A NEW RELEASE OF THE S^{3}M CODE

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1. Introduction

The SRIM code is often used for calculating physical quantities related to interaction of ions with matter [1]. The S^{3}M code enlarges the scope of SRIM by the addition of routines that: (1) process SRIM output data; (2) prepare SRIM input data; (3) convert SRIM output data into SRIM input data and (4) perform special transformations of SRIM output data. The first release of the S^{3}M code has been published in [2-4] and used by several groups for different applications [5-14].This paper presents a new release of the code that contains some additional routines and advanced features of displaying the results. Special attention is paid to the processing of the SRIM range file, which was not included in the previous release of the code.

2. Basic features of the S^{3}M code

The previous version of the S^{3}M code consisted of three types of modules: a data processing module, four statistical modules and two beam transport modules. The data processing module controls the standard file operations and data handling. In addition to this, it can be used to generate a beam input file to exchange data between different files or even different codes and to save processed files as an input for sub-sequent simulations.

The four statistical modules perform statistical analysis of the energy, momentum, position and angle distributions of ions leaving the target. The original data are recorded in the SRIM TRANSMIT.TXT file. A special filtering function allows rejecting ions with large deviations from the mean value of the distribution.

The two beam transport modules link the transport of ions in matter with the transport of ion beams in vacuum. One module converts the ensemble of particles to an ion beam represented by its sigma matrix. The other module performs the transfer matrix transformation of ion coordinates as defined in ion optics. The beam transport module allows calculating the beam transport in complex systems consisting of standard ion-optical elements as well as matter-containing elements like scattering foils, stripping foils, tandem accelerators, range shifters, vacuum windows, air gaps, etc. While the action of the standard ion-optical elements is represented by the transfer matrix, the action of the matter-containing elements is treated using Monte Carlo simulations. The S^{3}M code provides an interface and data conversion between those two approaches.

3. A new release of the S^{3}M code

The new release of the S^{3}M code is presently under development. It contains several additional routines and an advanced way of displaying the results. The first code-expansion concerns the processing of the SRIM range file, the SRIM RANGE_3D.TXT file. This file is recorded by SRIM upon a user request. It contains the final positions of the ions in the target. The ions are tabulated with their longitudinal (depth), and two lateral (transverse) coordinates, the horizontal one and the vertical one.

S^3M reads the RANGE_3D.TXT file and analyses the following quantities: (1) longitudinal projected range, (2) lateral range, and (3) radial range. At the same time, conversion of the SRIM coordinate system [X, Y, Z] to the beam-transport coordinate system [X, S, Z] is performed together with the unit conversion.[*]The basic statistical analysis provides the mean value, 1σ-value and 3σ-value of the pertinent distributions. In addition to this, histograms of all distributions can be plotted in an interactive way. Figure 1 shows an example of the range distributions for 50 MeV protons "implanted" to thyroid during a thyroid-tumor irradiation.

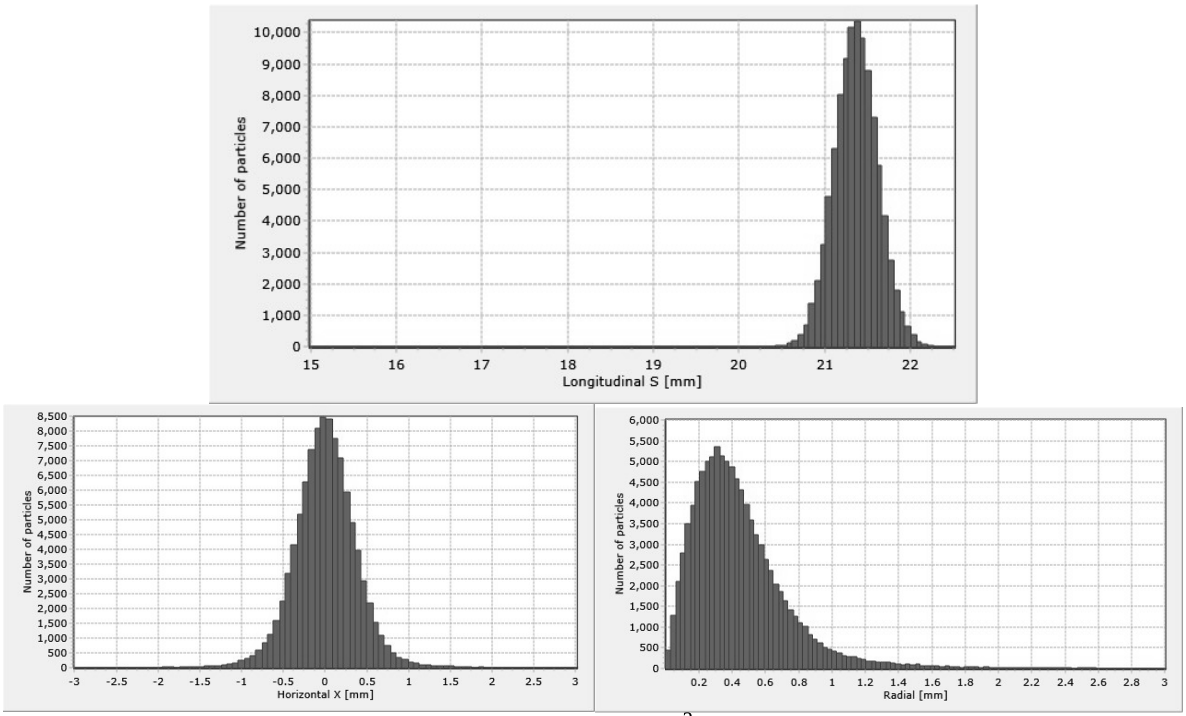

Fig.1: *Examples of distributions provided by the S^3M code for implanted ions: upper – projected range distribution, S; lower left – horizontal position distribution, X; lower right – radial range distribution, $(X^2+Z^2)^{1/2}$.*

While the projected range distribution is available also directly in SRIM, the other distributions are not. In addition to this, S^3M allows for additional manipulations with the histograms like setting a user-defined scale, resolution and logarithmic scale.

An important and new feature is also a possibility to produce correlation plots of all quantities calculated by S^3M. This possibility has been added to the code in order to investigate dispersion effects [15]. As an example, Figure 2 shows the SRIM plots of 50 MeV protons implanted into iron. There is no dispersion of the beam line in one plane, but there is some dispersion (D=0.05 m) in the other plane. The energy spread of the proton beam is 4%. It can be seen that in the plane of dispersion, a correlation between the particle range and its lateral position occurs, because the beam-line dispersion introduces correlation between the

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[*] The SRIM depth coordinate X corresponds to the beam-transport longitudinal coordinate S, the SRIM lateral coordinate Y corresponds to the beam-transport vertical coordinate Z and the SRIM lateral coordinate Z corresponds to the beam-transport horizontal coordinate X.

particle momentum and its lateral position in the beam. The particles with higher momenta are accumulated preferably on one side of the beam whereas the particles with lower momenta populate the opposite side of the beam. Particles with higher momenta have longer ranges compared to particles with lower momenta. This effect may deform implantation profiles in case of beam-transport lines that are not achromatic.

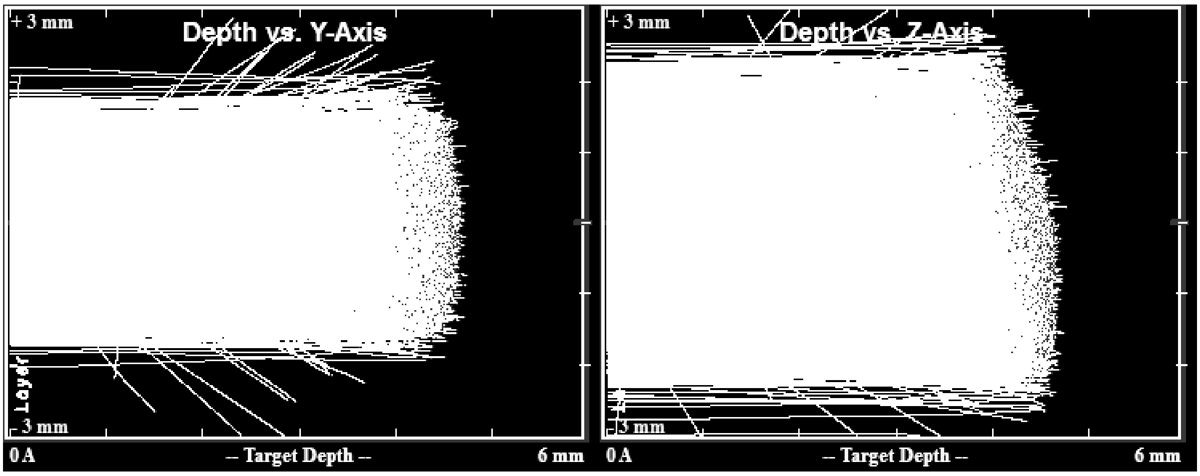

Fig.2: *Particle trajectories for 50 MeV protons in iron. Left panel – an achromatic beam line, no dispersion. Right panel – a beam line with 0.05 m dispersion; 4% energy spread.*

The corresponding correlation plots obtained from S^3M are shown in Figure 3.The particles` transverse (lateral) positions are plotted against their longitudinal (depth) positions in the target. Statistical analysis in terms of calculating correlation coefficient is included for any pair of quantities of interest.

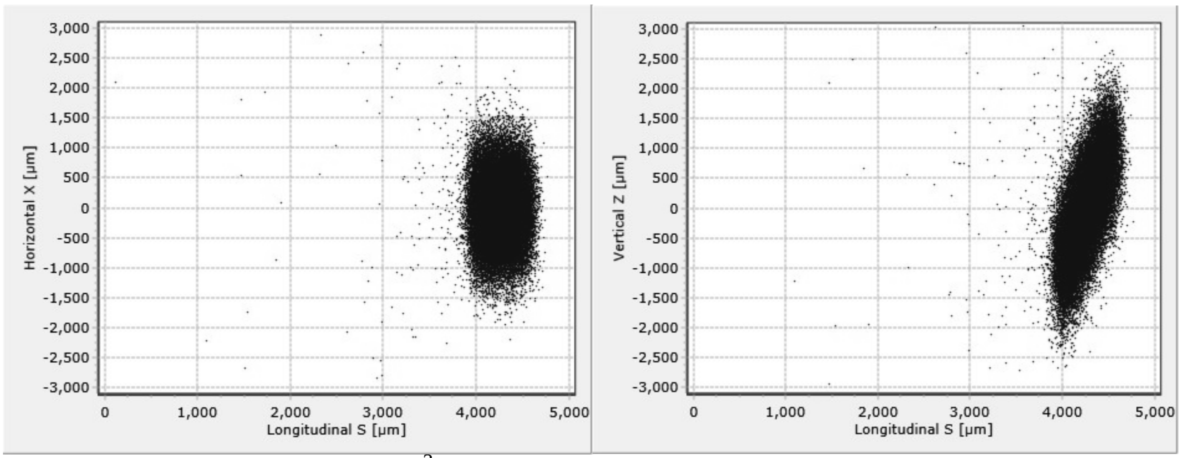

Fig.3: *Correlation plots from S^3M between the particles` transverse (lateral) positions and their longitudinal (depth) positions. Left panel – no dispersion. Right panel – a beam line with 0.05 m dispersion; 4% energy spread.*

4. Modules under development

There are several modules of the code that are still under development, namely:

- Statistical module for transmitted ions;
- Ion-optical module;
- Beam emittance module;
- Beam generation module.

All these modules are contained in the previous release of the code [2-4]. They are going to be integrated into the new programming environment and linked to the routines used in the range module presented in this paper.

The statistical module for transmitted ions is very similar to the range module. However, in case of the transmitted ions (the SRIM TRANSMIT.TXT file), there are more quantities to be calculated and analysed. Among them, the ion energy and momentum are of the biggest concern. The file of transmitted ions can also be converted back to the input TRIM.DAT file and used for subsequent SRIM calculation. The application of this strategy to particle CVD detector development has been described in Ref. [4].

The ion optical module performs the matrix transformations representing the action of ion optical elements. The particle coordinate vector is multiplied by the corresponding transfer matrix. This procedure can be repeated and the transformed files can be saved and analysed by the above described statistical tools in the same manner as the original TRANSMIT.TXT file.

Beam emittance module applies the correlation routines as described for the range file. The beam σ-matrix containing all the correlation coefficients between the terms of the particle coordinate vector can be easily generated this way.

The beam generation module generates the input TRIM.DAT for SRIM representing the real emittance pattern of the beam. It has been described in Ref. [3].

5. Results and discussion

The new release of the S^3M code reflects the experience and feedback provided by scientific community from using its previous version (which is still operational and available). New features have been added especially as far as the processing of the range file is concerned, which is the feature that was missing entirely in the previous release of the code. Manipulations with the plots became more interactive and flexible and many routines became general and universal. This applies, for example, to the correlation routines that can be now applied to any pair of the calculated quantities, not only to the beam emittance.

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