently used materials are available.

Figure 2 shows the window of input parameters for implantation simulation of hydrogen ions into silicon at 100 keV. The parameters to be supplied are: the ion type and its mass, the initial kinetic energy, the angle of incidence, the target in terms of layer thicknesses and compositions, the number of ions to be calculated, the plotting window and the output table files to be saved. The damage calculation option and the type of live plots to be displayed during calculation can be set with the choice windows.

The large number of information supplied by SRIM can constitute matter of study at different school levels and for different degrees of specialization. In this initial work, only the ions trajectories and the target atoms cascades will be treated. Physical background needed are the fundamentals of classical mechanics and electrodynamics.

The particular choices of the target material, of the ions and their energy could limit the generality of the study. However the aim of this paper is the suggestion of guidelines for the use of such research tool to teach ion-matter interaction. The SRIM version adopted is the 2000.39.

4.1 Qualitative exploration

4.1.1 Ion trajectories

Figure 3 shows the simulations of the trajectories of four ions with same initial kinetic energy (100 keV) impinging on silicon. The ions are H (Fig. 3a), C (Fig. 3b), Ge (Fig. 3c) and U (Fig. 3d). The horizontal axes report the depths and the vertical axes report the lateral displacements of the ions. It can be observed that the trajectories are finite in length and decrease with increasing the ion atomic number and mass. The trajectories appear not rectilinear and of irregular forms. Ions of the same kind produce almost similar shapes, while different ions present different features in their motion. For example, light ions as H travel in a straight way at the beginning and tracing hook-shaped trajectories at the end of their motion. Heavy ions as U travel in a more regular way, with light curves distributed within the whole track.

The statistics of the simulations can be improved by increasing the number of calculated ions. Figure 4 reports the simulations of 100 ions. The trajectories are contained within pear-shaped volumes of different dimensions and proportions. The region where the ions come at rest appears of cylindrical symmetry with the axis perpendicular to the target surface through the beam incidence point. Occasionally insulated trajectories, very long or with strong deflections, occur.

4.1.2 Recoils.

Figure 5 shows the simulations of one trajectory per ion type including the detailed calculation of full damage cascades. Green traces are the target atoms (recoils) tracks. For a more extensive exploration it is possible to do multiple ion simulations with the caution of clearing the screen to prevent confusion. The simulator allows the formation of the collisional cascades to be followed by switching the animation button.

Observing Figure 5, very few recoils are produced along light ion trajectories (H: 11, C: 518) and concentrated at the end of the track in correspondence of the hook. As ion mass and atomic number increase, the number of recoil increases (Ge: 1750, U: 2200) almost uniformly distributed along the track. Occasionally long trajectory recoils are produced.

4.2 Influence of the input parameters

In this section the input parameters will be varied. For a matter of simplicity the target composition will be kept constant, since having considered ions either lighter either heavier than silicon, the investigation does not loose generality.

4.2.1 Ion mass and atomic number

All the above qualitative observations exhibit dependence on the ion type. A question rises: is the control parameter the ion mass or the atomic number?

4.2.1.1 Trajectory length

Figure 6 reports the simulations for H and He ions with their correct masses (Fig. 6a and d) and with the inverted ones (Fig. 6b: H with mass 4 uma, Fig. 6c: He with mass 1 uma). Comparison between Fig. 6a and b and between Fig. 6c and d reveals that the mass increases the trajectory lengths, while comparison between Fig. 6a and c and between Fig. 6b and d reveals that the atomic number shortens the tracks. Same conclusions are deduced from similar simulations of Sn and U ions reported in Figure 7. Ion mass and atomic number have opposite effects and this leads to the conclusion that the atomic number prevails on the ion mass in determining the track lengths.

4.2.1.2 Trajectory shapes

To investigate the influence of the two parameters on the trajectory shape, simulations of H ions with the U mass and of U ions with the H mass can be used (Figure 8). Fig. 8a appears very similar to Fig. 3d and Fig. 8b appears very similar to Fig. 3a indicating that, in this case, the ion mass is the control parameter.

4.2.1.3 Recoil production

The simulations of Figure 8 are recalculated with full damage cascades and reported in Figure 9. It can be deduced that silicon atoms are displaced more efficiently by high atomic mass ions, either in terms of number (H: 2170 recoils/ion, U: 128 recoils/ion), either in terms of displacement from the ion track and dimension of the collisional cascade.

4.2.2 Ion energy

The kinetic energy of the impinging ions is expected to play a role in the recoil production (the displaced silicon atoms appear at first in the ending part of the ion track, see Fig. 5c, where the ion energy is low) other than, obviously, in the ion trajectory length. Figure 10 reports the simulations for C and U ions at different initial energies.

4.2.2.1 Trajectory length and shape

The trajectory lengths increase with ion initial energy (note the different depth axes). However the two physical quantities are not proportional, especially in the case of U. The shapes seem to be unaffected.

4.2.2.2 Recoil production

The number of recoils increases with ion initial energy (C at 10 keV: 108, C at 30 keV: 225, C at 60 keV: 325, C at 100 keV: 518; U at 10 keV: 262, U at 30 keV: 714, U at 60 keV: 1390, U at 100 keV: 2200). Moreover, observing Figure 10a, the displaced silicon atoms are roughly distributed along the whole ion track, while in Figure 10c they are less dense in the initial part. In the case of U ions the behavior appears the opposite: many recoils are produced along the track and fewer at the ending part of it.

It is useful for students to design and compile a table which summarizes the observations made. A suggestion is the following:

	Trajectory length	Trajectory shape	Recoil number
Ion mass	Y/N	Y/N	Y/N
Ion atomic number	Y/N	Y/N	Y/N

Ion initial energy	Y/N	Y/N	Y/N
Ion instantaneous energy	Y/N	Y/N	Y/N

The previous two activities, qualitative exploration and input parameter variation, constitute fundamental moments of the present didactic activity with SRIM, because they play the role of the experimental stage in a usual laboratory activity, with the advantage of offering large space to personal choices. In this sense, these activities are occasions for the students of measuring themselves in a research activity and of acquiring project skills and scientific method.

4.3 Identification of physical phenomena

From the above observations, physical phenomena can be recognized. In the following, some of them will be identified and described in a schematic way, leaving to the teacher the job of completing the treatment and the strategy with students.

4.3.1 Friction

Arguments: the ion trajectories are finite in length; the ion trajectories are not rectilinear
Properties: it depends on the ion atomic number; it depends on the instantaneous ion energy; it is not constant (exhibits different regimes within the same track)
Conclusion: it is of coulombian origin; there are two principal ways of loosing energy: as in a viscous medium and by collision with target atoms
Topics motion in a viscous medium; elastic and inelastic collisions

4.3.2 Energy loss as in a viscous medium

Arguments: trajectories present rectilinear parts
Properties: typical of light ions; more efficient at high instantaneous energy
Conclusion: model of coulombian collision of the ionized projectile with the electrons of the target
Topics: energy transfer from a projectile to mass orders of magnitude lighter; dependence of the charge of an ion on its velocity in matter

4.3.3 Energy loss due to target atom collision

Arguments: the trajectories present deflections; target atoms displacement (recoil production)
Properties: typical of heavy ions; more efficient at high energy
Conclusion: model of nuclear collision of the ion and the target atoms
Topics: equations of classical collisions; energy transfer from a projectile to target mass of comparable order of magnitude [7] Rutherford cross section [8]; nuclear charge screening due to electrons; interatomic potentials

4.4 Typical quantities of ion-matter interaction

The stochastic character of an ion implantation process requires the identification of measurable statistical quantities. Here will be mentioned the principal ones.

An implantation is performed in order to locate impurities at a desired depth and with a suitable profile in a material.

4.4.1 The principal quantity is then the projected range, defined as the average depth of the implanted ions. Moreover, a crucial point is the statistical width of the impurity distribution due to the so called straggling. Such quantity can be represented by the distribution standard deviation or by more sophisticated statistical parameters, such skewness and kurtosis, taking into account asymmetries in the ion distribution. SRIM supplies live graphs during simulation of the ion distribution with the corresponding statistical parameters which can be used to give the students a graphical representation of the ion implantation process.

4.4.2 An other important point in implantation technology is the damage caused in the target material. The damage can be represented in first approximation by the distribution of the target atoms taking part to the collisional cascade or the so called interstitials. Also in this case the principal quantity is the average depth of recoils, and, consequently, the standard deviation of their distribution.

4.4.3 The sites originally occupied by the displaced atoms are called vacancies and also contribute to the damage. The vacancy depth distribution is in most cases practically superimposed to that of the interstitials, however, for light target elements the interstitial distribution can result deeper.

SRIM supplies live plots both for interstitial and for vacancy distributions.

4.4.4 The energy loss of ions during their motion into matter is called stopping. Such phenomenon is roughly distinguished in the two contributions of the electronic friction and of the nuclear collisions.

4.4.4.1 The electronic stopping power $\left.\frac{dE}{dx}\right|_e$ is defined as the energy loss per unit depth due to the interaction with target electrons. Such quantity depends on the velocity (so the instantaneous energy) of the ion since, in the typical energy range of ion implantation, it can be comparable with the ion core electron velocities with a consequent stripping and increase of interaction. The electronic stopping power is energy dependent and initially increases with energy; after a maximum, roughly corresponding to the ion velocity similar to that of its core electrons (total electron stripping), the stopping decreases due to less and less interaction time spent by the ion near the electron.

4.4.4.2 The nuclear stopping power $\left.\frac{dE}{dx}\right|_n$ is defined as the energy loss per unit depth due to the collisions with the target atoms. It depends on ion energy since at low velocity the ion does not penetrate the electron cloud of the target atom with a consequent decrease of nuclear coulombian interaction. Also the nuclear stopping power reaches a maximum with increasing energy, then it decreases due to the decrease of interaction time.

Figure 11 reports the calculated stopping powers for the considered ions. Their dependence on ion atomic number and energy reflects the observations and the deductions reported above.

4.5 Elaboration of calculated data

An useful activity for students is now the numerical evaluation of the identified physical quantities. A first ability they can acquire is the use of statistical functions and methods of data elaboration and representation. SRIM supplies all the needed data in numerical tables for depth distributions of ions (RANGE.TXT), interstitials (RANGE.TXT) and vacancies (VACANCY.TXT).

A more complicated and not univocal job is the evaluation of the stopping powers (both electronic and nuclear) employing the data of calculated ions. Numerical tables do not supply these quantities, but give many informations about the ion motion and the collisional cascades (E2REC.TXT, COLLISON.TXT). This activity can be proposed to student as problem solving and then the outputs of the various adopted solutions can be compared with the stopping powers calculated (and employed) by SRIM as those plotted in Figure 11.

5. Conclusions

A possible didactic activity using SRIM has been proposed. The fundamentals of ion-matter interaction can be easily evidenced, recognized and investigated by means of simulations of the ion implantation process, overcoming all the constrains that an experimental activity imposes. The activity has been projected in a similar way to an experimental investigation, allowing the students to acquire method and ability as well as competencies in data handling and elaboration.

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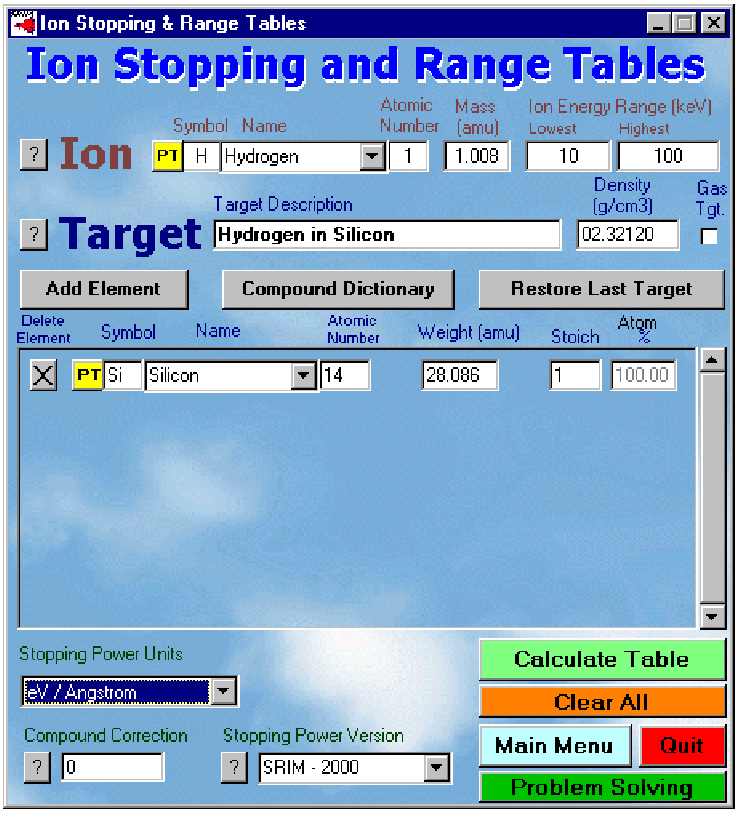


Ion Stopping and Range Tables

Ion: Symbol H, Name Hydrogen, Atomic Number 1, Mass (amu) 1.008, Ion Energy Range (keV) Lowest 10, Highest 100

Target: Target Description Hydrogen in Silicon, Density (g/cm3) 02.32120, Gas Tgt. ☐

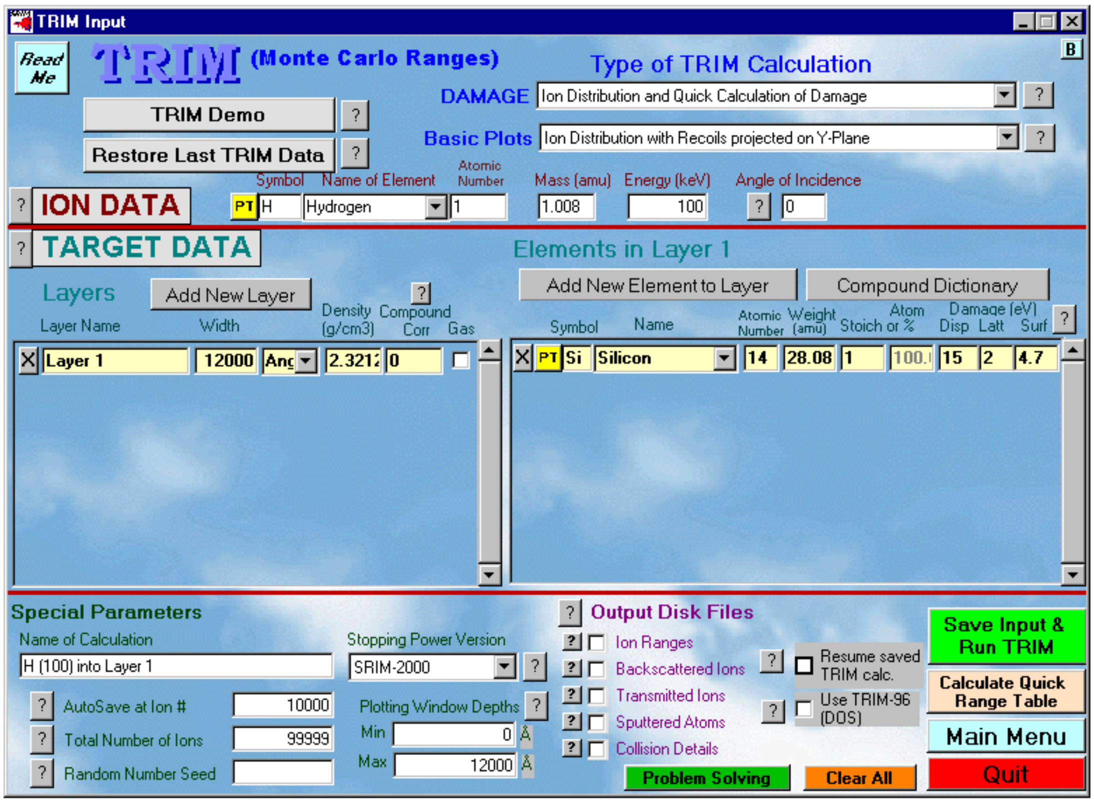
Element: Symbol Si, Name Silicon, Atomic Number 14, Weight (amu) 28.086, Stoich 1, Atom % 100.00

Stopping Power Units: eV / Angstrom

Compound Correction: 0

Stopping Power Version: SRIM - 2000

Figure 1. SRIM window of input parameters for stopping calculation.



TRIM (Monte Carlo Ranges)

Type of TRIM Calculation

DAMAGE: Ion Distribution and Quick Calculation of Damage

Basic Plots: Ion Distribution with Recoils projected on Y-Plane

ION DATA: Symbol H, Name of Element Hydrogen, Atomic Number 1, Mass (amu) 1.008, Energy (keV) 100, Angle of Incidence 0

TARGET DATA

Layers: Layer Name Layer 1, Width 12000 Ang, Density (g/cm3) 2.3212, Compound Corr 0, Gas ☐

Elements in Layer 1: Symbol Si, Name Silicon, Atomic Number 14, Weight (amu) 28.08, Stoich 1, Atom % 100., Damage (eV) Disp 15, Latt 2, Surf 4.7

Special Parameters

Name of Calculation: H (100) into Layer 1

Stopping Power Version: SRIM-2000

AutoSave at Ion #: 10000

Total Number of Ions: 99999

Random Number Seed:

Plotting Window Depths: Min 0 Å, Max 12000 Å

Output Disk Files:
- ☐ Ion Ranges
- ☐ Backscattered Ions
- ☐ Transmitted Ions
- ☐ Sputtered Atoms
- ☐ Collision Details

☐ Resume saved TRIM calc.

☐ Use TRIM-96 (DOS)

Figure 2. SRIM window of input parameters for implantation simulation.

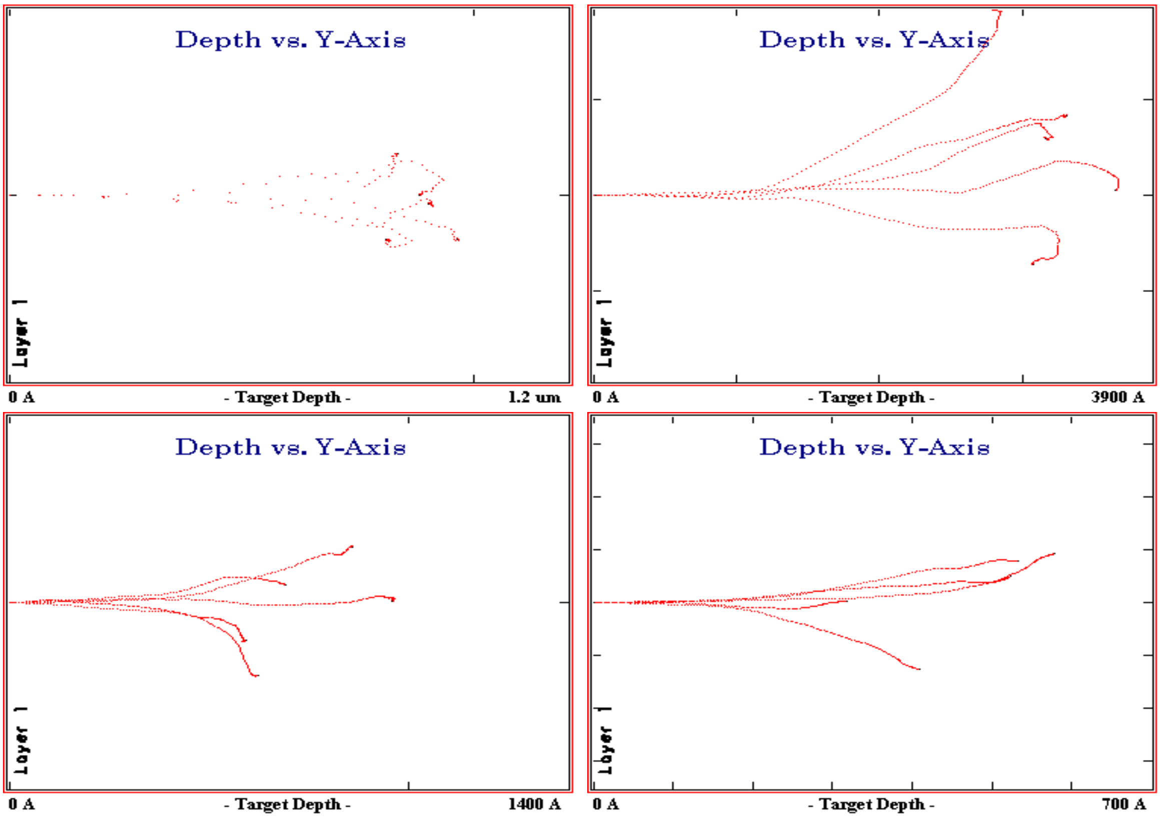


Figure 3. SRIM simulation of the trajectories of 5 a) H, b) C, c) Ge, d) U ions implanted in a Si target with energy of 100 keV.

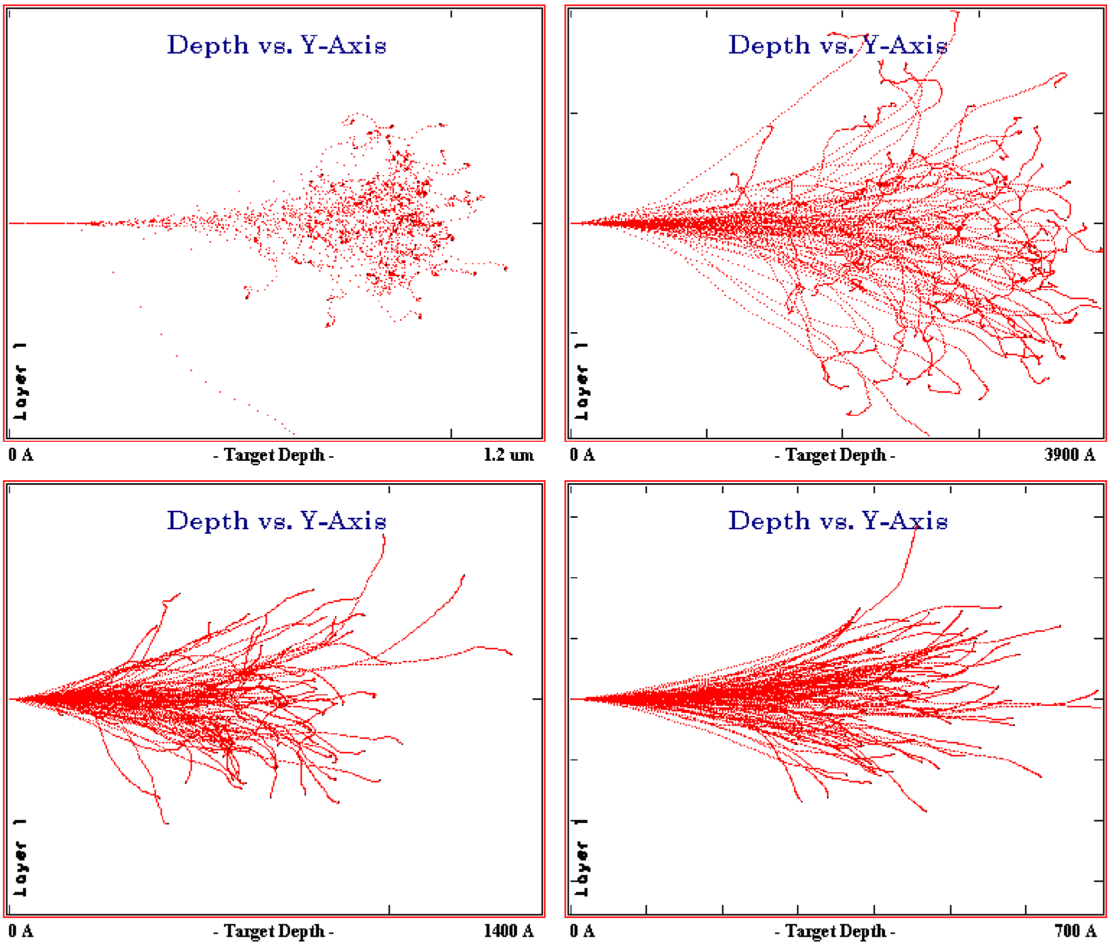


Figure 4. SRIM simulation of 100 ions of a) H, b) C, c) Ge, d) U with energy of 100 keV in Si.

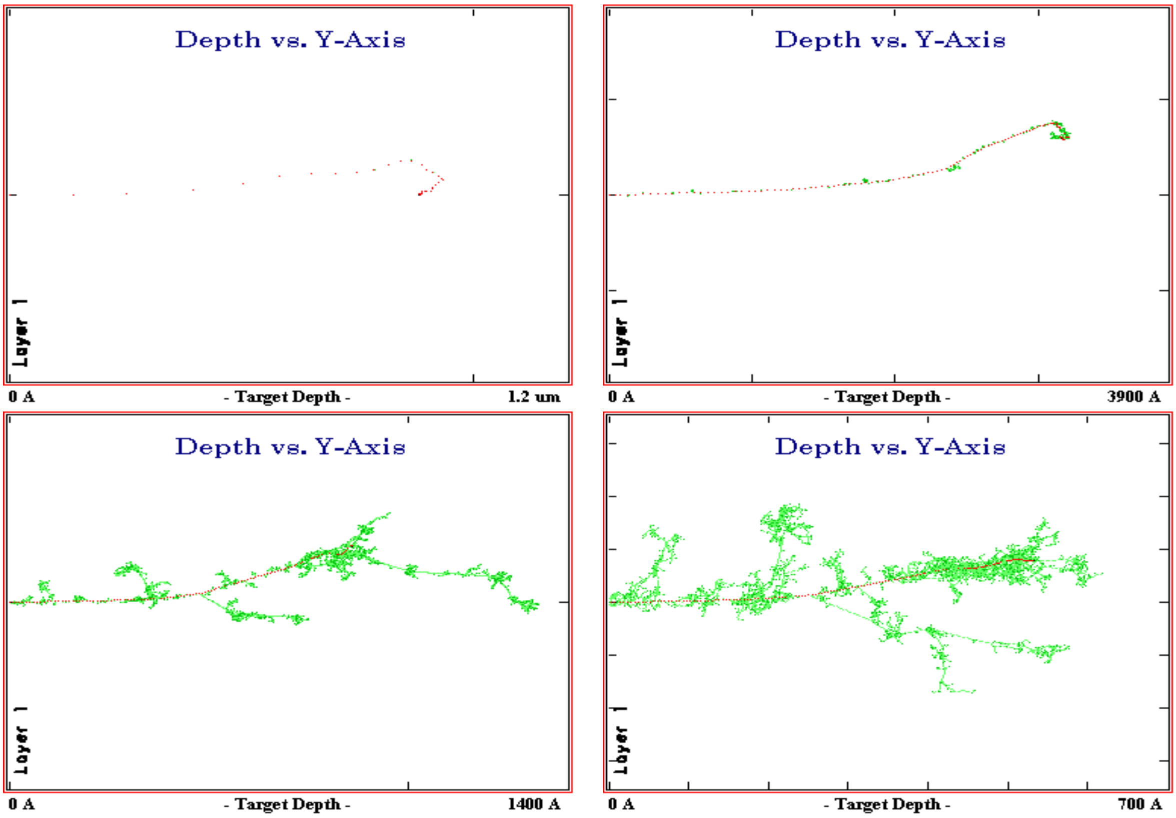


Figure 5. SRIM simulation including full damage cascade (marked in green) of a) H, b) C, c) Ge, d) U ion implanted in a Si target with energy of 100 keV.

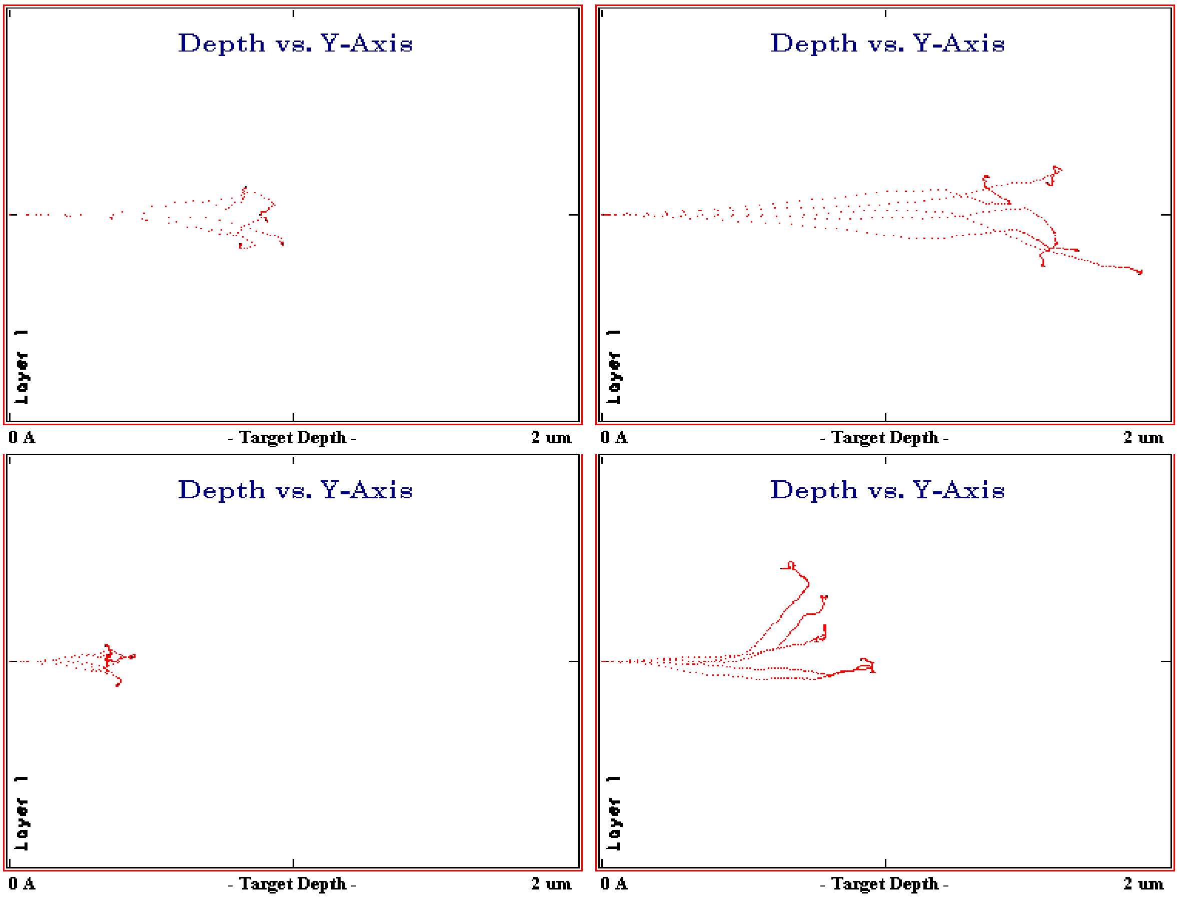


Figure 6. SRIM simulation of H and He ions into Si with the right masses (a and d) and with the inverted ones (b and c).

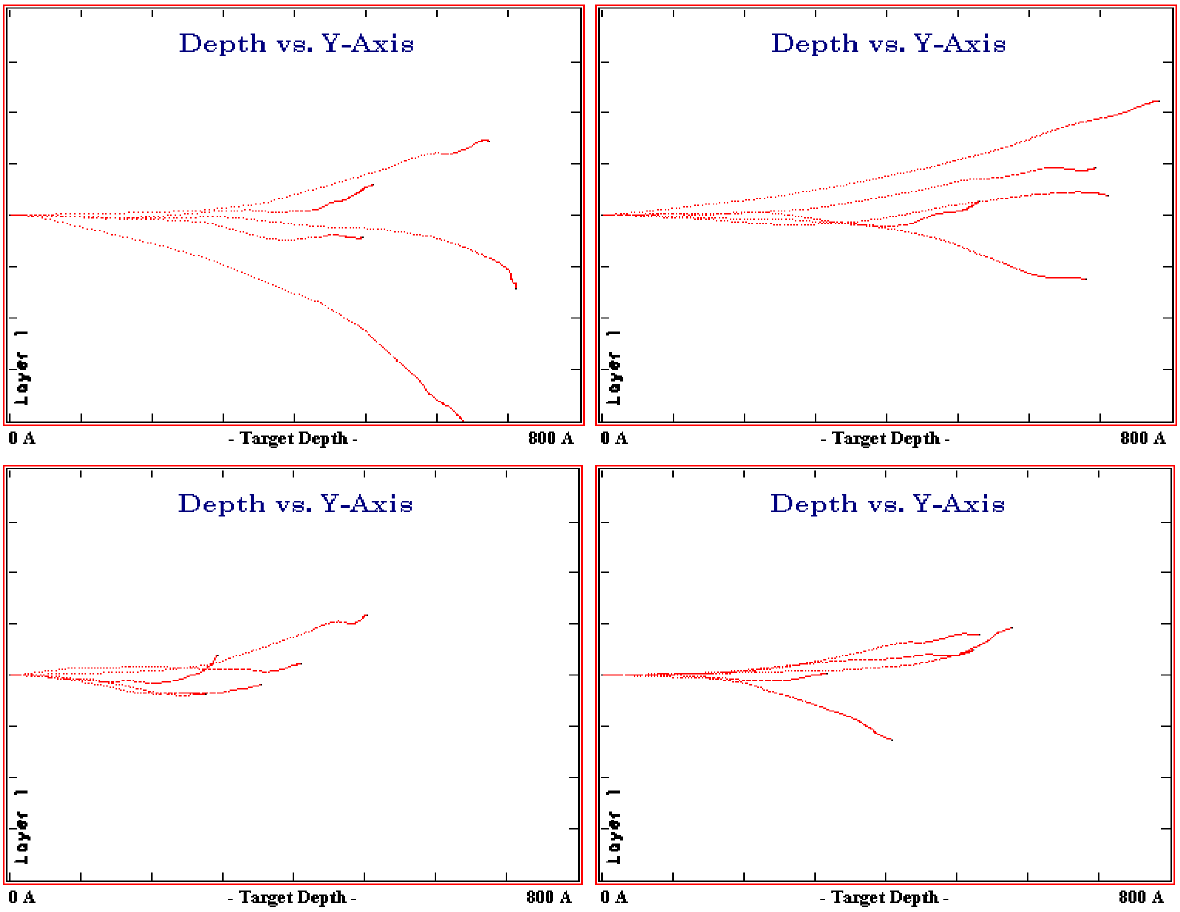


Figure 7. SRIM simulation of Sn and U ions into Si with the right masses (a and d) and with the inverted ones (b and c).

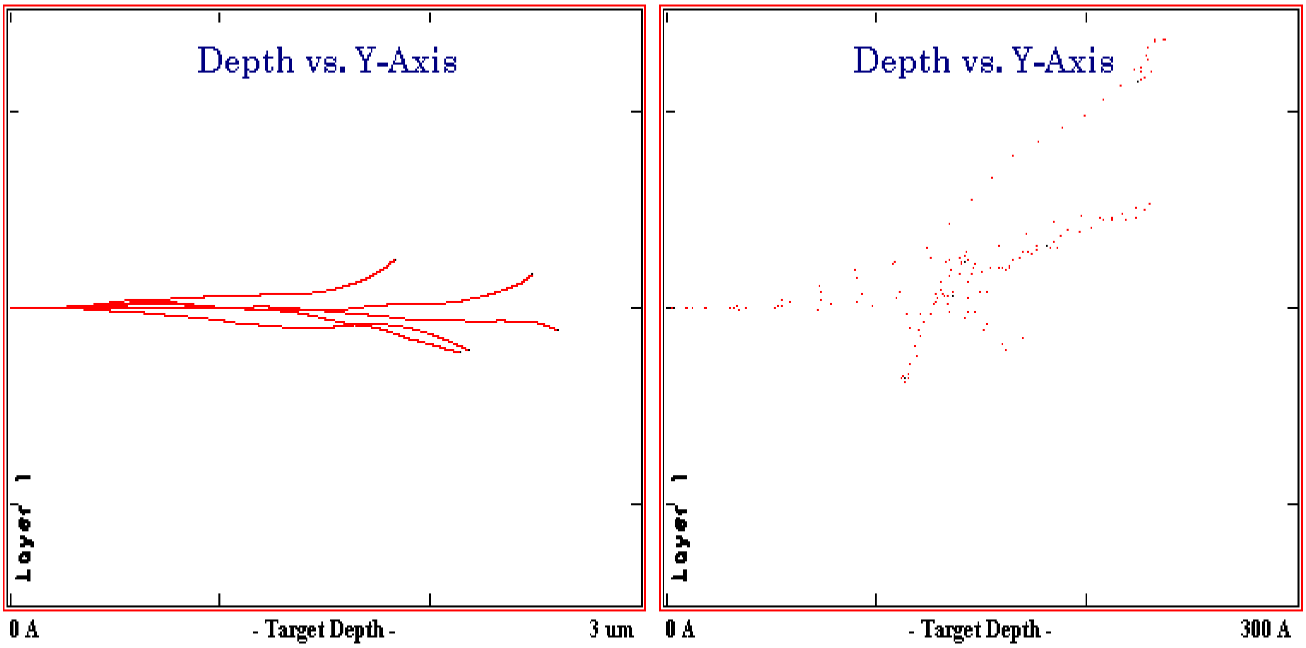


Figure 8. SRIM simulation of a) H ions with the U mass, and b) of U ions with H mass.

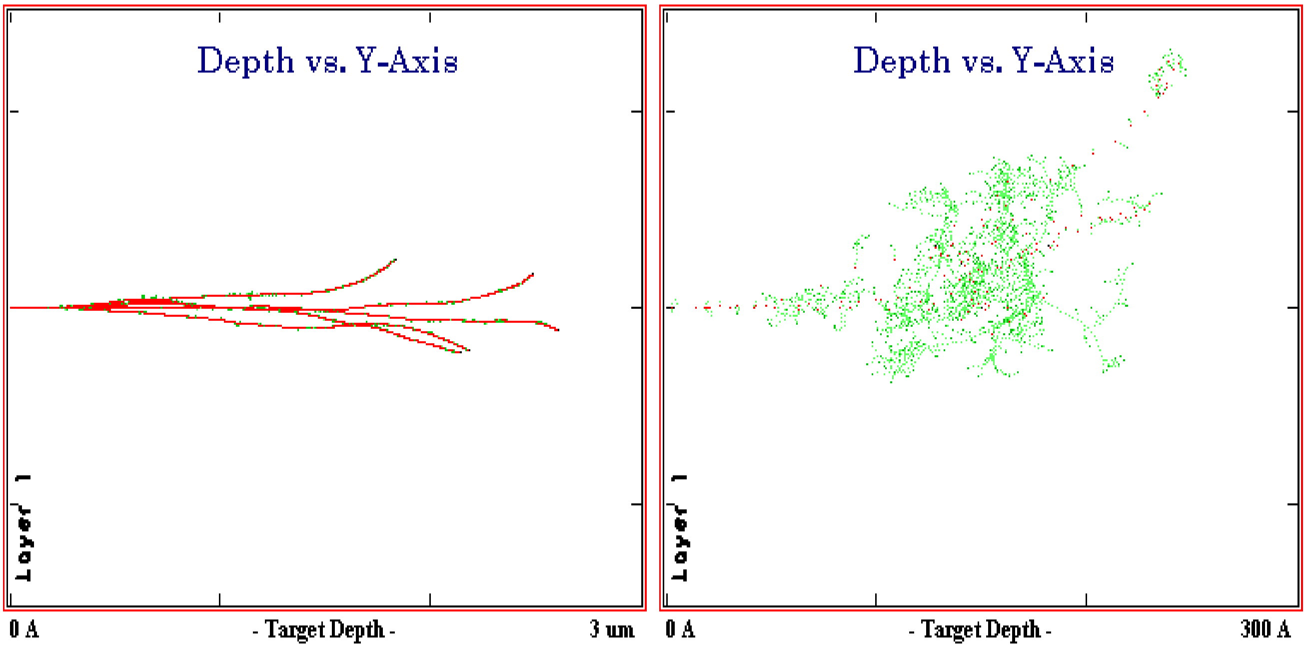


Figure 9. SRIM simulation including full damage cascade (marked in green) of a) H ions with the U mass, and b) of U ions with H mass.

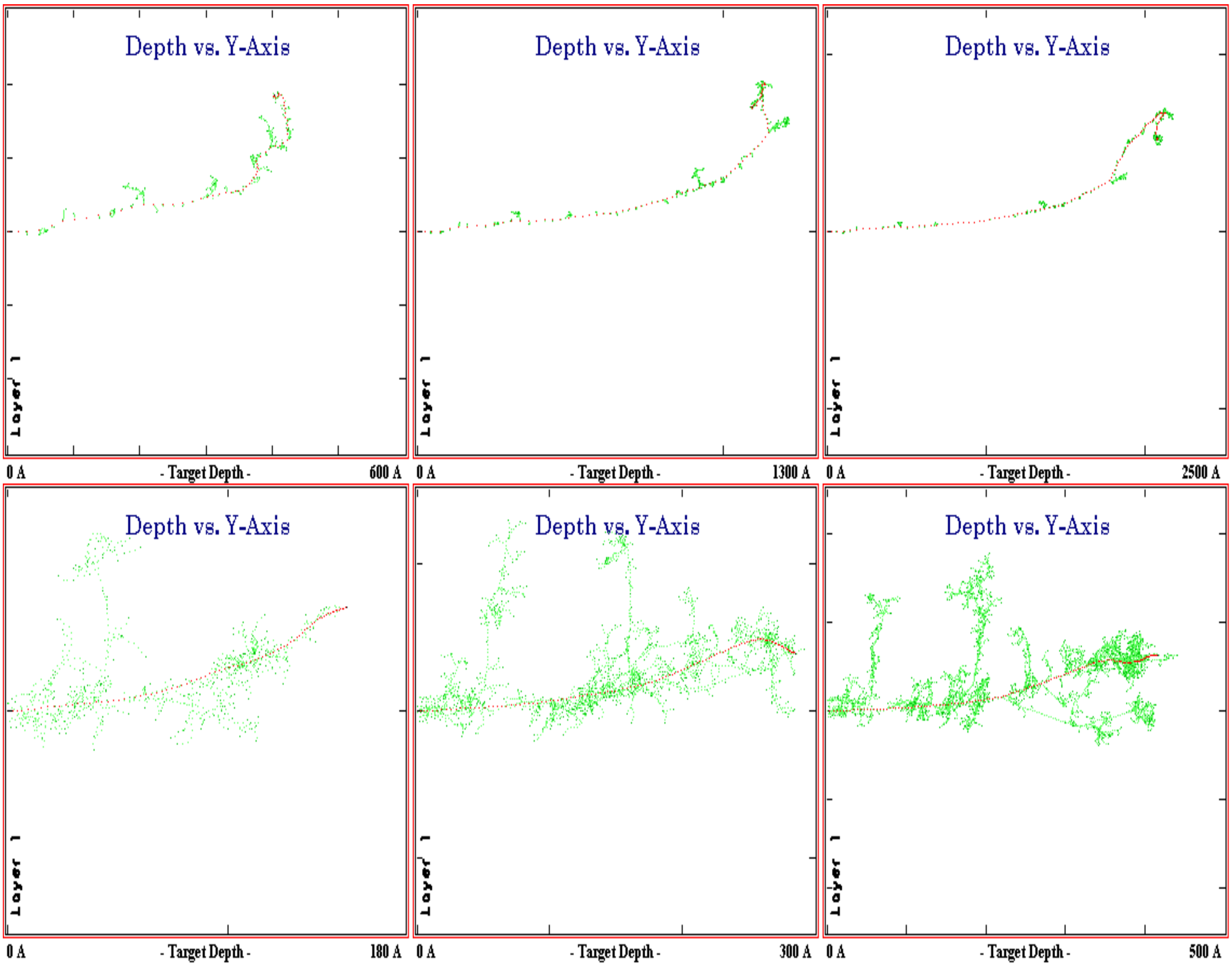


Figure 10. SRIM simulation including full damage cascade (marked in green) of C and U ions implanted in Si at different initial kinetic energies.

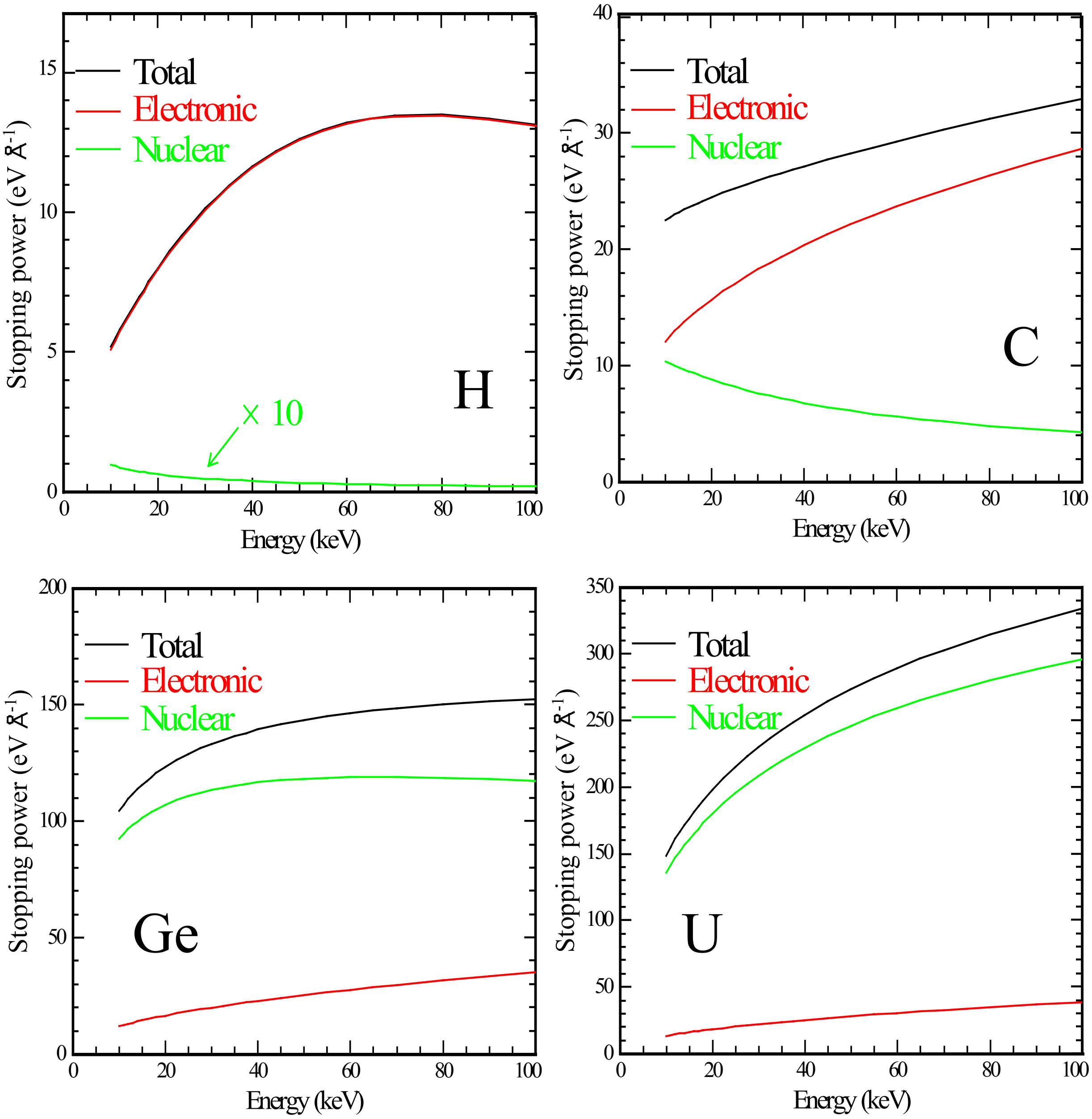


Figure 11. SRIM calculated stopping powers for H, C, Ge, and U ions in Si.