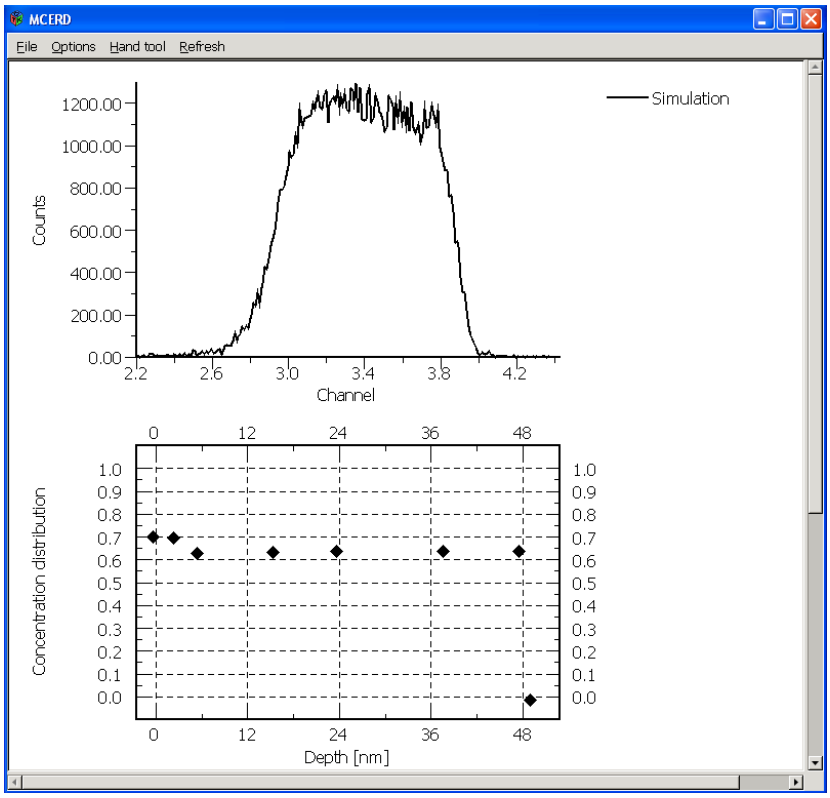
User manual for Monte Carlo simulation program: MCERD



Contents

1 Introduction

MCERD (written by Kai Arstila, 2001) is a Monte Carlo simulation program, which is used for simulations of ERD (Elastic Recoil Detection) measurements. User interface for the program was developed (Jouni Heiskanen, 2010) and this manual describes MCERD with the new easy-to-use interface. See ref. [1] which describes the MCERD code in detail.

Development of the user interface was supported by the IAEA (International Atomic Energy Agency) and user interface was the outcome of the project: 'Enhancing Nuclear Analytical Software for Monte Carlo Simulations of Heavy Ion Interactions in Materials'.

2 License and version of the program

Version: See modifications.txt about version history of MCERD. New version of MCERD can be downloaded on the web. This manual describes version 17122010 of MCERD.

License: See COPYING.txt

MCERD website:
<https://www.jyu.fi/fysiikka/en/research/accelerator/abasedmat/software/>

Note: You should have received modifications.txt and COPYING.txt when downloading MCERD.

3 Installation

This section describes how to install MCERD. MCERD includes already compiled binaries for Windows and Linux but if you wan't to compile MCERD yourself, see README.txt.

3.1 Installation instructions

MCERD uses GTK+ and GtkExtra libraries. You should have GTK+ (version 2.x) installed on your computer before running MCERD. GtkExtra (version 2.1.1) is included in the MCERD packet. In Linux you should have GTK+ installed already. You can check if GTK+ 2.x is installed on your system by typing:
pkg-config --modversion gtk+-2.0
it gives the version of your GTK+ if GTK+ 2.x is installed on your system.

3.1.1 Installing GTK+ on Windows

- Download GTK+ from <http://www.gtk.org/download.html>, select all-in-one bundle (e.g. version 2.16).
- Extract downloaded packet for example to C:\gtk.
- Add bin folder of the gtk (e.g. C:\gtk\bin) to Windows PATH environment variable. You can do this (in Windows XP) 'Control Panel' -> 'System' -> 'Advanced' -> 'Environment Variables'. Edit PATH (under 'System Variables'), and add the location of gtk bin folder to PATH.

3.1.2 Running MCERD

Download MCERD packet (zip or tar.gz) and extract it for example to C:\MCERD or /home/MCERD. Run MCERD binary located in MCERD folder (mcerd.exe in Windows and ./mcerd in Linux) to run the program.

Important: Use periods for decimal points in your system. You can set this (in Windows XP) 'Control Panel' -> 'Regional Settings'. Set your Regional Settings to 'English (United States)', then it should show a period for the 'Decimal Symbol'.

Important: If you get 'segmentation fault' error when running MCERD, check your stacksize limit. In Linux use command 'ulimit -s unlimited' before running the program. In Windows stacksize is reserved already during the compilation.

Note 1: Binaries in the MCERD packet are compiled using Windows XP (32-bit) and Linux (64-bit).

Note 2: If MCERD binary won't work in your architecture, try to compile it yourself. See README.txt in MCERD folder.

Note 3: Launch MCERD using command line, because some information during the simulation is printed in command line.

3.1.3 Problems with GtkExtra

GtkExtra library is included in MCERD packet. Packet includes libraries compiled using Windows XP (32-bit) and Linux (64-bit). If compiled library won't work in your architecture try to compile GtkExtra yourself:

- Download GtkExtra (version 2.1.1) from <http://gtkextra.sourceforge.net/>.
- Extract downloaded packet and run configure and makefile for getting GtkExtra library. Installation instructions comes with the GtkExtra packet.
- Copy this compiled GtkExtra library (e.g. libgtkextra-x11-2.0.a) to MCERD src folder and change variable 'gtkextralib' in makefile (winmake_mcerd.bat for Windows and Makefile for Linux) accordingly.
- Compile MCERD. See README.txt how to compile.

3.2 Files in the packet

You should have these files after extracting the MCERD packet:

MCERD folder:

- COPYING.txt and license.txt for license information
- default parameter files (default.dat.*)
- generate_sptables.exe for generating SRIM stopping powers (for Windows only)
- linuxmake script for compiling MCERD binary for Linux
- mcerd binaries for Windows and Linux
- modifications.txt for version history
- README.txt for compiling instructions
- SRModule.exe, SCOEF03.dat, SNUC03.dat used for generating SRIM stopping powers
- winmake.bat for compiling mcerd binary for Windows

MCERD\data folder:

- scoef.95a and scoef.95b coefficient tables for zbl96 stopping powers
- masses.dat file for isotope masses

MCERD\simulations folder:

- example simulations

MCERD\src folder:

- all source files
- makefiles for compiling MCERD (Windows and Linux)
- GtkExtra libraries for Windows and Linux

MCERD\src\gtkextra folder:

- GtkExtra source files and libraries

MCERD\src\zbl96-0.99a folder:

- zbl96 source files
- makefiles for compiling zbl96 (Windows and Linux)

MCERD\SRIM_documents folder:

- license and help file for SRIM (SRModule)

MCERD\stopping_data folder:

- generated SRIM stopping data

3.3 SRIM stopping powers

MCERD packet includes SRModule generated SRIM stopping power data [3] (in stopping_data folder) which includes stopping powers for all ion target combinations $Z \leq 83$ (generated by generate_sptables binary). You can generate stopping power data by running generate_sptables binary.

Note 1: SRIM stopping power data has to be in stopping_data folder located in the same folder with MCERD binary.

Note 2: SRIM stopping power data can be generated only in Windows.

Note 3: It takes approximately 30 minutes to generate SRIM stopping power data.

4 General information

4.1 Random number generator

Program uses Mersenne Twister pseudorandom number generator. Mersenne Twister provides a fast generation of high quality random numbers. Seed number is used for initializing Mersenne Twister, and same simulation can be repeated with the same seed number.

See <http://www.math.sci.hiroshima-u.ac.jp/~m-mat/MT/emt.html> for more information about Mersenne Twister.

4.2 Enhancements in the code for faster computing

Monte Carlo simulations are time consuming when simulating ERD measurements, and in MCERD a faster computing by means of enhancements in the code has been achieved. Code has following enhancements:

- Concept of virtual detector for increasing the probability for a detection of a recoil.
- Restriction of the solid angle of the recoils with presimulation procedure.
- Parameter for increasing the probability for a production of a recoil.
- Concept of statistical weights for recoils.

These enhancements are described more detail in ref. [1].

4.3 Thickness and densities for layers

Calculations of ion trajectories in MCERD are made in 'real' coordinates and that's why nanometres are used for thicknesses instead of atoms/cm^2. From that reason density for each layer has to be given.

4.4 Correct form for element names

When specifying layer elements, ion beam or recoil atom you have to give the name of the element, for example H or Si. For ion beam and recoil atom, you can use a specific isotope for giving also mass number of the element, for example 1H or 35Cl.

Note 1: There is a difference between lowercase and uppercase letters.

Note 2: For ion beam and recoil atom you have to use a specific isotope for unstable elements.

Note 3: Elements $Z \leq 102$ (No) can be used, see masses.dat for more accurate data which elements or isotopes can be used in simulations. SRIM stopping powers are limited only for $Z \leq 83$ (Bi). See 'Installation->SRIM stopping powers' for more information.

4.5 Stopping powers

Stopping powers for each layers (ion and recoil) is needed. Type ZBL when using ZBL values [2], type SRIM when using SRIM values [3] or you can give the name of the file if you wan't to use some other values for stopping powers.

4.5.1 ZBL

If you type ZBL, MCERD uses stopping powers from zbl96 program. Zbl96 is a program for calculating electronic and nuclear stopping powers according to the semiempirical model of Ziegler, Biersack and Littmark [2]. Zbl96 program is based on the version 96 of SRIM-code. Zbl96 comes with the MCERD.

4.5.2 SRIM

If you type SRIM, MCERD uses SRModule generated stopping powers. SRModule is a part of the SRIM and it generates SRIM stopping powers [3]. See 'Installation->SRIM stopping powers' for more information.

4.5.3 User defined values

You can give the name of the file (or path of the file if the file is in different folder than the program) which contains stopping powers for the ion in the specific layer for different velocities. Data points in the file has to be in correct format: Bohr velocity and stopping power (keV/nm).

Note 1: Use constant spacing velocities for data points.

Note 2: Give enough data points or the simulation is very slow (spacing of 100 000 m/s is recommended).

5 Using MCERD

5.1 File formats

Here all MCERD parameter and output files are explained. fname is the example for used filename.

File format for MCERD parameters is *.mcerd. For reading and saving parameters fname.mcerd is used, which contains all parameter files:

- fname.mcerd: main parameter file, simulation parameters
- fname.mcerd.det: detector parameters
- fname.mcerd.foil: detector foil parameters
- fname.mcerd.targ: target layers parameters
- fname.mcerd.rec: recoil material distribution parameters
- fname.mcerd.pre: presimulation parameters
- fname.mcerd.espe: energy spectrum parameters

File format for output files is *.mcerd.seednumber, after simulation MCERD generates output files which names are determined from used filename and seednumber:

- fname.mcerd.seednumber.erd: recoil data from main simulation
- fname.mcerd.seednumber.spe: energy spectrum data (channel, counts)
- fname.mcerd.seednumber.dist: distribution data (depth, concentration)
- fname.mcerd.seednumber.out: scattering table data
- fname.mcerd.seednumber.dat: general data from simulation
- fname.mcerd.seednumber.pre: calculated presimulation values
- fname.mcerd.seednumber.range: range or transmission data

5.2 Basic steps

These steps describes shortly how simulation is made in MCERD. All options and parameters are described more detail in this manual.

1. Adjust all parameters (detector, detector foils, target layers, recoil material distribution, presimulation and simulation parameters). See the description of each parameter in this manual.

2. Before running the simulation save for example to example_folder\ example_simulation.mcerd. After simulation example_folder includes all the parameter files and generated output files related to the specific simulation. See 'Using MCERD->File formats' for more information about parameter files and generated output files.

Note 1: Don't change file names or move/remove files afterwards if you wan't to modify simulated energy spectrum later.

Note 2: Save new simulation to new folder so there is no risk for overwriting already simulated data.

3. Run simulation

4. After simulation energy spectrum is generated. Recoil material distribution determined before the simulation is used for concentration distribution.

5. You can generate new energy spectrum by changing concentration distribution (in graph) and energy spectrum parameters.

6. You can open an experimental energy spectrum in the same graph with simulated energy spectrum for comparison.

7. Simulated energy spectrum data is automatically saved to *.spe file (channel vs counts) and concentration distribution data is automatically saved to *.dist file (depth vs concentration) every time when you generate a new energy spectrum.

8. You can open a simulated spectrum later for the new modification.

5.3 File menu

Here file handling (reading/saving) is described. fname is the example for used filename.

- **Open:** You can read all parameters from fname.mcerd file, it reads all parameter files relating to this file (fname.mcerd.*).
- **Read simulated data:** You can open a simulated spectrum (*.spe file). Program also reads parameters relating to the specific spectrum if the parameter files are in the same folder with spectrum file. Note that you can make changes to spectrum (change concentration distribution or energy spectrum parameters) only when the simulated data file (*.erd) is in the same folder with the spectrum file (*.spe).
- **Save/Save as:** Save parameters in the format *.mcerd. Before running the simulation, save with the different file name or use different seed number, if you don't want to overwrite an existing output files.

  Note 1: See 'Using MCERD->File formats' for more information about parameter files and generated output files.

  Note 2: Don't change file names or move/remove files afterwards if you wan't to modify simulated energy spectrum later.

  Note 3: Save new simulation to new folder so there is no risk for overwriting already simulated data.

5.4 MCERD parameters

5.4.1 Detector parameters

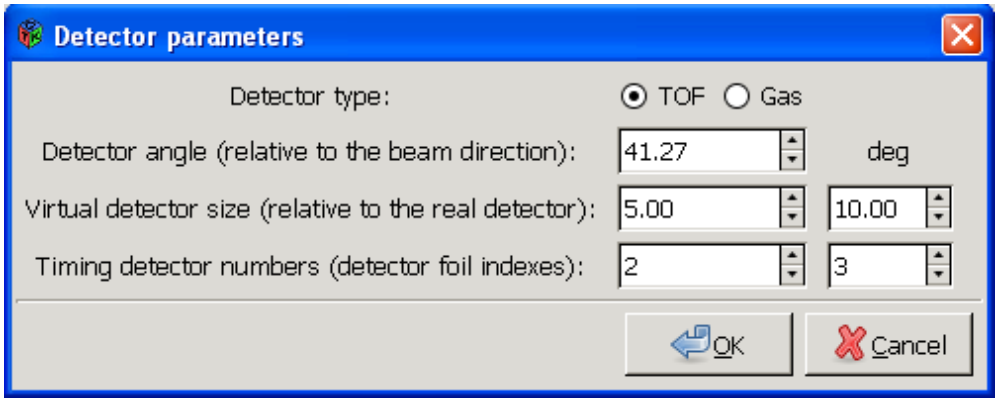


Figure 1: Detector parameters window.

- **Detector type:** Select time-of-flight (TOF), or gas detector.

Note 1: Different detector type needs different parameters.

Note 2: When you use gas detector, select energy resolution from energy spectrum parameters or you may get weird results.

- **Detector angle:** Detector angle relative to the ion beam $[0 - 360°]$.

  Note: Angle is measured between the ion beam and the surface normal of detector.

- **Virtual detector size:** Virtual detector size (width and height) relative to the real detector.

  Note 1: See: 'General information->Enhancements in the code for faster computing'.

  Note 2: Typical size of the virtual detector is five times as wide and ten times as high as the real detector.

  Note 3: Give values ≤ 1 for width and height if virtual detector is not used.

  Note 4: If you use virtual detector in the simulation, you can still choose whether to use virtual detector or not after simulation.

- **Timing detector numbers:** Select timing foils for detector. Give detector foil indexes which are used for timing foils.

  Note 1: Timing detector numbers are used only when TOF detector is selected.

  Note 2: Give indexes so that first number indicates the nearest foil from target.

  Example: If you have specified three detector foils so that there is filter before timing foils, use indexes 2 and 3 for timing foils (1 indicates the filter).

5.4.2 Detector foils

You can add or remove foils at the back of the other foils and you can add elements for each foil. Different foils are marked by foil tabs and you can choose different foil by clicking the tab. When specifying foils note that the leftmost tab corresponds to first foil (nearest from the target) and foils have to be in order with respect to their distances from the target.

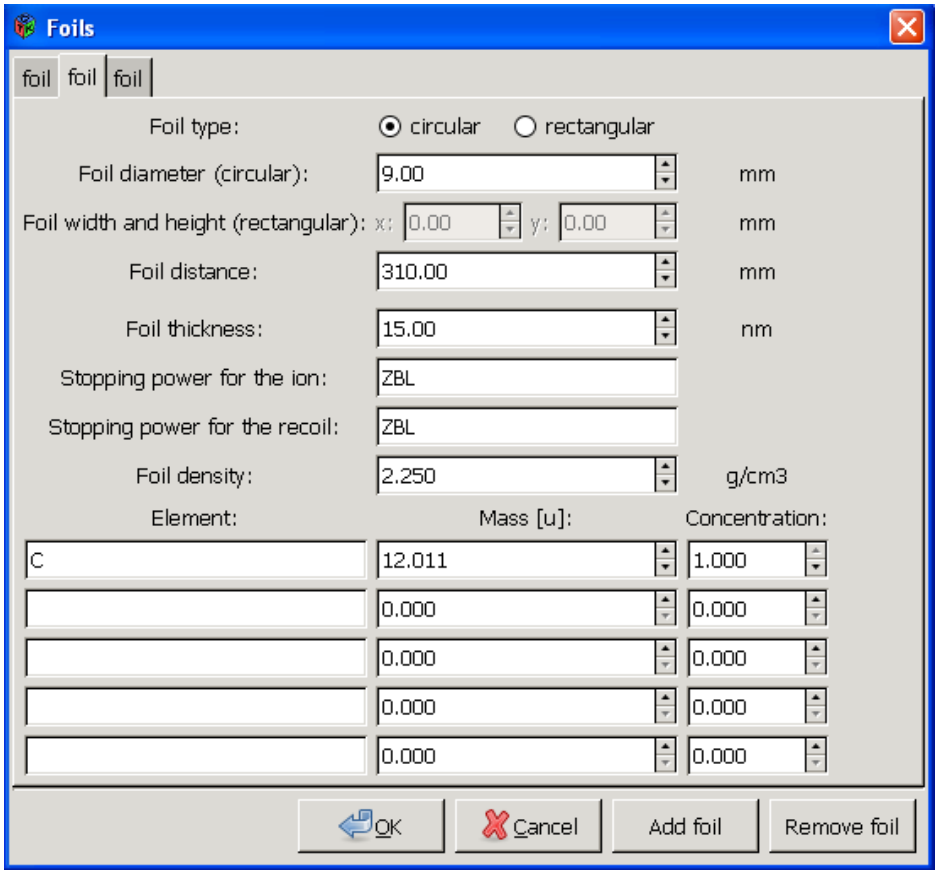


Figure 2: Detector foils window. Selected foil tab in the figure describes the first timing foil.

- **Foil type:** Select circular or rectangular foil.
- **Foil diameter:** Size of the foil in mm. Diameter for circular, width and height for rectangular.
- **Foil distance:** Foil distance from the target center in mm.

  Note: Foils have to be in order with respect to their distances (leftmost tab corresponds the nearest foil and rightmost tab corresponds the outermost foil from the target).
- **Foil thickness:** Foil thickness in nm.
- **Stopping powers:** Stopping powers for ion and recoil. Type ZBL or SRIM if you wan't to use ZBL or SRIM values for stopping powers. For user defined values give the name of the file where stopping powers will be read.

Note: See: 'General information->Stopping powers'.

- **Foil density** Foil density in g/cm^3.
- **Element table:** Specify what elements foil consists, and give masses in u and concentrations in at.%/100 for all elements.

  Note 1: See: 'General information->Correct form for element names'.

  Note 2: Concentrations need not to sum to 1, normalization is made automatically.

5.4.3 Target layers

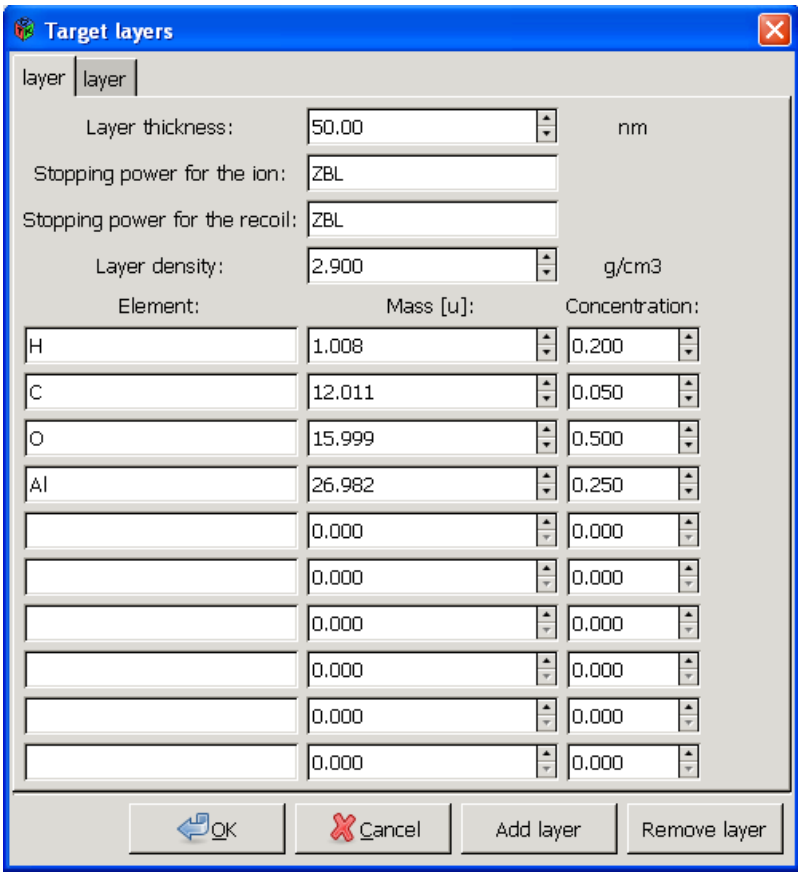


Figure 3: Target layers window. Selected layer tab in the figure describes the top layer of the target.

You can add or remove layers at the back of the other layers and you can add elements for each layers. Different layers are marked by layer tabs

and you can choose different layer by clicking the tab. When specifying layers note that the leftmost tab corresponds to top layer of the target.

- **Layer thickness:** Layer thickness in nm.

  Note: Give negative value if you wan't to use bulk thickness (for example for substrate).

- **Stopping powers:** Stopping powers for ion and recoil. Type ZBL or SRIM if you wan't to use ZBL or SRIM values for stopping powers. For user defined values give the name of the file where stopping powers will be read.

  Note: See: 'General information->Stopping powers'.

- **Layer density:** Layer density in g/cm^3.

- **Element table:** Specify what elements layer consists, and give masses in u and concentrations in at.%/100 for all elements.

  Note 1: See: 'General information->Correct form for element names'.

  Note 2: Concentrations need not to sum to 1, normalization is made automatically.

5.4.4 Recoil material distribution

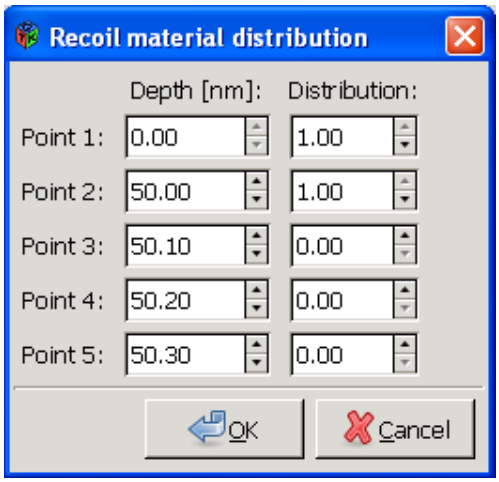


Figure 4: Recoil material distribution window. Here recoils are limited in the range: 0–50 nm.

Give data points for recoil material distribution (depth [nm] and distribution). With this distribution you can limit to certain depth in the target.

Note 1: Some values is needed for all points, and depth values must be in the order of magnitude (depth for point[i+1] > depth for point[i]).

Note 2: For getting the correct absolute concentrations, distribution has to be > 0 in the range of 0–10 nm.

Note 3: Concentration distribution graph is scaled using minimum and maximum depth values.

Note 4: See fig. 4 for example of used recoil material distribution.

5.4.5 Pre simulation parameters

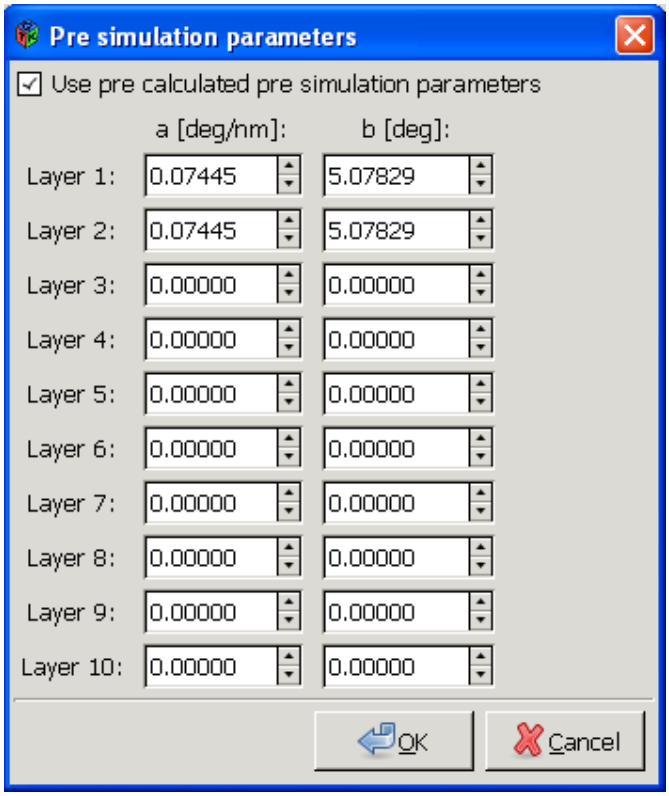


Figure 5: Pre simulation parameters window. Here pre calculated values for two target layers are used.

Here you can give linear fit parameters (half-angle vs. depth). If you tick 'use pre calculated pre simulation parameters', give recoiling solid angle fitted parameters (a [deg/nm] and b [deg]) for each target layers. Otherwise pre simulation parameters are calculated during the simulation (default).

Note 1: See: 'General information->Enhancements in the code for faster computing'.

Note 2: Pre simulation is made only when narrow simulation mode is selected (in recoil angle width).

Note 3: If pre simulation parameters are calculated during the simulation (default), these values are printed in the file: fname.mcerd.seednumber.pre

5.4.6 Simulation parameters

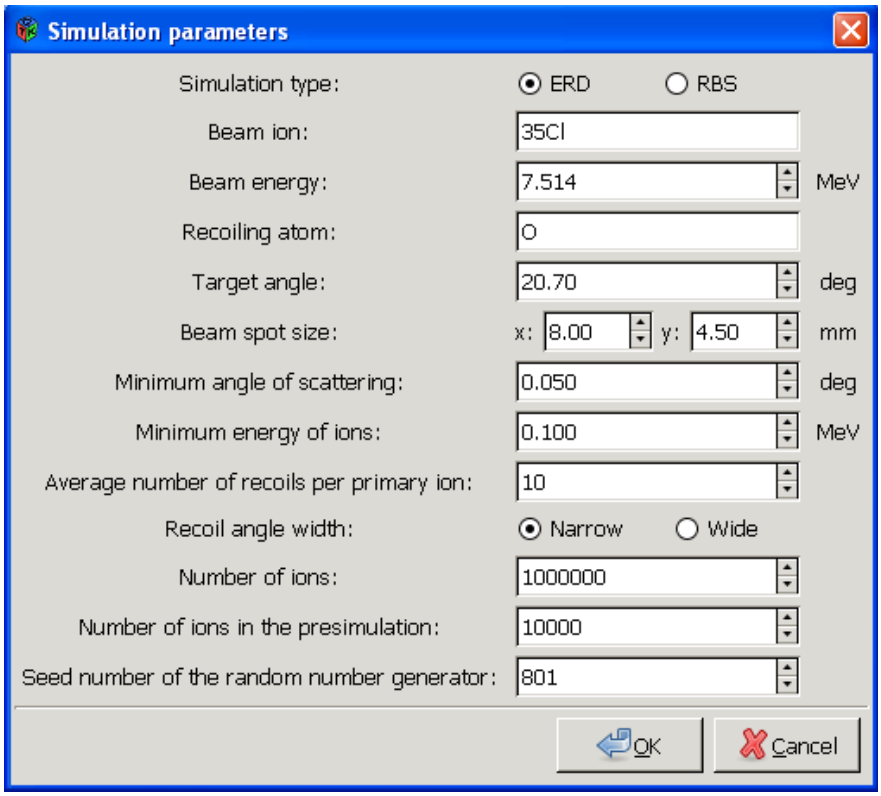


Figure 6: Simulation parameters window.

- **Simulation type:** Select ERD when detecting recoils from target and RBS when detecting primary ions.
- **Beam ion:** Element for ion beam.

  Note 1: See: 'General information->Correct form for element names'.

  Note 2: If you give only the name of the element, most abundant isotope is used.
- **Beam energy:** Beam energy in MeV.
- **Recoiling atom:** Give recoil atom when ERD is selected and atom where primary ions are recoiled from when RBS is selected.

  Note 1: See: 'General information->Correct form for element names'.

  Note 2: If you give only the name of the element, abundance of different isotopes is taken into account.
- **Target angle:** Target angle between the target and ion beam $[0 - 90°]$.

  Note: Angle is measured between the ion beam and the surface of the target.
- **Beam spot size:** Size of the beam spot (width and height) in mm.
- **Minimum angle of scattering:** Minimum angle of scattering in degrees. This gives mean path length for the simulation.

  Note: Typical value is $0{,}05°$ which yields a typical mean path length of a few nanometers.
- **Minimum energy of ions:** Minimum energy of ions in MeV.
- **Average number of recoils per primary ion:** The probability for a production of a recoiling atom can be increased when each ion produces several recoils.

  Note 1: See: 'General information->Enhancements in the code for faster computing'.

  Note 2: Typical value is 10.
- **Recoil angle width:** Select narrow (default) or wide simulation mode. With narrow simulation mode pre simulation procedure is used.

  Note 1: See: 'General information->Enhancements in the code for faster computing'.

Note 2: Simulation takes much longer with wide simulation mode than with the narrow simulation mode.

- **Number of ions:** Number of ions in the simulation.
- **Number of ions in the pre simulation:** Number of ions in the pre simulation when narrow simulation mode is selected.

  Note: Typically 10 000 ions is enough for pre simulation.
- **Seed number of the random number generator:** Seed number for the random number generator. This value is used for initializing the random number generator.

  Note 1: See: 'General information->Random number generator'.

  Note 2: Seed number is used in the output filenames, see 'Using MCERD->File formats'.

5.4.7 Energy spectrum parameters

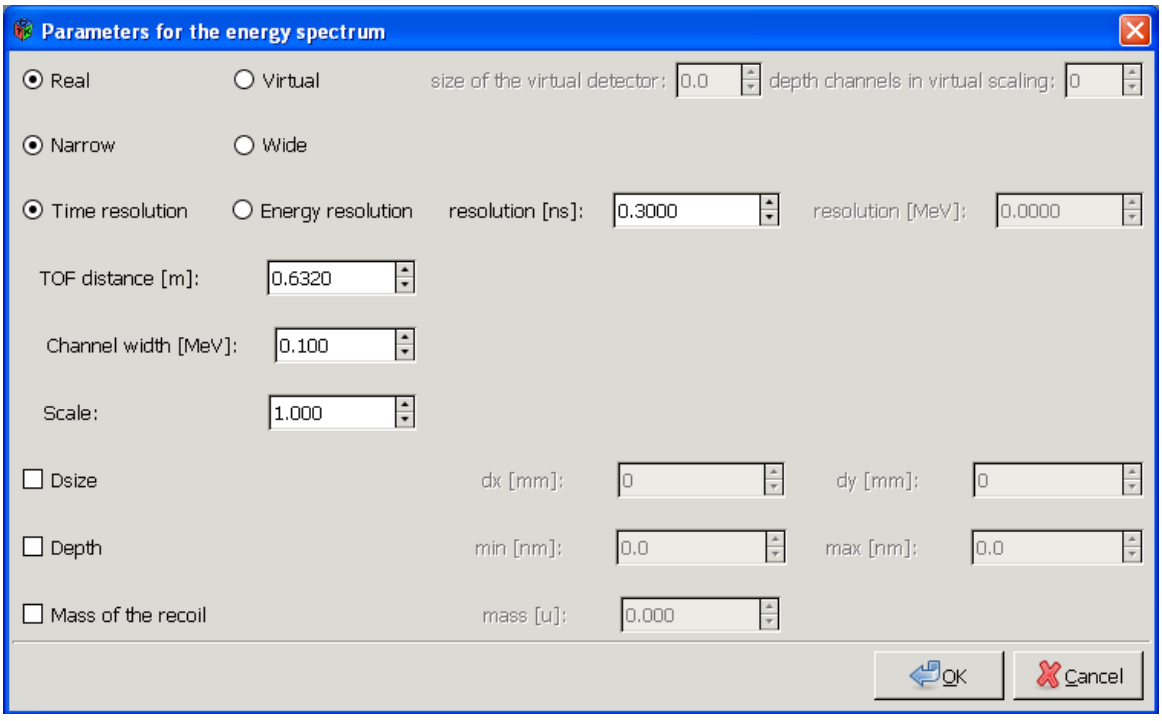


Figure 7: Energy spectrum parameters window.

These parameters affects only to energy spectrum (when generating energy spectrum from *.erd data file), so these parameters can be changed also after the simulation.

- **Real/virtual detector:** Select real (default) or virtual detector. If you select real detector, virtual detector is not used. Give scaling factor for virtual detector size and number of depth channels in virtual scaling when virtual detector is selected.

  Note 1: See: 'General information->Enhancements in the code for faster computing' for more information about virtual detector.

  Note 2: If you didn't use virtual detector in the simulation, selection of virtual detector has no effect.

- **Narrow/wide mode:** Select narrow (default) or wide mode. If you select real detector, virtual detector data points can be taken into account as a 'real' data points by selecting wide mode.

  Note: Wide mode has effect only when virtual detector is used in simulation and real detector is selected in energy spectrum parameters.

- **Time/energy resolution:** Select time or energy resolution and give resolution in ns or MeV.

  Note 1: For gas detector use only energy resolution.

  Note 2: When time resolution is used, recoil energies are calculated from the time signal.

- **TOF distance:** Time-of-flight length in m. Give distance between the timing foils.

  Note 1: TOF distance has to be the same with the timing foils distance (used in the simulation) or you may get weird results.

  Note 2: TOF distance is used only when time resolution is selected (for TOF detector).

- **Channel width:** Channel width for energy spectrum in MeV.

- **Scale:** Scale for energy spectrum.

- **Dsize:** Select this if you wan't to limit the detector size. Give dx and dy in mm.

- **Depth:** Select this if you wan't to limit the depth for recoils. Give minimum and maximum depth in nm.
- **Mass:** Select this if you want to use other value for recoils mass than what is used in the simulation. Give mass for recoils in u.

  Note: This mass value is used only for calculating recoil energies when time resolution is selected (for TOF detector).

5.5 Running simulation

Save before running the simulation. All the output files are generated in that folder where did you save, and output file names are determined from used filename and seednumber. See 'Using MCERD->File formats' for more information about the files. If you save new simulation to the new folder there is no risk for overwriting already simulated data. Run simulation by clicking 'Simulation' -> 'Run'. When simulation is ready output files are generated and energy spectrum/concentration distribution window will open.

5.6 Energy spectrum/concentration distribution window

This window includes energy spectrum and concentration distribution graph for simulated element, see fig. 8. Here you can generate new energy spectrum by changing concentration distribution and energy spectrum parameters. Experimental data can be also read in the same graph with the simulated data for comparison.

5.6.1 Energy spectrum

In energy spectrum counts with respect to energy channels for recoils is shown. By default one channel corresponds to one MeV energy. Energy spectrum is automatically scaled by using minimum and maximum values for energy, and maximum value for counts. Zooming can be made using a zoom tool by selecting 'Hand tool' -> 'Select Tool' -> 'Zoom'. You can read

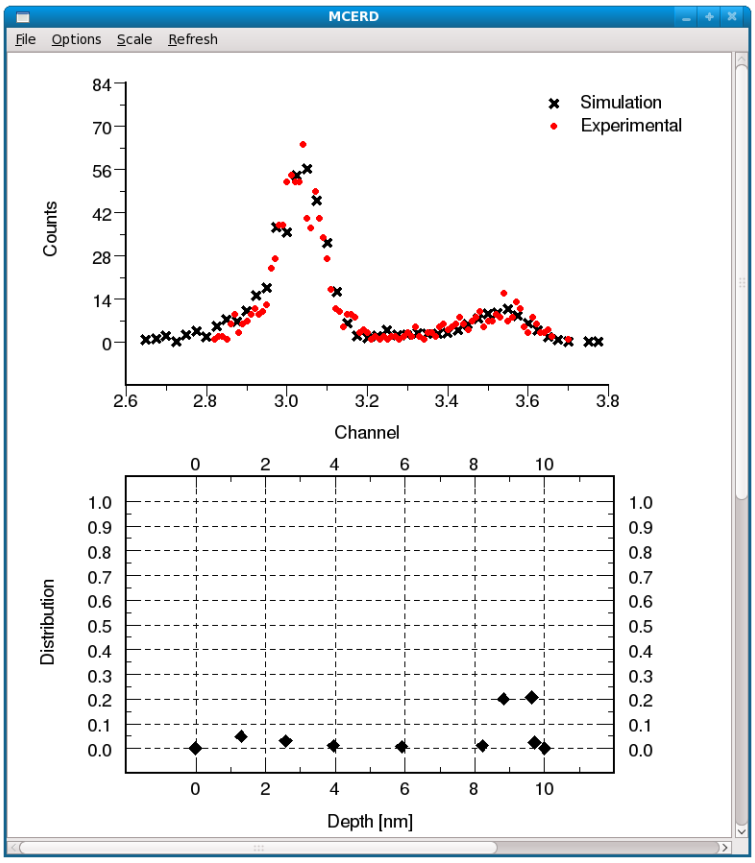


Figure 8: Simulated and experimental energy spectrum (above) and concentration distribution (below) for oxygen (C_xN_{1-x} target and 7,5 MeV ^{35}Cl ion beam).

experimental data in the same graph with the simulated energy spectrum in 'File' -> 'Read experimental data'.

5.6.2 Concentration distribution

In concentration distribution graph concentration (at.%/100) of the simulated element with respect to depth of the target (nm) is shown. After simulation recoil material distribution points is used for concentration distribution, and minimum and maximum depth values of these points is used for scaling the graph. Recoil material distribution is given before the simulation.

You can move distribution points by selecting 'Hand tool' -> 'Select tool'

-> 'Selection'. Drag and drop method is used for moving these points. Data points are automatically limited so that concentration is always [0,1] and depth [0,dmax], where dmax is the maximum depth given in recoil material distribution. Concentration distribution is interpolated from the given distribution points. Number of distribution points can be changed in 'Options' -> 'Number of distribution points'.

5.6.3 Experimental data

- **Read experimental data:** You can read experimental data in the same graph with the simulated data.

  Note 1: Data has to be in the format: channel vs. counts.

  Note 2: Scale (keV/channel) for experimental data is needed.

- **Remove experimental data:** You can remove experimental data.

5.6.4 Options

- **Energy spectrum parameters:** These can be changed before and after the simulation. See: 'Using MCERD->MCERD parameters->Energy spectrum parameters'.

- **Number of distribution points:** You can change the number of distribution points.

  Note 1: You loose 'active' distribution data when changing the number of distribution points.

  Note 2: New distribution points are drawn using constant spacing.

- **Export graph:** You can export energy spectrum or energy spectrum and distribution graph in the format *.ps

5.6.5 Zooming and data selection (Hand tool)

Choose a hand tool for zooming or moving distribution data points in 'Hand tool' -> 'Select tool' ->.

- **Normal:** You can move or resize graphs.
- **Selection:** You can move data points in concentration distribution graph.

  Note: Data points are automatically limited between certain depth and distribution limits.
- **Zoom:** You can zoom in energy spectrum graph by selecting the area.

  Note: When zooming, scaling for y-axis (counts) is made automatically so that data points won't be lost. So you can limit only the x-axis (energy) of the energy spectrum when zooming.
- **Hand tool -> Unzoom:** Zooming to original size.

5.6.6 Generating new energy spectrum (Refresh)

Every time when you generate a new spectrum ('Refresh' -> 'Refresh spectrum') following is done:

- Energy spectrum is generated from the data file (*.erd) using concentration distribution and energy spectrum parameters.
- Energy spectrum is generated to spectrum file (*.spe).
- Concentration distribution points are saved to distribution file (*.dist).

5.6.7 Saving

Here saving after the simulation is explained. fname is the example for used filename.

You can save all parameters in 'File' -> 'Save'. Energy spectrum and concentration data is automatically saved every time when you generate a new energy spectrum ('Refresh spectrum'). Energy spectrum data is saved to fname.mcerd.seednumber.spe and distribution data to fname.mcerd.seednumber.dist. See: 'Using MCERD->File formats' for more information about generated output files.

Note 1: 'File' -> 'Save' will save only used parameters, not spectrum or distribution data.

Note 2: Use the same filename (fname.mcerd) what you used for simulation.

5.7 How to use MCERD for getting the depth profile of the film

1. Adjust all the 'physical' parameters to correspond with experimental measurement and adjust also all 'non-physical' parameters. See description of each parameter in this manual.

2. Give some initial value for target thickness and element concentrations.

3. Save and run the simulation.

4. Read experimental data in the same graph with the simulated spectrum for comparison of simulated and experimental energy spectrum.

5. Change energy spectrum parameters (i.e. scale and channel width of the spectrum).

6. Find concentration distribution which gives the best match between simulated and experimental energy spectras.

7. If concentration distribution differs a lot from the target thickness and element concentrations determined before the simulation, simulation has to be done again with new target parameters (iteration).

8. Make simulation and comparison for all the elements in the target separately using same parameters.

9. Combine distribution data for all elements for getting the depth profile of the film.

5.8 Example simulations

MCERD packet includes example simulations:

- Al2O3_H: Al_2O_3-target, 7.5 Mev ^{35}Cl ion beam, TOF detector.
- LiNbO3_Li: $LiNbO_3$-target, 58 Mev ^{127}I ion beam, TOF detector.
- Al_Al: Al-target, 55 MeV ^{127}I ion beam, gas detector.

6 References

1 K. Arstila, T. Sajavaara, J. Keinonen, Nucl. Instr. and Meth. B 174 (2001) 163.

2 J. Ziegler, J. Biersack, U. Littmark, The Stopping and Range of Ions in Solids (Pergamon, New York, 1985).

3 J. Ziegler, J. Biersack, SRIM computer code, www.srim.org.