New GUI of the SATVAL code

Marcin Smolira, Juliusz Sielanko[*]

*Institute of Computer Science, Maria Curie-Skłodowska University,
pl. M.Curie-Skłodowskiej 1, 20-031 Lublin, Poland*

Abstract

In the paper we present the new version of the SATVAL code for Windows, equipped with the new graphical user interface (GUI). This graphic interface, created using the Power Builder, allows for the easiest preparation and management of data needed for the proper work of the program. The new GUI is addressed to two kinds of users: the advanced ones and the beginners.

1. Introduction

The SATVAL code was developed in the Institute of Physics of Maria Skłodowska Curie University in Lublin [1-3]. This is the Monte Carlo computer code, which may calculate the depth distribution of the ions implanted to the solid target and their kinetic phenomena associated with the ion energy loss like sputtering, cascade mixing effect and so on. The atomic cascades in the target are treated taking into account the dynamic change of composition during the target sample irradiation.

The code is permanently modified to increase its calculation possibilities of the above mentioned phenomena [4,5]. As the detailed description of the code was previously presented [1-5], only the general view of the program will be presented. The code may simulate the ion implantation phenomena, which is connected with modelling of slowing down of the energetic ions in solids. The rigorous treatment allows to obtain the depth profiles of implanted ions giving all required higher moments (*projected range Rp, standard deviation ΔRp, Skeew, Curtosis*) of the concentration distribution curve. The nuclear energy loss in a single collision is calculated from the scattering angle evaluation, the last one is obtained from the classical scattering integral for some interatomic potential. The electronic energy loss calculation method can be chosen in the code between the Lindhard-Scharff [6] and Oen-Robinson [7] models. The code

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[*]Corresponding author: *e-mail address*: jzs@tytan.umcs.lublin.pl

simulates also the sputtering effect. This phenomenon occurs when the near-surface atoms are removed from the target due to the irradiation of the target by the energetic ion beam. When a cascade of the target atoms, created by the primary ions, transfer to the target atom an energy greater than the *surface binding energy E_s* of that target, the atom may be sputtered. The E_s energy is commonly used as a heat of sublimation. The atom may be sputtered if its energy, normal to the surface, is above the surface binding energy, when it crosses the plane of the surface. The sputtering of a material is described by a s*puttering yield S*, which is defined as the mean number of sputtered target atoms per an incident ion.

The use of the code can be difficult for a person who is not accustomed to a rather complicated problem of the simulation of ion beam interaction with the solids. In many cases the user wants to know only a few basic data; such quantities as, for example, *Rp*, *S*, range distribution of implanted ions and etc. To avoid the problems with accomplishing all required input data we present a new version of the SATVAL code with the new GUI, which can simplify the use of the program as much as possible. The code is equipped now also with the option *automatic calculations*, when the user must choose only a few data related to the incident ion and the target atoms (atomic number Z, their mass M, Energy E and dose of irradiation D).

2. The new Satval for Windows

The new GUI of the Satval for Windows was created using a Power Builder language. It gives new posibilities for the interface. The Power Builder language was developed to cope with a large number of the data such as databases. To work properly, Satval needs a lot of input data, and as a result, a large number of the output data is created. The first version of the Satval for Windows allowed to change all required parameters of the simulation and these input data were saved in special files. In this case the user should know the basic theory of ion interactions with the solid surface and, in consequence, be able to cope with all parameters required to run the computer "experiment".

The new Satval for Windows offers two ways of preparing the input data: automatic and custom. The "custom" option looks like the old version of the program (Fig. 1). The user can set all parameters of the simulation, and only some simple data like atomic numbers, atomic masses and densities of the target are set automatically from the database after selection of ion names. The user should also model a composition of the target in the case when it has a binary form.

The "automatic" option simplifies significantly the use of the program. In this case all the parameters are chosen by the program automatically from the database tables as a widely used set of the parameters for the given ion-target system. Before making calculations, the user must only choose the kind of

primary ion and target atom. The target can be monoatomic or binary. When the
target is monoatomic the program needs the names of the primary ion and the
target atom. If the user chooses the option "binary" target, the program asks for
names of two components of the target, name of the primary ion and atomic
concentration of each compound. The target atomic concentration is computed
according to the fields where the relative rates of atomic concentration of the
first compound (number of the first compound atoms in the molecule) to that of
the second compound atoms should be indicated (Fig. 2 – last row of input data).
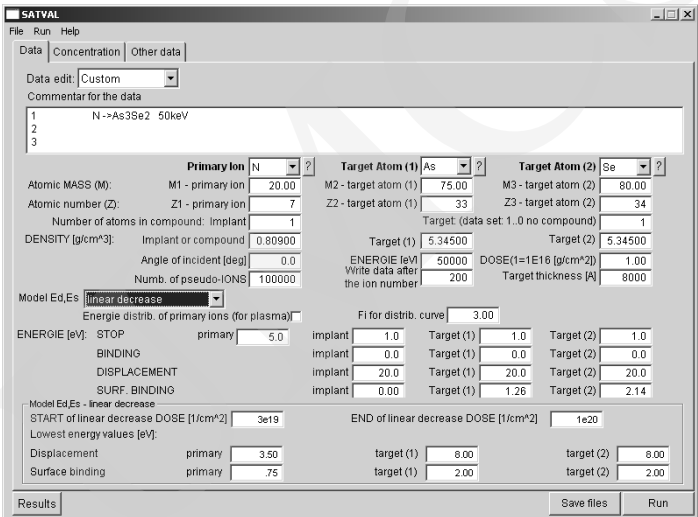Other data are set as a default.

Fig. 1. The main window of the GUI of the Satval code for advanced users

The new option of the GUI gives a possibility of monitoring simulation
results. During the program run the results of the calculations after some periods
(determined by the chosen number of counted particle) are saved automatically.
This number of particle can be set manually in the "custom" mode and should be
written to the field named "Write data after the ion number". In the "automatic"
mode the frequency of data saving depends on the number of pseudoions. The
equivalent number of particles is calculated by the program. The time of the
calculation as well as precision of calculation, is strictly related to the total
number of simulation particles, whose value can be chosen by the user (field
named "Numb.of pseudo-IONS" – see Fig. 2). Dividing the value of field
"Numb.of pseudo-IONS" by the value of "Write data after ion number" gives
the results of the number of automatically updating the satval.vip file. This file
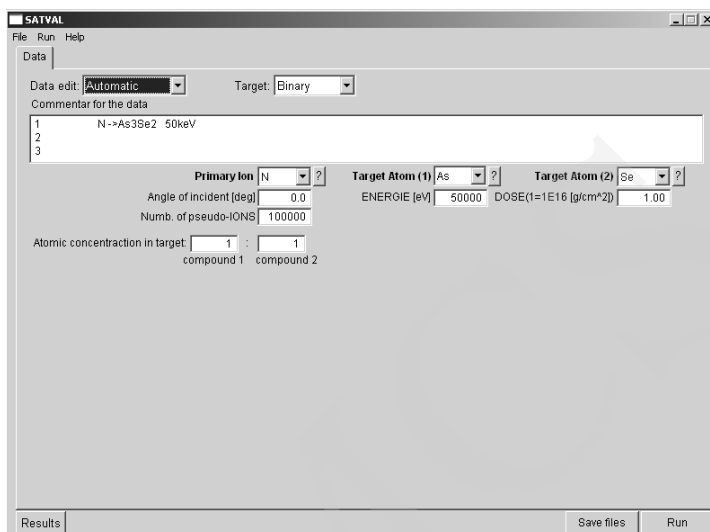contains all results of the simulation.

Fig. 2.The "data window" for the case of automatic setting of the input data

Thanks to the data visualization, the user may check the actual state of the calculations during the program run without its stopping and necessity of using the external programs (like grapher, origin) for treatment of the output data. If the input data are correct, the computing of the simulation may still work, but if from visualization of the results of the calculations it can be seen that some input data should be changed, the user can stop the program immediately and set the corrected input data. This function is especially useful for the "custom" option of the program, saves CPU time and makes use of code more easily (Fig. 3).

Using the Power Builder all data can be treated as the database. It allows the user to check the results of simulation in tables and graphs. The data are separated into five tables. Each table contains several columns. The data in each column relate to the others. This connection allows to create graphs, showing the results of calculations in a visual form. Thanks to using the database table, the user can decide, which data from the table should be used for graph creation (Fig. 4), and for watching simultaneusly the calculation results during the simulation.
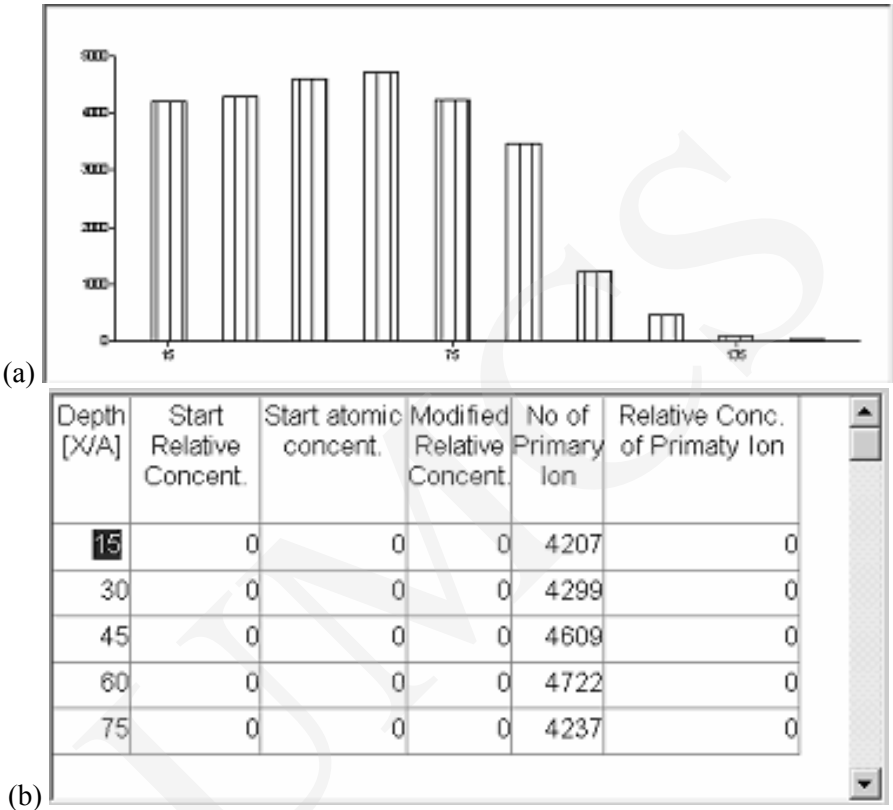
(a)

Depth [X/A]	Start Relative Concent.	Start atomic concent.	Modified Relative Concent.	No of Primary Ion	Relative Conc. of Primaty Ion
15	0	0	0	4207	0
30	0	0	0	4299	0
45	0	0	0	4609	0
60	0	0	0	4722	0
75	0	0	0	4237	0

(b)

Fig. 3. The graphic representation (3a) of the output data (*No. of Primary Ions* – 3b) calculated by the Satval code

Each table can be also exported to the external file like, for example, text file or excel datasheet etc., according to the user's decision. This function allows the user to save the computed data in the file, whose format depends on the external program he uses in further output data management (Fig. 5). Such a possibility eliminates the necessity of opening the satval.vip text file and converting the chosen part of the data to be used next in the external program such as Excel or Origin.
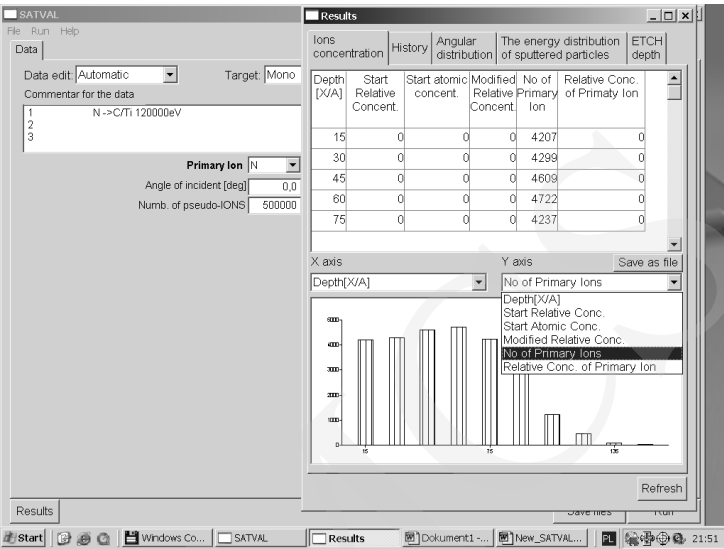
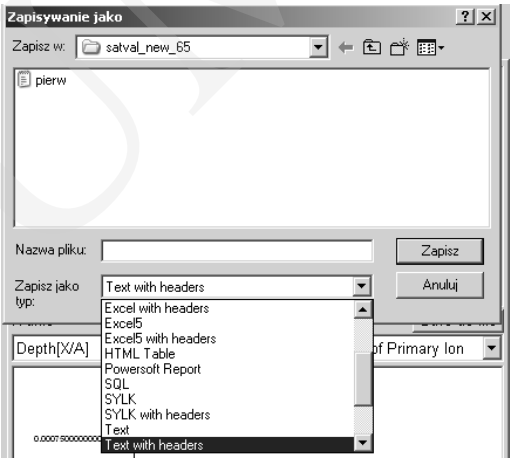Fig. 4. Choosing the data from the table, which should be used for graph creation

Fig. 5. Exporting output data to the external file

3. Conclusions

The new version of the Satval for Windows is equipped with the new graphical user interface added to the main program written in the Fortran language. The graphic interface, created using the Power Builder, allows for the easiest preparation and management of data needed for the proper work of the program. The new GUI is addressed to the kinds of users: the advanced ones and the beginners. The advanced user can set all parameters of the simulation of the experiment according to his own choice and knowledge of the phenomena of ion interaction with solids. The beginner should practically only choose the kind of

primary ions and target atoms to start the simulation, the other parameters are automatically calculated by the code. The results of simulation are displayed as tables and graphs, whose view depends only on the user. The output data can be exported to the external file with various formats. Using the new Satval for Windows is intuitive, so the user does not need a lot of time to learn how to operate the program.

References

[1] Sielanko J., Szyszko W., Surface Science, 161 (1985) 101.
[2] Sielanko J., Szyszko W., Nucl.Instr.and Meth., B16 (1986) 340.
[3] Szyszko W., Sielanko J., Phys.Stat.Sol. (A), 112 (1989) 315.
[4] Sielanko J., Hereć J., Elektronika, 7 (2001) 29.
[5] Sielanko J., Smolira M., Annales UMCS Informatica (2003).
[6] Lindhard J., Scharff M., Phys.Rev, 124 (1961) 128.
[7] Oen O.S., Robinson M.T., Nucl. Instr. and Meth., 132 (1976) 647.