

TITLE

Monte Carlo simulations of electron trajectories for samples with complex geometries

SHORT RUNNING TITLE

Simulation of electron trajectories for complex specimens

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SUMMARY

The MC-SET simulation program for electron trajectories has evolved to cater for complex specimens, easier simulation batch programming and better output data collection and analysis. This paper describes these aspects as implemented in MC-SET, and gives some results that were obtained.

INTRODUCTION

Monte Carlo simulations of electron trajectories contribute to our understanding of signal generation and imaging processes in electron beam instrumentation. To better achieve these aims the simulations must reflect current working conditions, both in terms of specimen characteristics and experimental equipment parameters.

The simulation process can be split into areas to be developed in parallel: sample definition, data input, physics of the interaction process, and data output. In addition to these it is also required that the simulation is widely available, and easy to use, reflecting a need for developing the user interface. A further consideration in the developmental process is the need for continuous improvement and changes to the simulation methods and programming methodologies.

The following table, based on Ritchie (2006) shows various characteristics of some simulation programs. To the original data in the table the last column and the last row were added, to place the MC-SET current simulation in context.

Name	Source	Bulk	Layers	GUI	Complex Samples	Spectrum Simulation	Prog	Last change
NISTMonte	Java	✓	✓		✓	✓	✓	2006
WinXRay		✓	✓	✓		✓		2006
Casino		✓	✓	✓				2002
Penelope	Fortran	✓	✓		✓	✓	✓	2006
Joy's	Basic	✓	✓	✓				?
NBSMonte	Fortran	✓	✓					?
Electron Flight Simulator		✓	✓	✓				1999
MC-SET	C++	✓	✓	✓	✓	✓	✓	2006

Table 1 - Various Monte Carlo electron trajectory simulation programs

To the above columns other characteristics could be added, such as easy of operation by "users" not involved in the program development, and speed of calculation. Of course, all the attributes have a great measure of subjectivity, and carry within each a large degree of variation between programs that possess the attribute in question.

This paper describes how developments in last three column-attributes in the above table have been implemented in a generally available Monte Carlo simulation program (Napchan 2006), that has been in continuous development and use in the past few years.

METHODS

Specimen definition and some calculation methods

The increase in computer power has allowed for the calculation to be carried out for specimens with even more complex geometries: beginning with bulk specimens, to layered materials, and finally to specimen with regions that have complex shapes. In most cases, these new complex shapes are related to actual physical specimens, but also

allow the creation of theoretical specimen conditions that might be related to yet unknown real specimens.

The following describe some of the options for defining specimens and beam conditions to be simulated in the current version of the simulation program:

1. Specimens can be composed of many elements of different compositions. Layer composition is chemically defined, and the average parameters needed for the simulation are calculated by a variety of methods.
2. Layer types can be either a slab layer or a particle layer. Both types are relatively simple to define, and allow rapid calculation of electron scattering.

Slab layers are defined by the 3D coordinates of two opposing points. In the current MC-SET the z dimension is along the layer thickness, and the x-y coordinates relate to the sample lateral extents.

A special case of a slab layer, for its composition, is a vacuum layer type, in which there are no scattering events during electron transversal: electrons enter and exit the later at the same angle, with no energy loss between these points.

A particle layer type is a 3D ellipsoid, defined by its centre point and three other dimensions along the x-y-z directions. When these dimensions are equal the particle is spherical, and when the ratio between dimensions in different directions is large it allows for elongated regions or disks to be defined.

As in real specimens, slab layers obviously can not occupy the same spatial position. Particle layers are defined without consideration to this principle, and are embedded within other slab layers. To quickly determine in which layer the beam is at every step in the simulation the following method is used: first the particle layers are checked, then the previous current layer, and finally the slab type layers.

3. The electron beam incidence point on the specimen is defined in 3D space, and can include a Gaussian distribution for the initial position of individual electrons. In addition, the beam angle of incidence can also be specified.

The physical principles used for the calculation are flexible enough to allow the use of methods based on different theories, in addition to be optimized for calculation speed. For example, elastic scattering can be simulated using Rutherford or Mott methods, and different models of random number generators can be selected. This paper does not deal with these options, apart from the specification that the simulation physics and related procedures should be modular.

Simulation results

Output from the simulation depends on the physical options selected for the particular simulation run. These can be one dimensional summary values, such as the backscattering electrons number and total energy, or two dimensional, such as various electron doses, but in the general case it will be three dimensional, and related to the defined specimen geometry.

One such output is the 3D electron beam energy distribution in the specimen. In the current simulation this consists of a 100x100x100 cubic matrix, the dimension of which is selected according to a pre-defined region of interest linked to the experimental conditions. This 3D energy matrix is used for the calculation of the 2D electron doses, by summing energy values in different differential areas. Additional information obtained from this matrix includes the total energy deposited in each layer, including the particle layer types. X-ray generation values can also be derived for each element of the energy matrix.

Individual electrons data is also processed and stored in 3D. For backscattered and transmitted electrons this includes: last trajectory point inside the specimen, exit point (allowing calculation of electron direction), energy at the exit. In addition to the exit parameters, for each backscattered electron the values of its deepest penetration point and energy in the specimen are given. Using the simulation program it is possible to further process this output data and create frequency distributions for the various output parameters.

All output values can be accessed using other analytical tools, and their format allows easy understanding of the data involved.

Batch programming and usage issues

The simulation consists basically of a point process, with a large number of electrons with basically the same starting conditions. A series of simulations in which one parameter is varied can be seen as a line-scan process: for example, simulation for a set of beam accelerating voltage, or for various beam positions along a specimen. This is one aspect of batch programming already implemented in the simulation. Any of the simulation parameters (such as beam voltage, beam tilt, beam position, etc) can be varied to yield a series of results. Most of the plot results presented in this work were produced using such batch technique for running the simulation.

A further aspect of batch programming is the further processing of large numbers of simulation results.

Two further aspect addressed in the design and implementation of the program are the relative easy user interface, that facilitates the program usage to users other than the software developers, and the coding in a high level language to allow for easier maintenance and participation of others in the development of the simulations.

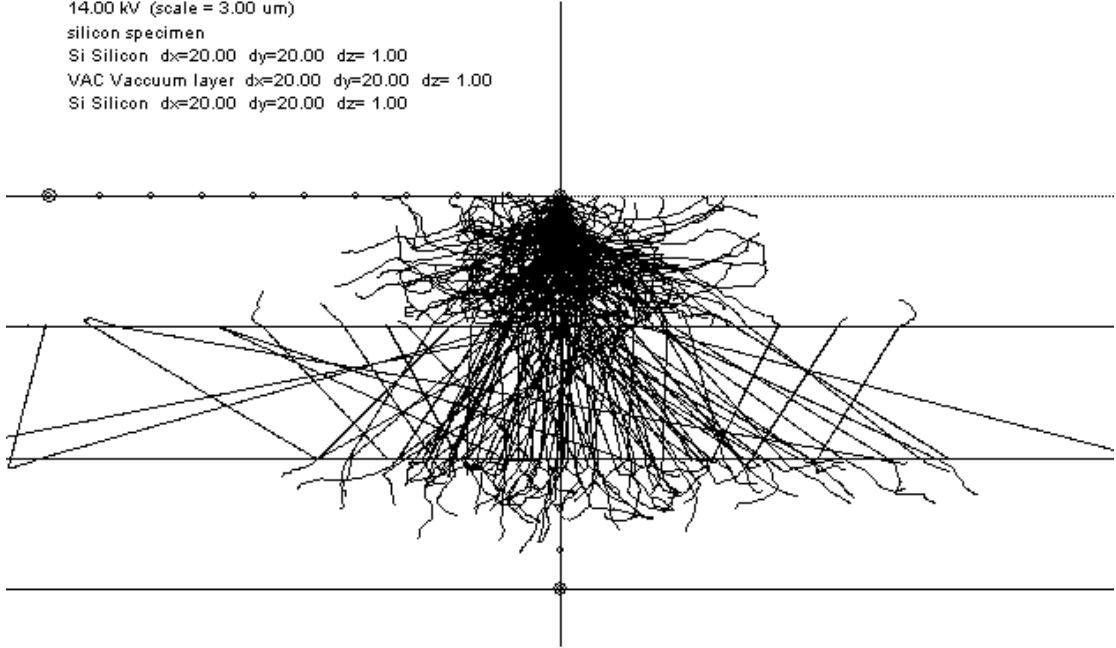
RESULTS

The second configuration includes recent developments of electron beam micro-columns and special specimen holders in which the beam passes through a window before reaching its intended destination². In this case the medium between the window itself and the device under investigation top surface could be either vacuum or non-vacuum, as in the configuration described previously

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Fig. 1(a) shows electron paths in a multi-layered specimen in which the 1 μm middle layer vacuum layer is confined between 1 μm Silicon layers. It can be seen that electrons transverse the middle layer without scattering. Fig. 1(b) shows the corresponding energy deposition as function of depth, known as the depth dose function, for this specimen: as expected, no energy is deposited in the middle layer.

Experiment description ...
14.00 kV (scale = 3.00 um)
silicon specimen
Si Silicon dx=20.00 dy=20.00 dz= 1.00
VAC Vacuum layer dx=20.00 dy=20.00 dz= 1.00
Si Silicon dx=20.00 dy=20.00 dz= 1.00



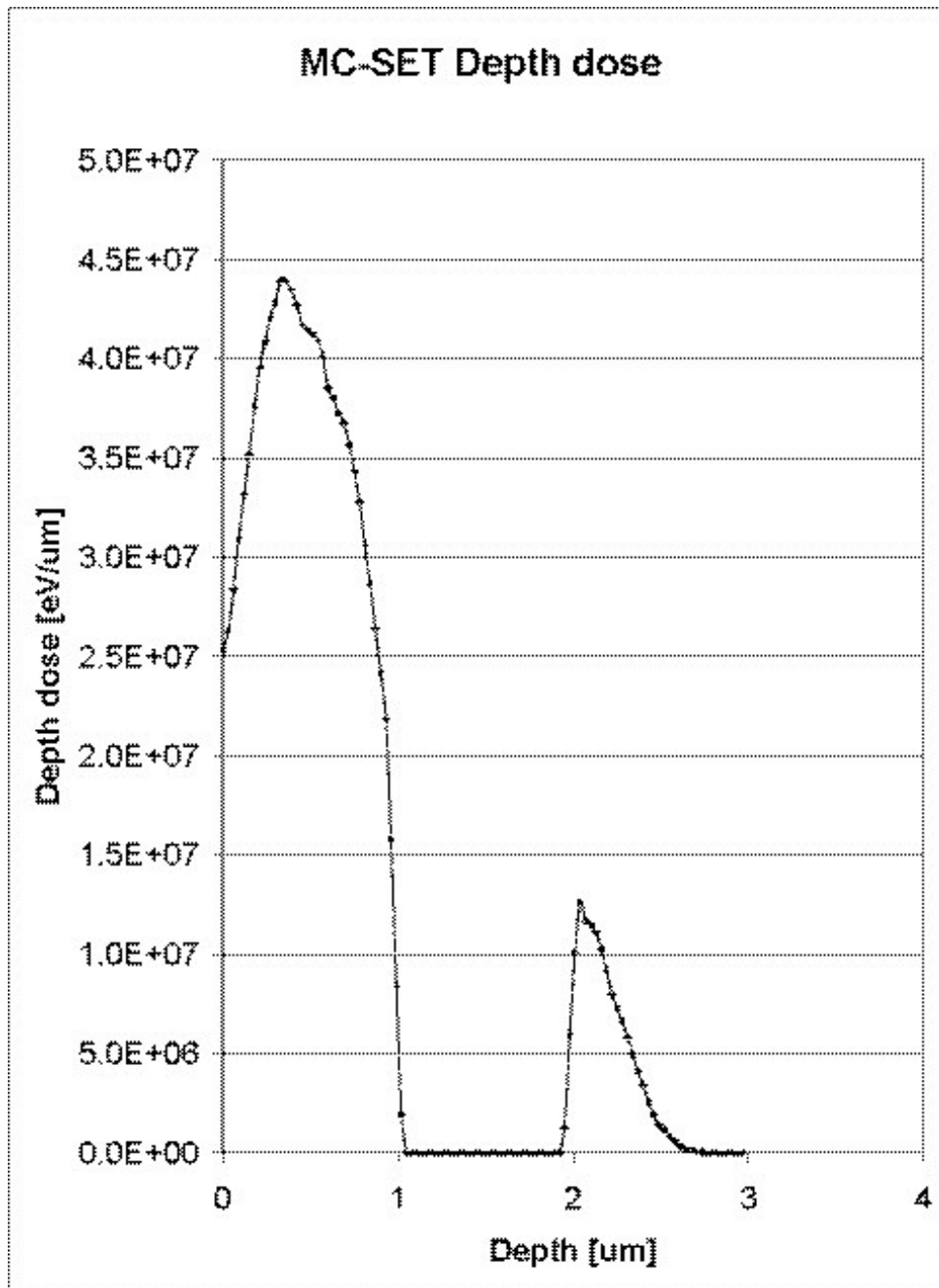


Fig. 1 - Simulation results for a multi-layered specimen consisting of a 1 um vacuum layer between two Silicon layers 1 um thick. (a) some electron trajectories; (b) depth dose function

DISCUSSION AND FUTURE WORK

Additional options for specimen and instrument definitions are under consideration and will be implemented later: porous materials, environmental SEM - which can be considered as a special case of the vacuum layer type.

ACKNOWLEDGMENTS

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